Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

Reinhold Kleiner
Universität Tübingen
Physikalisches Institut
An der Morgenstelle 14
72076 Tübingen
kleiner@uni-tuebingen.de

Overview of Invited Talks and Sessions

(Lecture Rooms H 0104, H 0110, H 2053, H 3005, H 3010, A 053, HFT-FT 101 and HFT-FT 131; Poster B)

Tutorial "Quantum Technologies (joint session HL/TT)"

HL 1.1	Sun	16:00–16:35	H 0105	**Quantum Technology - how is research funded?** — •Gerd Leuchs
HL 1.2	Sun	16:40–17:15	H 0105	**Superconducting Quantum Circuits** — •Rudolf Gross
HL 1.3	Sun	17:15–17:50	H 0105	**Josephson junction based interferometers and amplifiers** — •Sebastian Kempf
HL 1.4	Sun	17:50–18:25	H 0105	**Manipulation of quantum bits based on defect centres in diamond** — •Oliver Benson

Plenaries

PLV IV	Mon	14:00–14:45	H 0104	**Fast Parametric Interactions Between Superconducting Quantum Circuits** — •Raymond W Simmonds
PLV VII	Wed	8:30– 9:15	H 0105	**Nanoscale thermal imaging of dissipation in quantum systems** — •Eli Zeldov

Focus on Topology

Plenaries

PLV II	Mon	8:30– 9:15	H 0105	**Imaging Topological Electrons in Low Dimensions: from the Inorganic to the Organic** — •Michael F. Crommie
PLV XI	Thu	8:30– 9:15	H 0105	**Emergent properties and functions of topological magnets** — •Yoshinori Tokura

Symposium "Topology in Condensed Matter Physics (SYTO)"

See SYTO for the abstracts of the symposium.

SYTO 1.1	Wed	9:30–10:00	H 0105	**Beyond Topologically Ordered States: Insights from Entanglement** — •B. Andrei Bernevig
SYTO 1.2	Wed	10:00–10:30	H 0105	**Topological Magnon Materials** — •Ingrid Mertig
SYTO 1.3	Wed	10:30–11:00	H 0105	**Topological Order of Interacting Polymers on a Substrate** — •Vincenzo Vitelli
SYTO 1.4	Wed	11:15–11:45	H 0105	**Quantization of Heat Flow in Fractional Quantum Hall States** — •Moty Heiblum
SYTO 1.5	Wed	11:45–12:15	H 0105	**Currents and Phases in Quantum Rings** — •Kathryn Moler

Focus Session "Chiral Topological Superconductors and Majorana Fermions" (organized by TT)

TT 32.1	Tue	9:30–10:00	H 0104	**Spin-Triplet Superconductivity in the Ruthenate** — •Yoshiteru Maeno
TT 32.2	Tue	10:00–10:30	H 0104	**Paths Towards Chiral d-wave Superconductivity** — •Ronny Thomale
TT 32.3	Tue	10:30–11:00	H 0104	**Towards the Design of Majorana Bound States in Artificially Constructed Magnetic Atom Chains on Elemental Superconductors** — •Roland Wiesendanger
TT 32.4	Tue	11:15–11:45	H 0104	**Design of Majorana Modes: From Magnetic Skyrmions to Dimensional Tuning** — •Dirk Morr
TT 32.5	Tue	11:45–12:15	H 0104	**Experimental Hints of Topological Superconductivity in Hybrid Ferromagnet-Superconductor Systems** — •Tristan Cren

Focus Session "Topological Defects in Superconductors and Magnets" (organized by TT)

TT 60.1	Wed	15:00–15:30	H 0104	**Stability and Emergent Electrodynamics of Skyrmions** — •Christian Pfleiderer
TT 60.2	Wed	15:30–16:00	H 0104	**Optical Manipulation of Single Flux Quanta** — •Philippe Tamarat
TT 60.3	Wed	16:00–16:30	H 0104	**Skyrmion Lattices in Random and Ordered Potential Landscapes** — •Charles Reichhardt
TT 60.4	Wed	16:45–17:15	H 0104	**Hedgehog Spin-Vortex Crystal Magnetic Order in Superconducting $CaK(Fe_{1-x}M_x)_4As_4$ (M=Co, Ni)** — •Anna Böhmer
TT 60.5	Wed	17:15–17:45	H 0104	**Geometric Frustration and Ratchet Effect of Vortices in an Artificial-Spin/Superconductor Hybrid** — •Zhi-Li Xiao

Focus Session "Quantum Turbulence and Imaging of Quantum Flow of Superfluids" (organized by TT)

TT 77.1	Thu	9:30–10:00	H 0104	**Quantum Turbulence: New Aspects of an Old Problem** — •Carlo F. Barenghi
TT 77.2	Thu	10:00–10:30	H 0104	**Numerical Simulation of Quantum Turbulence** — •Makoto Tsubota
TT 77.3	Thu	10:30–11:00	H 0104	**Visualising Pure Quantum Turbulence in Fermionic Superfluid** — •Viktor Tsepelin
TT 77.4	Thu	11:15–11:45	H 0104	**Experimental Exploration of Intense Quantum Turbulence with He-II** — •Philippe-E. Roche
TT 77.5	Thu	11:45–12:15	H 0104	**Visualization of Superfluid Helium Flows** — •Marco La Mantia

Focus Sessions "Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions I–III" (organized by MA)

See MA for the abstracts of the talks.

MA 40.1	Thu	9:30–10:00	H 1012	**Understanding Spin-Charge Conversion in Topological Insulators** — •Aurelien Manchon
MA 40.5	Thu	11:15–11:45	H 1012	**Interfacial spin-orbitronic: Rashba interfaces and topological insulators as efficient spin-charge current converters** — •Juan-Carlos Rojas-Sanchez
MA 47.1	Thu	15:00–15:30	H 1012	**Spin orbit fields at the Fe/GaAs(001) interface** — •Christian Back
MA 57.1	Fri	9:30–10:00	H 1012	**Manipulation of interface-induced Skyrmions studied with STM** — •Kirsten von Bergmann
MA 57.6	Fri	11:30–12:00	H 1012	**Magnonics in skyrmion-hosting chiral magnetic materials** — •Markus Garst

Invited Talks not included in Focus Sessions and Symposia

TT 9.1	Mon	9:30–10:00	HFT-FT 101	**Unconventional Superconductivity in Quantum-Dot Systems** — •Stephan Weiss
TT 5.8	Mon	11:30–12:00	H 3005	**Superconductivity in $YbRh_2Si_2$** — •Erwin Schuberth

TT 34.1	Tue	9:30–10:00	H 2053	**Non-Equilibrium Spin- and Charge Transport Phenomena in Superconductor-Ferromagnet Hybrid Structures** — •Torsten Pietsch
TT 49.1	Wed	9:30–10:00	H 2053	**Parametric Amplification in Josephson Circuits with Non-Centrosymmetric Nonlinearity** — •Alexander Zorin
TT 51.1	Wed	9:30–10:00	H 3010	**Electronic Squeezing of Pumped Phonons: Negative U and Transient Superconductivity** — •Dante M. Kennes
TT 50.8	Wed	11:30–12:00	H 3005	**Critical Phonon Softening Near a Structural Instability at $T = 0$** — •Oliver Stockert
TT 61.1	Wed	15:00–15:30	H 2053	**Quantum Thermodynamics on Superconducting Qubits** — •Jukka Pekola
TT 62.1	Wed	15:00–15:30	H 3010	**Efficient Simulation of Quantum Thermalization and Dynamics** — •Frank Pollmann
TT 93.1	Thu	15:00–15:30	H 2053	**Non-Markovian Quantum Thermodynamics: Second Law and Fluctuation Theorems** — •Robert S Whitney
TT 94.6	Thu	16:30–17:00	H 3010	**Discrete Time Crystals** — •Roderich Moessner
TT 103.1	Thu	17:15–17:45	H 2053	**From Fundamental Principles to Applications: Cryogenic Micro-Calorimeters** — •Christian Enss

Other Focus Sessions organized by TT

"Recent Developments in Computational Many Body Physics"

TT 2.1	Mon	9:30–10:00	H 0104	**Revealing Fermionic Quantum Criticality from New Monte Carlo Techniques** — •Zi Yang Meng
TT 2.2	Mon	10:00–10:30	H 0104	**Computational Approaches to Many-Body Localization** — •David J. Luitz
TT 2.3	Mon	10:30–11:00	H 0104	**Tensor Network Techniques and Dynamical Systems** — •Ignacio Cirac
TT 2.4	Mon	11:15–11:45	H 0104	**Digital Quantum Simulation** — •Bela Bauer
TT 2.5	Mon	11:45–12:15	H 0104	**Quantum Monte Carlo Simulation of Coupled Fermion-Boson Systems** — •Martin Hohenadler
TT 2.6	Mon	12:15–12:45	H 0104	**Machine Learning Methods for Quantum Many-Body Physics** — •Giuseppe Carleo

"Mesoscopic Superconductivity and Quantum Circuits"

TT 105.1	Fri	9:30–10:00	H 0104	**New Hardware Components for Scalable Quantum Computers** — •David DiVincenzo
TT 105.2	Fri	10:00–10:30	H 0104	**Quantum Communcation with Propagating Microwaves** — •Frank Deppe
TT 105.3	Fri	10:30–11:00	H 0104	**Dynamics of a Qubit While Simultaneously Monitoring its Relaxation and Dephasing** — •Benjamin Huard
TT 105.4	Fri	11:15–11:45	H 0104	**Estimating the Error of an Analog Quantum Simulator by Additional Measurements** — •Michael Marthaler
TT 105.5	Fri	11:45–12:15	H 0104	**On-demand distribution of quantum information between superconducting cavity quantum memories** — •Wolfgang Pfaff
TT 105.6	Fri	12:15–12:35	H 0104	**Quantum Simulation of Light-Matter Interaction** — •Jochen Braumüller

Other Symposia with TT Participation

Symposium "2D Materials (SYDM)"

See SYDM for the abstracts of the symposium.

SYDM 1.1	Thu	15:00–15:30	H 0105	**Bending, pulling, and cutting wrinkled two-dimensional materials** — •Kirill Bolotin
SYDM 1.2	Thu	15:30–16:00	H 0105	**Ultrafast valley and spin dynamics in single-layer transition metal dichalcogenides** — •Alejandro Molina-Sanchez

SYDM 1.3	Thu	16:00–16:30	H 0105	**Interlayer excitons in layered semiconductor transition metal dichalcogenides** — •Steffen Michaelis de Vasconcellos
SYDM 1.4	Thu	16:45–17:15	H 0105	**Exploring exciton physics in liquid-exfoliated 2D materials** — •Claudia Backes
SYDM 1.5	Thu	17:15–17:45	H 0105	**A Progress Report on Electron Transport in MXenes; A New Family of 2D Materials** — •Michel Barsoum

Other Joint Focus Sessions

"Quantum Nanophotonics in Solid State Systems: Status, Challenges and Perspectives I–II " (organized by HL)

See HL for the abstracts of the talks.

HL 16.1	Tue	9:30–10:00	EW 201	**Exploring the limits of position measurement with optomechanics** — •Tobias J. Kippenberg
HL 16.2	Tue	10:00–10:30	EW 201	**On-chip integration of superconducting single photon detectors** — •Wolfram Pernice
HL 16.5	Tue	11:15–11:45	EW 201	**Integrated III-V nonlinear quantum optical devices** — •Gregor Weihs
HL 16.12	Tue	14:00–14:30	EW 201	**Hybrid waveguide platforms for quantum optics** — •Michal Bajcsy
HL 25.1	Wed	9:30–10:00	EW 201	**The quantum knitting machine: a quantum dot as device for deterministic production of cluster states of many entangled photons** — •David Gershoni
HL 25.7	Wed	11:30–12:00	EW 201	**Exploiting the Bright and the Dark Side of Deterministic Solid-State Quantum-Light Sources** — •Tobias Heindel

"Frontiers of Electronic-Structure Theory: Correlated Electron Materials I-VIII"(organized by O)

See O for the abstracts of the talks.

O 31.1	Tue	10:30–11:00	HL 001	**Control and prediction of molecular crystal properties by multilevel strategies** — •Jan Gerit Brandenburg
O 31.2	Tue	11:00–11:30	HL 001	**Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing** — •Viktor Ivády
O 31.3	Tue	11:30–12:00	HL 001	**Recent advances in first-principles modelling of correlated magnetic materials** — •Yaroslav Kvashnin
O 31.4	Tue	12:00–12:30	HL 001	**A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces** — •Reinhard J. Maurer
O 31.5	Tue	12:30–13:00	HL 001	**Temperature effects in spin-orbit physics from first principles** — •Bartomeu Monserrat
O 62.1	Wed	10:30–11:00	HL 001	**Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications** — •Katarzyna Pernal
O 72.1	Wed	15:00–15:30	HL 001	**Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design** — •Gabriel Kotliar
O 102.1	Thu	15:00–15:30	HL 001	**Recent developments in FCIQMC: real-time propagation and improved convergence with walker number** — •Ali Alavi

"Exploiting Spintronics for Unconventional Computing" (organized by MA)

See MA for the abstracts of the talks.

MA 24.1	Wed	9:30–10:00	H 1012	**Control of Mesoscopic Magnetism for Computation** — •Laura Heyderman
MA 24.3	Wed	10:15–10:45	H 1012	**Spin waves for unconventional computing and data processing** — •Philipp Pirro
MA 24.4	Wed	11:00–11:30	H 1012	**p-bits, p-transistors and p-circuits** — •Kerem Camsari
MA 24.6	Wed	11:45–12:15	H 1012	**Bits and Brains: New materials and brain-inspired concepts for low energy information processing** — •Theo Rasing

"Chaos and Correlation in Quantum Matter" (organized by DY)

See DY for the abstracts of the talks.

DY 36.1	Wed	9:30–10:00	EB 107	**Computing quantum thermalization dynamics: from quantum chaos to emergent hydrodynamics** — •Ehud Altman
DY 36.6	Wed	11:15–11:45	EB 107	**Quantum Thermalization Dynamics: From Information Scrambling to Emergent Hydrodynamics** — •Michael Knap

"Emergent Phenomena in Driven Quantum Many-Body Systems" (organized by DY)

See DY for the abstracts of the talks.

DY 55.1	Thu	9:30–10:00	EB 107	**Nuclear and electronic dynamics in ultrafast photoinduced charge separation** — •Carlo Andrea Rozzi
DY 55.2	Thu	10:00–10:30	EB 107	**Theory of pump-probe spectroscopy: Ultrafast laser engineering of ordered phases and microscopic couplings** — •Michael Sentef

All sessions

TT 1.1–1.4	Sun	16:00–18:25	H 0105	**Tutorial: Quantum Technologies (joint session HL/TT/TUT)**
TT 2.1–2.6	Mon	9:30–12:45	H 0104	**Focus Session: Recent Developments in Computational Many Body Physics (joint session TT/DY)**
TT 3.1–3.13	Mon	9:30–13:00	H 0110	**Superconductivity: Properties and Electronic Structure I**
TT 4.1–4.13	Mon	9:30–13:00	H 2053	**Superconductivity: Qubits I**
TT 5.1–5.12	Mon	9:30–13:00	H 3005	**f-Electron Systems and Heavy Fermions I**
TT 6.1–6.13	Mon	9:30–13:00	H 3010	**Quantum Magnets and Molecular Magnets (joint session TT/MA)**
TT 7.1–7.13	Mon	9:30–13:00	A 053	**Topological Semimetals I**
TT 8.1–8.13	Mon	9:30–13:00	A 151	**Topological Insulators I (joint session HL/TT)**
TT 9.1–9.12	Mon	9:30–13:00	HFT-FT 101	**Quantum Dots, Quantum Wires, Point Contacts**
TT 10.1–10.14	Mon	9:30–13:15	EB 301	**Heusler Compounds, Semimetals and Oxides (joint session MA/TT)**
TT 11.1–11.10	Mon	9:30–12:45	EMH 225	**Ferroelectric Domain Walls I (joint session KFM/TT)**
TT 12.1–12.10	Mon	10:00–12:45	EB 107	**Dynamics in Many-Body Systems: Interference, Equilibration and Localization I (joint session DY/TT)**
TT 13.1–13.11	Mon	10:30–13:15	MA 043	**Graphene: Electronic Properties, Structure and Substrate Interaction I (joint session O/TT)**
TT 14.1–14.10	Mon	10:30–13:00	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)**
TT 15.1–15.14	Mon	15:00–18:45	H 0104	**Dual-Method Approaches to Quantum Many-Body Systems I**
TT 16.1–16.9	Mon	15:00–17:30	H 0110	**Superconductivity: Properties and Electronic Structure II**
TT 17.1–17.8	Mon	15:00–17:00	H 2053	**Superconductivity: Qubits II**
TT 18.1–18.9	Mon	15:00–17:30	H 3005	**f-Electron Systems and Heavy Fermions II**
TT 19.1–19.12	Mon	15:00–18:15	H 3010	**Frustrated Magnets - Spin Liquids - Theory**
TT 20.1–20.14	Mon	15:00–18:45	A 053	**Topological Semimetals II**
TT 21.1–21.9	Mon	15:00–17:30	A 151	**Topological Insulators II (joint session HL/TT)**
TT 22.1–22.10	Mon	15:00–17:45	HFT-FT 101	**Superconductivity: Topological Defects in Superconductors and Magnets (joint session TT/MA)**
TT 23.1–23.6	Mon	15:00–16:30	MA 043	**Graphene: Adsorption, Intercalation and Doping I (joint session O/TT)**
TT 24.1–24.6	Mon	16:45–18:15	MA 043	**Graphene: Adsorption, Intercalation and Doping II (joint session O/TT)**
TT 25.1–25.9	Mon	15:00–17:15	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)**

TT 26.1–26.12	Mon	15:00–18:30	EB 301	**Skyrmions I (joint session MA/KFM/TT)**
TT 27.1–27.10	Mon	15:00–18:30	EMH 225	**Ferroelectric Domain Walls II (joint session KFM/TT)**
TT 28.1–28.18	Mon	15:00–19:00	Poster B	**Poster Session: Topological Topics**
TT 29.1–29.16	Mon	15:00–19:00	Poster B	**Poster Session: Cryogenic Particle Detectors and Cryotechnique**
TT 30.1–30.7	Mon	15:00–19:00	Poster B	**Poster Session: Disordered Quantum Systems**
TT 31.1–31.9	Mon	15:30–17:45	EB 107	**Dynamics in Many-Body Systems: Interference, Equilibration and Localization II (joint session DY/TT)**
TT 32.1–32.7	Tue	9:30–12:45	H 0104	**Focus Session: Chiral Topological Superconductors and Majorana Fermions**
TT 33.1–33.8	Tue	9:30–11:30	H 0110	**Nanotubes and Nanoribbons**
TT 34.1–34.12	Tue	9:30–13:00	H 2053	**Superconductivity: Tunneling and Josephson Junctions**
TT 35.1–35.13	Tue	9:30–13:00	A 053	**Superconductivity: Fe-based Superconductors - 122 and Theory**
TT 36.1–36.10	Tue	9:30–12:15	HFT-FT 101	**Correlated Electrons: 1D Theory**
TT 37.1–37.13	Tue	9:30–13:15	EB 301	**Skyrmions II (joint session MA/TT/KFM)**
TT 38.1–38.12	Tue	9:30–12:45	EB 407	**Magnetocaloric Effects (joint session MA/TT)**
TT 39.1–39.17	Tue	9:30–15:45	EW 201	**Focus Session: Quantum Nanophotonics in Solid State Systems I (joint session HL/TT)**
TT 40.1–40.11	Tue	10:00–13:00	H 3010	**Dual-Method Approaches to Quantum Many-Body Systems II**
TT 41.1–41.10	Tue	10:15–13:00	H 3005	**Frustrated Magnets - Spin Liquids - Experiments**
TT 42.1–42.10	Tue	10:15–13:00	HFT-FT 131	**Charge Order**
TT 43.1–43.10	Tue	10:30–13:15	MA 043	**Graphene: Electronic Properties, Structure and Substrate Interaction II (joint session O/TT)**
TT 44.1–44.5	Tue	10:30–13:00	HL 001	**Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)**
TT 45.1–45.5	Tue	11:45–13:00	H 0110	**Nano- and Optomechanics**
TT 46.1–46.13	Tue	18:15–20:30	Poster A	**Poster Session: Graphene (joint session O/TT)**
TT 47.1–47.12	Wed	9:30–12:45	H 0104	**Frustrated Magnets - Iridates and Fe-based Materials**
TT 48.1–48.6	Wed	9:30–12:15	H 1012	**Focus Session: Exploiting Spintronics for Unconventional Computing (joint session MA/TT)**
TT 49.1–49.12	Wed	9:30–13:00	H 2053	**Superconductivity: Superconducting Electronics I**
TT 50.1–50.12	Wed	9:30–13:00	H 3005	**Quantum-Critical Phenomena I**
TT 51.1–51.12	Wed	9:30–13:00	H 3010	**Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)**
TT 52.1–52.13	Wed	9:30–13:00	HFT-FT 101	**Superconductivity: Fe-based Superconductors - FeSe and LiFeAs**
TT 53.1–53.7	Wed	9:30–11:15	HFT-FT 131	**Quantum Impurities and Kondo Physics**
TT 54.1–54.8	Wed	9:30–12:15	EB 107	**Focus Session: Chaos and Correlation in Quantum Matter (joint session DY/TT)**
TT 55.1–55.11	Wed	9:30–12:45	EMH 225	**Multiferroic Oxide Thin Films and Heterostructures I (joint session KFM/TT/MA)**
TT 56.1–56.12	Wed	9:30–13:15	EW 201	**Focus Session: Quantum Nanophotonics in Solid State Systems II (joint session HL/TT)**
TT 57.1–57.5	Wed	10:00–11:15	A 053	**Topological Semimetals III**
TT 58.1–58.9	Wed	10:30–13:00	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)**
TT 59.1–59.5	Wed	11:45–13:00	A 053	**Topological Insulators I (joint session TT/MA)**
TT 60.1–60.5	Wed	15:00–17:45	H 0104	**Focus Session: Topological Defects in Superconductors and Magnets (joint session TT/MA)**
TT 61.1–61.6	Wed	15:00–16:45	H 2053	**Superconductivity: Superconducting Electronics II and Cryotechnique**
TT 62.1–62.12	Wed	15:00–18:30	H 3010	**Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)**
TT 63.1–63.7	Wed	15:00–16:45	A 053	**Topology: Quantum Hall Systems**
TT 64.1–64.12	Wed	15:00–18:15	HFT-FT 101	**Frustrated Magnets - α-$RuCl_3$ and Cu-based Materials**
TT 65.1–65.13	Wed	15:00–18:30	HFT-FT 131	**Quantum-Critical Phenomena II**
TT 66.1–66.8	Wed	15:00–17:00	EB 202	**Spintronics (joint session MA/TT)**

TT 67.1–67.14	Wed	15:00–18:30	EB 301	**Skyrmions III (joint session MA/TT/KFM)**
TT 68.1–68.12	Wed	15:00–18:15	EB 407	**Topological Insulators and Weyl Semimetals (joint session MA/TT)**
TT 69.1–69.10	Wed	15:00–18:15	EMH 225	**Multiferroic Oxide Thin Films and Heterostructures II (joint session KFM/TT/MA)**
TT 70.1–70.10	Wed	15:00–17:45	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)**
TT 71.1–71.9	Wed	15:00–17:30	EW 203	**Quantum Information Systems (joint session HL/TT)**
TT 72.1–72.98	Wed	15:00–19:00	Poster B	**Poster Session: Correlated Electrons**
TT 73.1–73.10	Wed	15:30–18:15	EB 107	**Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)**
TT 74.1–74.9	Wed	16:00–18:30	H 3005	**Molecular Electronics and Photonics**
TT 75.1–75.6	Wed	17:00–18:30	H 2053	**Superconductivity: Mesoscopic Superconductivity and Quantum Circuits**
TT 76.1–76.6	Wed	17:00–18:30	A 053	**Topology: Other Topics**
TT 77.1–77.5	Thu	9:30–12:15	H 0104	**Focus Session: Quantum Turbulence and Imaging of Quantum Flow of Superfluids**
TT 78.1–78.8	Thu	9:30–12:30	H 1012	**Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions I (joint session MA/TT)**
TT 79.1–79.12	Thu	9:30–12:45	H 2053	**Superconductivity: Superconducting Electronics - Circuit QED**
TT 80.1–80.13	Thu	9:30–13:00	H 3005	**Graphene**
TT 81.1–81.7	Thu	9:30–11:15	H 3010	**Nonequilibrium Quantum Many-Body Systems III**
TT 82.1–82.13	Thu	9:30–13:00	A 053	**Topological Insulators II (joint session TT/MA)**
TT 83.1–83.12	Thu	9:30–12:45	HFT-FT 101	**Superconductivity: (General) Theory**
TT 84.1–84.7	Thu	9:30–11:15	HFT-FT 131	**Fluctuations and Noise**
TT 85.1–85.6	Thu	9:30–11:30	EB 107	**Focus Session: Emergent Phenomena in Driven Quantum Many-Body Systems (joint session DY/TT)**
TT 86.1–86.11	Thu	9:30–13:30	EMH 225	**Ferroics and Multiferroics (joint session KFM/TT/MA)**
TT 87.1–87.9	Thu	10:30–12:45	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)**
TT 88.1–88.6	Thu	11:30–13:00	H 3010	**Quantum-Critical Phenomena III**
TT 89.1–89.5	Thu	11:30–12:45	HFT-FT 131	**Disordered Quantum Systems**
TT 90.1–90.3	Thu	12:00–12:45	EB 107	**Coherent Quantum Dynamics (joint session DY/TT)**
TT 91.1–91.12	Thu	15:00–18:15	H 0104	**Correlated Electrons: Method Development**
TT 92.1–92.10	Thu	15:00–18:00	H 1012	**Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions II (joint session MA/TT)**
TT 93.1–93.7	Thu	15:00–17:00	H 2053	**Quantum Coherence and Quantum Information Systems (joint session TT/MA)**
TT 94.1–94.12	Thu	15:00–18:30	H 3010	**Correlated Electrons: Other Theoretical Topics**
TT 95.1–95.10	Thu	15:00–17:45	HFT-FT 131	**Cold Atomic Gases, Superfluids, Quantum Fluids and Solids**
TT 96.1–96.10	Thu	15:00–17:45	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)**
TT 97.1–97.9	Thu	15:00–17:30	EW 201	**Spintronics (joint session HL/TT)**
TT 98.1–98.23	Thu	15:00–19:00	Poster B	**Poster Session: Superconductivity**
TT 99.1–99.53	Thu	15:00–19:00	Poster B	**Poster Session: Transport**
TT 100.1–100.9	Thu	15:30–18:00	H 3005	**Frustrated Magnets - Pyrochlore Oxides**
TT 101.1–101.10	Thu	15:30–18:15	HFT-FT 101	**Correlated Electrons: Other Materials**
TT 102.1–102.9	Thu	16:00–18:30	A 053	**Topology: Majorana Fermions**
TT 103.1–103.4	Thu	17:15–18:30	H 2053	**Superconductivity: Cryogenic Particle Detectors**
TT 104	Thu	18:45–20:00	H 3005	**Annual General Meeting of the Low Temperature Physics Division**
TT 105.1–105.8	Fri	9:30–13:05	H 0104	**Focus Session: Mesoscopic Superconductivity and Quantum Circuits**

TT 106.1–106.13	Fri	9:30–13:00	H 0110	**Complex Oxides: Bulk Properties, Surfaces and Interfaces (joint session TT/MA/KFM)**
TT 107.1–107.9	Fri	9:30–12:45	H 1012	**Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions III (joint session MA/TT)**
TT 108.1–108.9	Fri	9:30–12:00	H 2053	**Topological Superconductors**
TT 109.1–109.10	Fri	9:30–12:15	H 3005	**Frustrated Magnets - (General) Theory**
TT 110.1–110.8	Fri	9:30–11:45	H 3010	**Superconductivity: Fe-based Superconductors - 1111 and Others**
TT 111.1–111.9	Fri	10:30–12:45	HL 001	**Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:45–20:00 Room H 3005
All TT members are invited to attend!

TT 1: Tutorial: Quantum Technologies (joint session HL/TT/TUT)

This tutorial features both the high hopes in Europe regarding quantum technologies and the underlying physics of several promising routes towards economically relevant quantum information science as well as the physics of a whole range of novel quantum devices.

Organized by Christian Enss (Heidelberg) and Erich Runge (Ilmenau) on behalf of the divisions TT and HL.

Time: Sunday 16:00–18:25 Location: H 0105

Tutorial TT 1.1 Sun 16:00 H 0105

Quantum Technology - how is research funded? — •Gerd Leuchs — Max Planck Institute for the Science of Light, Erlangen, Germany

Quantum technology is a field in physics which experienced considerable growth recently and is about to generate real world applications with significant economic potential. Scientists and research oriented companies succeeded raising the awareness of politicians in Germany and Europe.
As a consequence, the European Quantum Flagship, which will be supported by national initiatives (in Germany, QUTEGA, a BMBF funded project), is currently in the process of being established. The goal is to provide infrastructural and financial support to projects associated to Quantum Technologies. The major focus is on connecting scientific groups with players from industry who are interested in investing into emerging quantum technologies such as quantum communication, quantum metrology, quantum simulation and quantum computing.
For younger scientists, the structure and the political initiation process of such funding initiatives is often lacking transparency. As the national coordinator of the quantum initiative in Germany, I will try to shed some light on this topic by reporting about the currently ongoing foundation of the Quantum Flagship and the associated national initiatives. Since the final structure of the Flagship is not yet fully established, I will also share my experience with similar projects from the past.

5 min. break

Tutorial TT 1.2 Sun 16:40 H 0105

Superconducting Quantum Circuits — •Rudolf Gross — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — Physik-Department, TU-München, Garching, Germany — Nanosystems Initiative Munich, München, Germany

Superconducting quantum circuits, consisting of inductors, capacitors and Josephson junctions, can be flexibly engineered using modern thin film and micro/nano-fabrication techniques. These quantum electronic circuits behave quantum coherently with coherence times approaching the millisecond regime. They are successfully used to study fundamental quantum effects and develop components for applications in quantum technology. Examples are the tailoring of light-matter interaction, the development of sources and detectors for quantum light, or the implementation of quantum information processing, quantum metrology and quantum simulation systems. Meanwhile, several companies such as Google, IBM or Intel have started the race towards a universal quantum computer based on a superconducting hardware platform.

Superconducting quantum circuits can also be successfully coupled to nano-mechanical and magnetic systems. In the resulting hybrid quantum systems different quantum degrees of freedom can be strongly coupled, allowing for the coherent exchange of elementary excitations such as pho-tons, phonons and magnons on a single quantum level.

I will give an introduction into the field of superconducting quantum circuits and address recent advancements in the rapidly growing field of superconducting quantum technology.

Tutorial TT 1.3 Sun 17:15 H 0105

Josephson junction based interferometers and amplifiers — •Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Advances in science, health care or other areas of everyday life are often accompanied by progress in physical instrumentation. The development of ultra-sensitive detectors and sensors is therefore of great importance and will not only influence our understanding of nature but also future examination methods in medical care or search strategies for natural resources. Quantum technology plays an important role in these developments as superconducting quantum devices (SQDs) are among the most sensitive measurement instruments presently existing and enabling fascinating investigations of tiniest signals.

Josephson junction based interferometers and amplifiers are a special class of SQDs which are very well suited for measuring variations of tiny magnetic fields or any other physical quantity that can be naturally converted into magnetic flux. They are based on the Josephson effects as well as magnetic flux conservation and are used not only for measuring biogmagnetic signals as induced for instance by the electrical currents within the human brain but also to read out cryogenic particle detectors, to explore mineral deposits within geoscience or for magnetic sensing at nanoscale level.

I will give an introduction into this fascinating field, discuss different kinds of devices such as the well-known superconducting quantum interference device and highlight several applications for which Josephson junction based interferometers and amplifiers are a key technology.

Tutorial TT 1.4 Sun 17:50 H 0105

Manipulation of quantum bits based on defect centres in diamond — •Oliver Benson — Institut für Physik der Humboldt-Universität zu Berlin, Newtonstrasse 15, 12489 Berlin

Quantum information processing relies on initialisation, manipulation, read-out and transmission of individual quantum bits. Defect centres in diamond are an example of stable, optically addressable single quantum systems in a solid-state matrix [1-4]. Their electronic states couple efficiently to light, and their energy level structure allows for long spin coherence time in the ground state. Moreover, coupling to nuclear spins in the diamond host provides storage of quantum bits for seconds. With this all ingredients for a full quantum information processing (QIP) architecture are present in one material platform. In this presentation, we introduce the fundamental concepts of QIP in diamond. We then describe recent breakthroughs, such as stationary to flying quantum bit conversion and entanglement of distant quantum bits [5]. Other applications of defect centres in diamond for quantum sensing [6] will be discussed as well.

[1] F. Jelezko and J. Wrachtrup, Phys. Status Solidi A, 203, 3207 (2006). [2] V. Acosta, P. Hemmer, MRS Bull. 38, 127 (2013). [3] J. R. Weber, et al., PNAS 107, 8513 (2010). [4] I. Aharonovich, et al., Rep. Prog. Phys. 74, 076501 (2011). [5] H. Bernien, et al., Nature 497, 86 (2013) [6] S. Hong, et al., MRS Bull. 38, 155 (2013).

TT 2: Focus Session: Recent Developments in Computational Many Body Physics (joint session TT/DY)

This focus session provides an overview of recent achievements and new directions in the domain of computational many body physics. Numerical simulations provide invaluable insights in fermion quantum criticality, many body localization as well as in coupled fermion-boson systems. Tensor networks offer immense possibilities to tackle problems in and out of equilibrium. Finally, new directions such as machine learning and quantum computations will greatly impact the field. All these themes and methods will be discussed by the invited speakers.

Organization: Fakher F. Assaad, Universität Würzburg; Reinhard Noack, Philipps-Universität Marburg

Time: Monday 9:30–12:45 Location: H 0104

Invited Talk TT 2.1 Mon 9:30 H 0104

Revealing Fermionic Quantum Criticality from New Monte Carlo Techniques — •Zi Yang Meng — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

In this talk, I will present recent developments in the numerical investigations of fermionic quantum criticality in the form of Fermi surfaces coupled to various critical bosonic fluctuations. The thence obtain itinerant quantum critical points reveal rich and fundamental physics that has immediate impact on both theoretical and experimental investigations in the correlated electrons systems such as Cu- and Ir-based superconductors, heavy-fermion systems as well as the interacting topological state of matter and phase transitions. These developments are made possible due to the insightful model design as well as the timely algorithmic developments in the Monte Carlo techniques.

Invited Talk TT 2.2 Mon 10:00 H 0104

Computational Approaches to Many-Body Localization — •David J. Luitz — Physik Department T42, Technische Universität München, Germany

In the past decade, enormous progress has been made in the understanding of the phenomenon of many-body localization, a dynamical phase of matter in strongly disordered interacting quantum systems far from equilibrium. In particular, the understanding of the phase transition from an extended phase at weak disorder to a localized phase at strong disorder relies heavily on state of the art numerical studies. The numerically accessible system sizes have recently been increased substantially by the introduction of advanced exact numerical techniques: Exact sparse diagonalization as well as matrix product state (MPS) techniques permit the calculation of highly excited eigenstates of the system, whereas exact Krylov space time evolution methods and MPS time evolution methods can be used to study the nonequilibrium dynamics in generic many-body systems. I will give a short survey of current exact numerical techniques (cf [1] for a detailed discussion) to study the MBL phase as well as the transition regime and highlight some results obtained by these approaches.
[1] D. J. Luitz, Y. Bar Lev, Annalen der Physik 529, 1600350 (2017)

Invited Talk TT 2.3 Mon 10:30 H 0104

Tensor Network Techniques and Dynamical Systems — Nicola Pancotti[1], Michael Knapp[2], David Huse[3], Mari Carmen Banuls[1], and •Ignacio Cirac[1] — [1]Max-Planck Institut für Quantenoptic, Garching, Germany — [2]Technical University of Munich, Garching, Germany — [3]University of Princeton, Princeton, US

Tensor networks can be used to efficiently describe the equilibrium properties of many-body quantum systems with local interactions. However, they fail to describe their dynamics, at least for long times. In this talk we will present several methods based on tensor networks to extract dynamical properties of one dimensional spin chains. In particular, we will show how one can construct matrix product operators that quasi commute with the system Hamiltonian, and how this is related to the thermalization process.

15 min. break.

Invited Talk TT 2.4 Mon 11:15 H 0104

Digital Quantum Simulation — •Bela Bauer — Station Q, Microsoft Research, Santa Barbara, CA 93106-6105, USA

Recent improvements in the control of quantum systems make it appear feasible to build a quantum computer within a decade. One of the most promising applications for a quantum computer is the simulation of quantum systems that have thus far eluded numerical simulation on conventional supercomputers. In this talk, I will review the relevant models of quantum computation and survey some potential applications for a small quantum computer. I will then focus on the particular case of simulating complex materials. We show that this important and challenging problem can be tackled using a hybrid quantum-classical algorithm that incorporates the power of a small quantum computer into a framework of classical embedding algorithms.

Invited Talk TT 2.5 Mon 11:45 H 0104

Quantum Monte Carlo Simulation of Coupled Fermion-Boson Systems — Manuel Weber, Fakher Assaad, and •Martin Hohenadler — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

Problems of fermions coupled to bosonic degrees of freedom can be found in a variety of contexts in condensed matter physics. The bosons may represent, for example, quantum lattice, spin, or orbital fluctuations. Numerical simulations of such problems are challenging because of the bosonic Hilbert space, the different time scales for the fermion and boson dynamics, and the absence of efficient sampling methods for the bosons. In this talk, recent advances in quantum Monte Carlo simulations are presented. By integrating out the bosons, the original problem can be reformulated in terms of fermions with a retarded interaction. The latter can be simulated efficiently by continuous-time quantum Monte Carlo methods. Especially in combination with global updates, simulations can be carried out on system sizes currently inaccessible by any other method. Applications to be presented include the problem of competing electron-phonon couplings as well as charge-density-wave transitions in one and two dimensions.

Invited Talk TT 2.6 Mon 12:15 H 0104

Machine Learning Methods for Quantum Many-Body Physics — •Giuseppe Carleo — ETH Zurich, Institute for Theoretical Physics Wolfgang-Pauli-Str. 27 8093 Zurich - Switzerland

Machine-learning-based approaches are being increasingly adopted in a wide variety of domains, and very recently their effectiveness has been demonstrated also for many-body physics [1-4]. In this talk I will present recent applications to quantum physics.

First, I will discuss how a systematic machine learning of the many-body wave-function can be realized. This goal has been achieved in [1], introducing a variational representation of quantum states based on artificial neural networks. In conjunction with Monte Carlo schemes, this representation can be used to study both ground-state and unitary dynamics, with controlled accuracy. Moreover, I will show how a similar representation can be used to perform efficient Quantum State Tomography on highly-entangled states [5], previously inaccessible to state-of-the art tomographic approaches.

I will then briefly discuss, recent developments in quantum information theory, concerning the high representational power of neural-network quantum states.
[1] Carleo, Troyer, Science 355, 602 (2017).
[2] Carrasquilla, Melko, Nature Physics 13, 431 (2017).
[3] Wang, Physical Review B 94, 195105 (2016).
[4] van Nieuwenburg, Liu, Huber, Nature Physics 13, 435 (2017).
[5] Torlai, Mazzola, Carrasquilla, Troyer, Melko, Carleo, arXiv: 1703.05334.

TT 3: Superconductivity: Properties and Electronic Structure I

Time: Monday 9:30–13:00 Location: H 0110

TT 3.1 Mon 9:30 H 0110

Paramagnetic Meissner effect in Nb: 20 years after — •Michael Koblischka[1], Crosby Chang[2], Thomas Hauet[2], and Ladislav Pust[3] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Institut Jean Lamour, UMR CNRS-Université de Lorraine, 54506 Vandœvre-lès-Nancy, France — [3]ELI Beamlines, Institute of Physics AS CR, Za Radnici 835, 25241 Dolni Brezany, Czech Republic

The paramagnetic Meissner effect (PME) was investigated in Nb samples which showed the PME already 20 years ago [1]. Magnetization measurements ($M(T)$ and $M(H)$)were performed using different magnetometers (QD SQUID MPMS3 and PPMS). We could reproduce the same PME behavior of the samples, despite the long storage time. In this contribution, we compare the old results from 1997 to the new data. The $M(T)$-data reveal the same principal features at the superconducting transition, and the $M(H)$-data measured close to the superconducting transition exhibit a change of the shape of the magnetization loops as in the original experiments. Furthermore, we also observe the features of the PME transition to much higher fields as reported previously. The measurements proof that the sample surfaces were not altered due to storage.

[1] L. Pust, L. E. Wenger, M. R. Koblischka, PRB 58, 14191 (1998)

TT 3.2 Mon 9:45 H 0110

Strong coupling superconductivity in the aperiodic high-pressure phase of bismuth — •Konstantin Semeniuk[1], Philip Brown[1], Stephen Hodgson[1], Diandian Wang[1], Bartomeu Monserrat[2,1], Chris Pickard[3,4], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Dept. of Physics and Astronomy, Rutgers University, Piscataway, USA — [3]Dept. of Materials Science, University of Cambridge, UK — [4]Advanced Institute for Materials Research, Tohoku University, Japan

Application of hydrostatic pressure to elemental materials surprisingly often leads to the emergence of structurally complex phases [1]. Examples include aperiodic structures consisting of two incommensurate sublattices, seen in high pressure phases of bismuth, antimony, barium and other elemental metals. Aside from crystallographic characterisation, not many experiments have been conducted to explore the electronic and vibrational properties of these systems. We examine the incommensurate host-guest structure of high pressure bismuth, Bi-III, which superconducts below 7 K and has an anomalously large gradient of resistivity against temperature below 50 K. We attribute its properties to the existence of sliding modes, or phasons, which cause enhanced electron-phonon scattering at low temperature and boost electron-phonon coupling constant to $\lambda \simeq 2.8$, indicating unusually strong coupling superconductivity for an element.

[1] M. I. McMahon, R. J. Nelmes, Chem. Soc. Rev. 35(2006)943.

TT 3.3 Mon 10:00 H 0110

Nonequilibrium transport in ultrathin aluminium films near the vortex-unbinding transition — •Klaus Kronfeldner, Lorenz Fuchs, and Christoph Strunk — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We analyze $I(V)$-characteristics and ac-susceptibility of epitaxial aluminium films with thicknesses below 8 nm. The Berezinskii-Kosterlitz-Thouless transition temperature T_{BKT} is determined from the superfluid stiffnesses that are extracted from both measurement techniques. For the dc-measurement the power-law criterion with slope 3 in $\log(V)$ vs. $\log(I)$ is used to determine T_{BKT}. While the two independently identified values for T_{BKT} are in good agreement for the lowest voltages V, at higher V a pronounced concave curvature is visible in the $\log(V)$ vs. $\log(I)$ plot. This curvature is traced back to both changes in the superfluid stiffness and self-heating in presence of a driving current.

TT 3.4 Mon 10:15 H 0110

Superfluid stiffness vs. electric resistance in the vicinity of the Berezinskii-Kosterlitz-Thouless transition in ultrathin aluminum films — •Lorenz Fuchs, Klaus Kronfeldner, Imke Gronwald, Dieter Schuh, Dominique Bougeard, and Christoph Strunk — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We present superconducting properties of ultrathin aluminum films with thicknesses below 8 nm. Transport measurements are carried out in a low-noise DC configuration with IV curves spanning a voltage range of 6 orders of magnitude. Resistances are extracted from the linear parts of the curves in the zero-bias limit. Discontinuous jumps by a factor of up to 10^5 are observed above a critical current $I_c(T)$ at low temperature T. For moderate voltages we find a power-law dependence $V \propto I^{\alpha(T)} = I^{1+\pi J_s(T)/T}$. Superfluid stiffness $J_s(T) \propto 1/\lambda^2$, which is directly related to the magnetic penetration depth λ, is measured by a two-coil mutual inductance setup. We see clear signatures of a Berezinskii-Kosterlitz-Thouless transition in the low-resistance tail of the transition curve. Critical temperatures agree within a few mK for the different methods. $\alpha(T)$ extracted from IV curves and independently calculated from $J_s(T)$ are compared.

TT 3.5 Mon 10:30 H 0110

Unconventional superconductivity in Mo_8Ga_{41} — •Valeriy Verchenko[1], Rustem Khasanov[2], Zurab Guguchia[2], Alexander Tsirlin[3], Miroslav Marcin[4], and Andrei Shevelkov[1] — [1]Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen PSI, Switzerland — [3]Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany — [4]Institute of Experimental Physics, Slovak Academy of Sciences, Košice, Slovakia

Among intermetallics, gallium cluster phases - the compounds, which crystal structures are built by gallium-based polyhedra with high coordination numbers - are promising candidates for unconventional superconductivity. In this class of compounds, $ReGa_5$, Mo_8Ga_{41}, Mo_6Ga_{31}, Rh_2Ga_9 and Ir_2Ga_9 are known to superconduct at low temperatures. Among the series, Mo_8Ga_{41} exhibits the largest superconducting transition temperature of $T_C = 9.7$ K in zero magnetic field. In our study, we focused on Mo_8Ga_{41}, aiming at the investigation of its macro- and microscopic properties. For this purpose, thermodynamic measurements as well as muon spin spectroscopy technique were employed. According to the specific heat measurements and transverse-field muon spin rotation/relaxation experiments, we classify Mo_8Ga_{41} as a strong-coupled superconductor with two s-wave superconducting gaps.

TT 3.6 Mon 10:45 H 0110

Two-gap superconductivity in the $Ag_xMo_6S_8$ Chevrel Phase — •Manuel Feig[1,2], Matej Bobnar[2], Christoph Hennig[3], Igor Veremchuk[2], Andreas Leithe-Jasper[2], and Roman Gumeniuk[1,2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Straße 23, 09599 Freiberg, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [3]European Synchrotron Radiation Facility, 71, Avenue des Martyrs, Grenoble, France

The Rietveld refinement of HR-PXRD data on the superconducting $Ag_{0.92}Mo_6S_8$ confirmed the Chevrel-like structure: SG $R\bar{3}$, a = 9.3065 Å and c = 10.8310 Å. Magnetization measurements revealed a superconducting transition at $T_c = 7.9$ K. The lower and upper critical magnetic fields $B_{c1} = 12$ mT and $B_{c2} = 3.5$ T were deduced from the hysteresis. In contrast, measurements of the electrical resistivity in different magnetic fields resulted in $B_{c2} = 7.4$ T as well as the GL-coherence length $\xi_{GL} = 67$ Å, the GL-parameter $\kappa = 33$ and the London penetration depth $\lambda_L = 2204$ Å. The specific heat jump at the superconducting transition $\Delta c_p/\gamma T_c = 1.77$ is well above the value predicted by BCS theory (1.43), whereas the energy gap ratio $\Delta(0)/k_BT_c = 1.55$ obtained from an exponential fit of the electronic specific heat c_{el} from 0.35 K to 4 K is smaller than the theoretically predicted value of 1.76. In agreement with the isostructural $SnMo_6S_8$ and $PbMo_6S_8$ Chevrel phases [1], $Ag_{0.92}Mo_6S_8$ is a two-band superconductor with the gap ratios $\Delta_1/k_BT_c = 2.39$ (95%) and $\Delta_2/k_BT_c = 1.03$ (5%).

[1] A.P. Petrović et al., Phys. Rev. Lett., 106, 017003 (2011)

TT 3.7 Mon 11:00 H 0110

Strain-enhanced three-gap superconductivity in monolayer MgB_2 — •Alex Aperis[1], Jonas Bekaert[2], Bart Partoens[2], Milorad V. Milošević[2], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]University of Antwerp, Antwerp, Bel-

gium

Starting from first principles, we show the formation and evolution of superconducting gaps in MgB_2 at its ultrathin limit. Atomically thin MgB_2 is distinctly different from bulk MgB_2 in that surface states become comparable in electronic density to the bulk like σ and π bands. Solving the anisotropic Eliashberg equations with *ab initio* calculated input for electrons, phonons and the electron-phonon coupling, we show that monolayer MgB_2 develops three distinct superconducting gaps, on completely separate parts of the Fermi surface due to the emergent surface contribution. These gaps hybridise nontrivially with every extra monolayer added to the film owing to the opening of additional coupling channels. Furthermore, we reveal that the three-gap superconductivity in monolayer MgB_2 is robust over the entire temperature range that stretches up to a considerably high critical temperature of 20 K. The latter can be boosted to T_c>50 K under biaxial tensile strain of $\sim 4\%$, which is an enhancement that is stronger than in any other graphene-related superconductor known to date.

15 min. break.

TT 3.8 Mon 11:30 H 0110

Hidden nesting as the origin of strong electron-phonon coupling — •Philipp Kurzhals, Frank Weber, Rolf Heid, and John-Paul Castellan — Institute for Solid-State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

We report a combined inelastic neutron scattering and density-functional theory investigation of a phonon anomaly in the superconductor YNi_2B_2C assigned to strong electron-phonon coupling.

Band structure calculations indicate that the Fermi surface in the material is not nested in the sense that there is no singularity in the electronic joint density of states at the wavevector $\boldsymbol{q}_{\mathbf{anom}} = (0.55, 0, 0)$ that could define the phonon anomaly.

We measured the evolution of the strong-coupling phonon mode in a volume of reciprocal space around $\boldsymbol{q}_{\mathbf{anom}}$ to unravel the momentum dependence of electron-phonon coupling expressed in the softening and broadening of single phonon modes and compared it to predictions of *ab-initio* lattice dynamical calculations.

Our combined results hint at a hybrid approach, in which a small enhancement of the nesting properties is boosted by a concomitant increase of the electron-phonon coupling matrix elements at the same wavevector $\boldsymbol{q}$.

TT 3.9 Mon 11:45 H 0110

Is there a relation between $T_{c,max}$ and the superexchange strength J? — •Silvia Müllner[1], Dirk Wulferding[1,2], Peter Lemmens[1,2], Meny Shay[3], Gil Drachuck[3], Wayne Crump[4], Jeff Tallon[4], and Amit Keren[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Phys. Dep., Technion Haifa, Israel — [4]RRI, Victoria Univ., New Zealand

Using Raman scattering the magnetic superexchange strength J can be directly determined via two-magnon scattering. Two earlier Raman scattering investigations on HTSC have shown contradicting relations between J and $T_{c,max}$. We present new Raman scattering results of various RE123 HTSC with different J and their relation with $T_{c,max}$. Work supported by GIF 1171-486 189.14/2011.

[1] Wulferding, et al., PRB 90, 104511 (2014).
[2] Tallon, PRB 90, 214523 (2014).
[3] Ellis, et al., PRB 92, 104507 (2015).

TT 3.10 Mon 12:00 H 0110

Why T_c is so low in high-T_c cuprates: importance of the dynamical vertex structure — •Motoharu Kitatani[1], Thomas Schäfer[2,3], Hideo Aoki[4], and Karsten Held[1] — [1]Vienna University of Technology, Vienna, Austria — [2]Collège de France, Paris, France — [3]École Polytechnique, Palaiseau, France — [4]Advanced Industrial Science and Technology (AIST), Ibaraki, Japan

We have applied the dynamical vertex approximation (DΓA), one of the diagrammatic extensions of the dynamical mean field theory (DMFT), for studying d-wave superconductivity in the repulsive Hubbard model on a square lattice. The result well reproduces the cuprate superconducting phase diagram, with a reasonable T_c and a superconducting dome. We have also decomposed the vertex correction contributions to T_c and traced back the dominant scattering processes, and found that local particle-particle diagrams strongly screen the bare interaction near the Fermi level, which act to suppress the pairing interaction. We shall discuss in detail how the dynamical vertex structure passes from the local vertex to the magnetic vertex (spin-fluctuations) to the pairing interaction.

TT 3.11 Mon 12:15 H 0110

Terahertz and infrared spectroscopic study of in-gap excitations in epitaxial $DyBa_2Cu_3O_7$ superconducting films — •Robert Dawson, Timofei Larkin, Daniel Putzky, Georg Christiani, Gennady Logvenov, Alexander Boris, and Bernhard Keimer — Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Investigations of the electronic ground state properties of high-temperature cuprate superconductors have revealed a complex array of competing forms of order, suggesting the existence of dipole-active excitations at low energies which evolve across a wide range of doping levels. Unfortunately, the strong optical response of the superconducting condensate below T_c masks low energy spectral features and makes their direct measurement challenging. To address this issue we have combined the three complementary phase-sensitive techniques of millimeter-wave interferometry, high-resolution time domain terahertz spectroscopy, and infrared ellipsometry to sensitively probe the in-gap states of $DyBa_2Cu_3O_7$ epitaxial films grown by atomic-layer-by-layer oxide MBE. We have obtained the continuous complex dielectric function in the spectral range of 0.5meV to 0.5eV and have observed its evolution as a function of temperature between 7K and 300K. We observe significant spectral weight accumulation at frequencies below 500GHz in the superconducting state, with 30% of the total charge carrier density remaining uncondensed even at temperatures below $T_c/10$. We will discuss this result and its implications for the evolution of the spectral weight distribution in the DBCO-1237 compound.

TT 3.12 Mon 12:30 H 0110

Transmission x-ray microscopy at low temperatures: watching superconductors at work — •Julian Simmendinger[1], Stephen Ruoss[1], Joachim Albrecht[2], and Gisela Schütz[1] — [1]Max Planck Institute for Intelligent Systems, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Research Institute for Innovative Surfaces FINO, Beethovenstr. 1, D-73430 Aalen, Germany

Scanning transmission x-ray microscopy has been used to image electric currents in superconducting films at temperatures down to 20 K. The magnetic stray field of supercurrents in a thin YBaCuO film is mapped into a soft-magnetic coating of permalloy. The so created local magnetization of the ferromagnetic film can be detected by dichroic absorption of polarized x-rays. To enable high-quality measurements in transmission geometry the whole heterostructure of ferromagnet, superconductor and single-crystalline substrate has been thinned to an overall thickness of less than 1 micron. With this novel technique local supercurrents can be analyzed in a wide range of temperatures and magnetic fields. A magnetic resolution of less than 100nm together with simultaneuosly obtained nanostructural data allow the correlation of local supercurrents with the micro- and nanostructure of the superconducting film.

TT 3.13 Mon 12:45 H 0110

Single-gap superconductivity in Nb-doped $SrTiO_3$ and superconducting dome probed by microwave spectroscopy — Markus Thiemann[1], Manfred H. Beutel[1], Martin Dressel[1], Nicholas R. Lee-Hone[2], David M. Broun[2,3], Evangelos Fillis-Tsirakis[4], Hans Boschker[4], Jochen Mannhart[4], and •Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, Canada — [3]Canadian Institute for Advance Research, Toronto, Canada — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany

$SrTiO_3$ exhibits a superconducting dome (critical temperature T_c up to 0.4 K) upon doping with Nb, which successively fills multiple bands at the Fermi level. Using superconducting microwave stripline resonators at frequencies 2 to 23 GHz and temperatures down to 0.02 K, we probe the low-energy optical response of superconducting $SrTiO_3$ with charge carrier concentration from 0.3 to 2.2×10^{20} cm^{-3} across the superconducting dome. We find single-gap behavior [1] although several electronic bands are superconducting in $SrTiO_3$, and this presence of a single energy gap 2Δ due to gap homogenization over the Fermi surface is consistent with the amount of defect scattering observed in Nb-doped $SrTiO_3$. Furthermore, we determine T_c, 2Δ, and the superfluid density throughout the superconducting regime of Nb-doped $SrTiO_3$, and all three quantities exhibit the characteristic dome shape as a function of Nb concentration.

[1] M. Thiemann *et al.*, arXiv:1703.04716

TT 4: Superconductivity: Qubits I

Time: Monday 9:30–13:00 Location: H 2053

TT 4.1 Mon 9:30 H 2053

Dissipation by normal-metal traps in transmon qubits — •Roman-Pascal Riwar[1,2], Robert J. Schoelkopf[2], Leonid I. Glazman[2], and Gianluigi Catelani[1] — [1]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Departments of Physics and Applied Physics, Yale University, New Haven, CT 06520, USA

Quasiparticles are an intrinsic source of relaxation and decoherence for superconducting qubits. Recent works have shown that normal-metal traps may be used to evacuate quasiparticles, and potentially improve the qubit life time. Here, we investigate how far the normal metals themselves may introduce qubit relaxation. We identify the ohmic losses inside the normal metal and the tunnelling current through the normal metal-superconductor interface as the relevant relaxation mechanisms. We show that the ohmic loss contribution depends strongly on the device and trap geometry, as a result of the inhomogeneous electric fields in the qubit. The correction of the quality factor due to the tunnelling current on the other hand is highly sensitive to the nonequilibrium distribution function of the quasiparticles. Overall, we show that even when choosing less than optimal parameters, the presence of normal-metal traps does not affect the quality factor of state-of-the-art qubits.

TT 4.2 Mon 9:45 H 2053

Coupling transmons to traveling waves by strongly blockaded EIT — •Felix Motzoi and Klaus Molmer — Dept. of Physics and Astronomy, Aarhus University, Denmark

There are numerous proposals for entangling superconducting qubits on separated chips, which can be used for modular computing architectures. Here, we present a method that employs itinerant traveling waves, without the need for the light to be stored in the cavity or interact directly with the qubit. Rather, an EIT mechanism is controlled dispersively by the qubit in the cavity (by shifting it in and out of resonance), effectively performing a CPHASE operation. By using an ancillary transmon qubit, the light-matter coupling strength can be greatly enhanced without negatively affecting the coherence time of the device. Such a scheme can be used with coherent light fields and without the need for measurement, offering potential for high practicality.

TT 4.3 Mon 10:00 H 2053

Using Superconducting Qubits for analog Quantum Simulation — •Oscar Gargiulo[1,2], Stefan Oleschko[1,2], Phani Muppalla[1,2], Maximilian Zanner[1,2], Aleksei Sharafiev[1,2], and Gerhard Kirchmair[1,2] — [1]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Technikerstraße 21a, A-6020 Innsbruck, Austria — [2]Institute for Experimental Physics, University of Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria

In this talk I want to present the research activities of the Superconducting Quantum Circuits group at the Institute for Quantum Optics and Quantum Information in Innsbruck. I will give an introduction to circuit quantum electrodynamics and our 3D circuit QED architecture. I will show how we want to use this architecture to realize a platform for quantum many body simulations of dipolar XY models on 2D lattices using state of the art circuit QED technology. The central idea is to exploit the naturally occurring dipolar interactions between 3D superconducting qubits to simulate models of interacting quantum spins. The ability to arrange the qubits on essentially arbitrary geometries allows us to design spin models with more than nearest-neighbor interaction in various geometries.

TT 4.4 Mon 10:15 H 2053

Fast flux control of 3D transmon qubits — •Stefan Oleschko[1,2], Oscar Gargiulo[1,2], Phani Muppalla[1,2], Maximilian Zanner[1,2], Aleksei Sharafiev[1,2], and Gerhard Kirchmair[1,2] — [1]Institute for Quantum Optics and Quantum Information, Austrian Academy of Sciences, Technikerstraße 21a, A-6020 Innsbruck, Austria — [2]Institute for Experimental Physics, University of Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria

An important feature in analog quantum simulation experiments with superconducting qubits [1] is the possibility to change the frequency of SQUID-based transmon qubits by applying magnetic flux. Implementing fast flux control on a transmon remains challenging in the 3D cavity architectures due to the presence of a massive metallic cavity. Here we introduce a new approach for fast flux control of 3D transmon qubits. We use a magnetic hose similar to the one proposed by C. Navau et al [2] to guide a fast flux pulse from the outside to the inside of a microwave cavity. This hose enables us to locally circumvent any magnetic shielding effects such as the appearance of eddy currents in cavities made out of copper or the Meissner effect in superconducting cavities made out of aluminum. First experiments show that the transition frequency of a transmon can be tuned within 50 nanoseconds. Besides the high speed, the frequency shift is precise, without showing any ringing or hysteresis. Using a magnetic hose with an aluminum cavity preserves the benefits of a superconducting cavity, like providing magnetic field shielding and a high internal quality factor, along with the possibility to fast-tune individual qubits.

TT 4.5 Mon 10:30 H 2053

Transmon qubit circuits based on semiconductor/superconductor core/shell nanowire Josephson junctions — •Patrick Zellekens[1,2], Steffen Schlör[3], Tobias Ziegler[1,2], Nicolas Güsken[1,2], Torsten Rieger[1,2], Benjamin Bennemann[1,2], Mihail Ion Lepsa[1,2], Detlev Grützmacher[1,2], Martin Weides[3], and Thomas Schäpers[1,2] — [1]Peter Gruenberg Institute 9, Forschungszentrum Juelich, 52425 Juelich, Germany — [2]JARA - Fundamentals of Future Information Technologies — [3]Physikalisches Institut, Karlsruher Institut für Technologie

State-of-the-art qubits, like the transmon, are typically tuned in frequency by a magnetic field. Our goal is to fabricate and characterize an electrically tunable qubit in the GHz regime, using a semiconductor nanowire Josephson junction as nonlinear element. Thereby it is possible to tune the resonance frequency of the qubit without a magnetic flux bias. The main limitation for the qubit performance is the semiconductor-superconductor interface as well as the coherence properties of the surrounding circuit. In order to address this issue and to optimize the interface properties, an in-situ fabrication approach was chosen, in which the nanowire is directly covered with a superconducting shell. Subsequently, Josephson junctions are fabricated and electrically characterized at low temperature. Finally, implementations as building blocks for 2-dimensional transmon qubits based on TiN will be shown.

TT 4.6 Mon 10:45 H 2053

Flux-Noise Spectroscopy on a Superconducting Transmon Qubit — •Tim Wolz[1], Andre Schneider[1], Jochen Braumüller[1], Alexey V. Ustinov[1,2], and Martin Weides[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Russian Quantum Center, Moscow, Russia — [3]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany

Superconducting qubits can act as noise sensors because their decoherence times under certain pulse sequences can be linked to the system's noise power spectral density (PSD). These sequences also set the observable frequency range of the PSD. The PSD during free evolution of the qubit can be obtained with a dynamical decoupling (CPMG-) pulse sequence, which renders the qubit only susceptible to noise within a narrow frequency band. The PSD during driven evolution is measured with a so-called spin-locking sequence, during which only noise at the Rabi frequency can affect the qubit. Both protocols were successfully tested on a flux qubit by Bylander [1] and Yan [2]. In this work, we apply these two protocols to a tunable concentric transmon [3], overcome the challenge of the transmon's low anharmonicity by using DRAG pulses and compare the PSDs of free and driven evolution. Our results show a clear $1/f$ dependence in both cases, as well as a white spectrum at frequencies above 1 MHz during free evolution. The successful application of these protocols to a transmon permits magnetic noise sensing with such a qubit in future experiments.

[1] J. Bylander *et al.*, Nat. Phys. (2011).
[2] F. Yan *et al.*, Nat. Comm. (2013).
[3] J. Braumüller *et al.*, Appl. Phys. Lett. (2016)

TT 4.7 Mon 11:00 H 2053

Adding ZZ-coupling to transmon qubits — •Alexander Stehli[1], Jochen Braumüller[1], Hannes Rotzinger[1], Andre

Schneider[1], Martin Weides[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]Russian Quantum Center, National Institute of Science and Technology MISIS, Moscow, Russia

Versatile quantum elements enable higher connectivity for quantum computing or the quantum simulation of intricate physics using only few physical qubits. In superconducting quantum circuits, the transmon qubit is the most widely used architecture, owed to its robustness and good coherence properties. While typical transmon designs solely allow for an XX-interaction between neighboring qubits, the concentric transmon [1] was predicted to feature an additional ZZ-coupling [2]. It is mediated by the non-vanishing dc magnetic field of the qubits in the flux-biased state.

In this work, we explore the possibility of ZZ-interaction between two concentric transmon qubits. The qubits are galvanically coupled to maximize their mutual inductance, which is proportional to this effect. In time-resolved microwave measurements, we determine the ZZ-coupling strength from a shift of the qubit transition frequency. First experiments indicate a coupling strength on the order of several MHz.

[1] J. Braumüller *et al.*, Appl. Phys. Lett. **108**, 032601 (2016)
[2] J.-M. Reiner *et al.*, Phys. Rev. A **94**, 032338 (2016)

15 min. break.

TT 4.8 Mon 11:30 H 2053

Qubit readout using a transmon with a V-shaped energy diagram — Remy Dassonneville, Luca Planat, Javier Puertas, Farshad Foroughi, Cecile Naud, Wiebke Guichard, Nicolas Roch, and •Olivier Buisson — University Grenoble Alpes & CNRS, Institut Néel, F-38000 Grenoble, France.

The most widely used scheme to perform qubit readout in cQED relies on the dispersive coupling between a qubit and a harmonic oscillator. However, despite important progresses, implementing a fast and high fidelity readout remains nowadays a major challenge. Indeed, inferring a qubit state is limited by the trade-off between speed and accuracy due to Purcell effect and transitions induced by readout photons in the resonator. To overcome this, we introduce a new device: a transmon with a V-shaped energy diagram, embedded in 3D architecture. It is made of two transmons coupled via a large inductance[1]. The resulting circuit presents two qubits longitudinally coupled called qubit and ancilla. Using symmetry rules[2], the ancilla can be strongly coupled to the cavity while the qubit remains uncoupled. However due to their strong longitudinal coupling, the qubit state can still be inferred through the ancilla state. A theoretical study[3] has predicted a QND readout with fidelity as high as 99.9

[1] É. Dumur, et al, Phys. Rev. B 92, 020515(R) (2015).
[2] É. Dumur, et al, IEEE Trans. Appl. Supercond. 26, 1700304 (2016).
[3] I.Diniz, et al, , Phys. Rev. A 87, 033837 (2013).

TT 4.9 Mon 11:45 H 2053

Decoherence mechanisms in transmon qubits: Ultra-low frequency noise and switching events — •Steffen Schlör[1], Andre Schneider[1], Jürgen Lisenfeld[1], Martin Sandberg[2], David P. Pappas[2], Alexey V. Ustinov[1], and Martin Weides[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]National Institute of Standards and Technology, Boulder, USA — [3]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Today's quantum computers made of highly coherent superconducting qubits are already capable to find the electronic ground state of small molecules [1]. The complexity and number of qubits on single chips having gate fidelities at or beyond the threshold for fault-tolerant quantum computing [2] keeps growing. Their longer operation times shift the focus towards decoherence mechanisms and fluctuations occurring on time scales of hours or even days.

We present the results of such long-term measurements of a high-coherent, non-tunable transmon qubit. We perform simultaneous measurements of the qubit's relaxation and dephasing rates as well as resonance frequency shifts and analyze their correlations. These yield information about the microscopic origin of decoherence mechanisms, their interacting with the qubit, and their fluctuation dynamics. From a spectral noise analysis, we obtain evidence for the presence of a small number of dominant fluctuators.

[1] A. Kandala et al., Nature **549**(7671), 2017
[2] R. Barends et al., Nature **508**(7497), 2014

TT 4.10 Mon 12:00 H 2053

Parametrically activated two-qubit interactions in a superconducting qubit system — •Marc Ganzhorn[1], Marco Roth[2], Gian Salis[1], Nikolaj Moll[1], Sebastian Schmidt[3], and Stefan Filipp[1] — [1]IBM Research, Zurich, Switzerland — [2]RWTH, Aachen, Germany — [3]ETH, Zurich, Switzerland

A current bottleneck for quantum computation is the realization of high-fidelity two-qubit operations in arrays of more than two coupled qubits. Gates based on parametrically driven tunable couplers offer a convenient method to entangle multiple qubits by selectively activating different interaction terms in the effective Hamiltonian. Here we present experimental results on a system comprising fixed-frequency superconducting transmons capacitively coupled to a tunable coupler (in this case a flux tunable qubit). The two-qubit interactions are activated via a parametric frequency modulation. We realize different types of interactions with fidelities up to 97% by adjusting the frequency and phase of this modulation. Our experimental findings are backed by numerical simulations, revealing that the fidelities of these two qubit operations are limited by the coherence of the tunable coupler. Finally, using such a set of single and two qubit interactions, simulation of quantum systems such as molecules or spin systems could be realized.

TT 4.11 Mon 12:15 H 2053

Suppression of the low-frequency decoherence by Bell-state motion — •Andrey Vasenko[1] and Dmitri Averin[2] — [1]National Research University Higher School of Economics, 101000 Moscow, Russia — [2]Department of Physics and Astronomy, Stony Brook University, SUNY,Stony Brook, NY 11794, USA

As demonstrated recently, in the realistic situation when the low-frequency noises are uncorrelated among different physical superconducting qubits, transfer of individual logical qubits in arrays of physical qubits can be used to suppress the low-frequency decoherence of quantum information encoded in the logical qubits [1]. The purpose of this work is to show that, if the quantum information is encoded in the Bell-type logical states, the transfer of these states through an array of physical qubits implements simultaneously the motion-induced and spin-echo suppression of decoherence leading to a qualitatively stronger tool against the low-frequency noise than is provided by the two approaches separately [2]. We also discuss the coexistence of the motion-induced suppression of decoherence and more complicated dynamic decoupling-schemes, like Carr-Purcell pulse sequence.

[1] D. V. Averin, K. Xu, Y. P. Zhong, C. Song, H. Wang, and Siyuan Han, Phys. Rev. Lett. 116, 010501 (2016).
[2] D.V. Averin and A.S. Vasenko, in preparation.

TT 4.12 Mon 12:30 H 2053

In-situ tunable environment for superconducting qubits — •J. Goetz[1], M. Silveri[1,2], K. Y. Tan[1], M. Partanen[1], A. M. Gunyho[1], D. Hazra[1], V. Vesterinen[1,3], J. Hassel[3], L. Grönberg[3], H. Grabert[4], and M. Möttönen[1] — [1]QCD Labs, Department of Applied Physics, Aalto University, Aalto, Finland — [2]University of Oulu, Research Unit of Theoretical Physics, Oulu, Finland — [3]VTT Technical Research Centre of Finland Ltd, VTT, Finland — [4]University of Freiburg, Department of Physics, Freiburg, Germany

Superconducting quantum circuits hold great potential in providing revolutionizing practical applications such as quantum sensing or computing. However, in many cases noise limits the operation and the fidelity of these circuits. Here we introduce a concept that exploits noise instead of trying to reduce it. Our concept uses photon-assisted single-electron tunneling as a controlled source for dissipation in superconducting qubits. We show how the recently developed quantum-circuit refrigerator [1], QCR, is suitable to control the dynamics of superconducting qubits. In our experiments, the QCR works as a voltage-controlled environmental bath for the qubit. The qubit-bath coupling strength can be tuned over several orders of magnitude on a nanosecond timescale. Such a tunable environment is promising for fast qubit reset and studies of dissipative open quantum circuits. Our highly integrable circuit architecture may prove useful in the initialization of qubit arrays and in dissipation-assisted quantum annealing.

[1] K. Y. Tan, et al., Nature Commun. 8, 15189 (2017)

TT 4.13 Mon 12:45 H 2053

Rapid High-Fidelity Multiplexed Readout of Superconduct-

ing Qubits — •Johannes Heinsoo, Christian Kraglund Andersen, Ants Remm, Sebastian Krinner, Yves Salathe, Theodore Walter, Simone Gasparinetti, Jean-Claude Besse, Anton Potocnik, Christopher Eichler, and Andreas Wallraff — ETH Zürich

The duration and fidelity of qubit readout is a critical factor for applications in quantum information processing as it limits the fidelity of algorithms, which reuse qubits after measurement or apply feedback based on the measurement result. In this talk we discuss the results of a fast multiplexed readout experiment performed on five qubits with readout resonators populated for less than 200 ns. We find that the probability of assigning the individual qubit to be in the state we intended to prepare, is above 95% for all five measured qubits. In addition, the data shows that individual Purcell filters used in this experiment lead to reduced measurement induced dephasing of the qubits we did not intend to measure.

TT 5: f-Electron Systems and Heavy Fermions I

Time: Monday 9:30–13:00 Location: H 3005

TT 5.1 Mon 9:30 H 3005

X-ray absorption study of Sn and Cd substituted $CeCoIn_5$ — Kai Chen[1,6], Fabio Strigari[1], Martin Sundermann[1,2,3], Stefano Agrestini[2], Zhiwei Hu[2], Davide Betto[4], Kurt Kummer[4], Javier Herrero[5], Steffen Wirth[2], and •Andrea Severing[1,2] — [1]University of Cologne, Institute of Physics II, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [5]ALBA Synchrotron, Barcelona, Spain — [6]present address: SOLEIL Synchrotron, Saclay, France

In a previous soft x-ray absorption investigation of the crystal-electric field wave function of the $CeRh_{1-x}Ir_xIn_5$ substitution series we showed that changes in the cerium wave function correlate with the phase diagram while these changes anticorrelate with the lattice anisotropy. Here we will present the crystal-electric field wave functions for two other related substitution series: $CeCo(In_{1-x}Cd_x)_5$ and $CeCo(In_{1-y}Sn_y)_5$. The parent compound $CeCoIn_5$ is an unconventional superconductor (T_c=2.3 K) with a field-induced antiferromagnetic quantum critical point inside the superconducting dome. The substitution of tiny amounts of In by Cd or Sn suppresses superconductivity. Sakai *et al.* suspected that Cd and Sn doping has a different impact on hybridization. Our soft x-ray absorption results strongly support this conjecture and show that M-edge XAS is a very sensitive probe of the direction dependence of hybridization.

TT 5.2 Mon 9:45 H 3005

Magnetic field dependence of the zone-center excitation in the heavy-fermion metal CeB_6 — •P. Y. Portnichenko[1], S. E. Nikitin[1,2], S. V. Demishev[3], A. V. Semeno[3], H. Ohta[4], A. V. Dukhnenko[5], N. Yu. Shitsevalova[5], V. B. Filipov[5], Z. Huesges[6], Z. Lu[6], A. Schneidewind[7], and D. S. Inosov[1] — [1]TU Dresden, Germany — [2]MPI-CPfS Dresden, Germany — [3]GPI of RAS, Moscow, Russia — [4]Kobe University, Japan — [5]IMPS, Kiev, Ukraine — [6]HZB, Berlin, Germany — [7]JCNS, Jülich, Germany

The heavy-fermion metal CeB_6 with a simple cubic crystal structure is characterized by a rich magnetic-field – temperature phase diagram. Neutron scattering experiments showed an intense ferromagnetic collective mode that dominates the magnetic excitation spectrum. ESR measurements revealed a significant anisotropy of the g-factor as a function of the applied field direction. The g-factor remains temperature independent and isotropic for field directions like [110] or [111], but shows a noticeable anomaly for $\mathbf{B} \parallel [100]$. Knowing that the energy of the ESR resonance matches perfectly with that of the field-induced INS excitation, we expected a corresponding softening of the zone-center mode in field parallel to [100]. However, our results show absolutely no temperature effect on the g-factor at high fields. We observe significant difference of the resonance energy upon change of the field direction. Observed difference of the resonance energy can be explained either by anisotropy or by redistribution of the spectral weight between two collective magnetic modes, which we perceive as a change of the resonance energy.

TT 5.3 Mon 10:00 H 3005

Doping-induced redistribution of magnetic spectral weight in substituted hexaborides $Ce_{1-x}La_xB_6$ and $Ce_{0.7}Nd_{0.3}B_6$ — •S. E. Nikitin[1,2], P. Y. Portnichenko[2], A. V. Dukhnenko[3], N. Yu. Shitsevalova[3], V. B. Filipov[3], Y. Qiu[4], J. A. Rodriguez-Rivera[4,5], J. Ollivier[6], and D. S. Inosov[2] — [1]MPI CPfS, Dresden, Germany — [2]TU Dresden, Germany — [3]I.M. Frantsevich Inst. for Problems of Materials Sci. of NAS, Kiev, Ukraine — [4]NIST Center for Neutron Research, Maryland, USA — [5]University of Maryland, USA — [6]ILL, Grenoble, France

CeB_6 is a model example of intriguing heavy-fermion physics. At zero field it exhibits a complex magnetic phase diagram with antiferromagnetic (AFM) and "hidden order" phases, which is associated with the ordering of Ce^{3+} antiferroquadrupolar (AFQ) moments. Our recent ARPES and INS measurements have shown that both propagation vectors of AFQ and AFM phases are dictated by the nesting instability of the Fermi-surface. In this work we have extended this approach to probe the evolution of the electronic properties cerium hexaboride upon La and Nd substitutions. We observe that strong diffuse peak at the corner of the Brillouin zone, which coincides with the propagation vector of the elusive AFQ order in CeB_6, is rapidly suppressed by both La and Nd doping, like the AFQ order itself and the corresponding spectral weight is transferred to the $X(\frac{1}{2}00)$ point. Our results provide direct evidence that the complex magnetic phase diagrams of substituted hexaborides are dictated by the evolution of the Fermi-surface upon effective "hole"-like doping.

TT 5.4 Mon 10:15 H 3005

Investigation of the surface properties of SmB_6 by STM — •Lin Jiao[1], Sahana Rössler[1], Priscila F. S. Rosa[2,3], LiuHao Tjeng[1], Zachary Fisk[2], Frank Steglich[1], and Steffen Wirth[1] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, University of California, Irvine, California, USA — [3]Los Alamos National Laboratory, Los Alamos, New Mexico, USA

We present scanning tunneling microscopy and spectroscopy measurements on SmB_6, which is a candidate material for a topological Kondo insulator. The measurements were conducted on non-reconstructed (001) surfaces [1,2] at temperatures down to 0.35 K. At these low temperatures, we observe several well-resolved states within the hybridization gap of SmB_6. The temperature evolution of the tunneling spectra indicates two energy scales, in line with bulk and surface Kondo effect, respectively [3]. Moreover, we can put our results into perspective with the predicted existence of topologically protected surface states. In this respect, we will also present spectroscopic as well as resistivity results on substituted samples $(Sm_{1-x}R_x)B_6$ for R = Gd, Y, Yb and, in particular, discuss the influence of magnetic substituents on the topological surface states.

[1] S. Rößler *et al.*, Proc. Natl. Acad. Sci. USA **111**, 4798 (2014).
[2] S. Rößler *et al.*, Phil. Mag. **96**, 3262 (2016).
[3] L. Jiao *et al.*, Nat. Commun. **7**, 13762 (2016).

TT 5.5 Mon 10:30 H 3005

DFT+DMFT simulations of rare-earth hexaborides — •Florian Sohn[1], Steffen Backes[4], Salvatore R. Manmana[1], Roser Valentí[3], and Peter E. Blöchl[1,2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für theoretische Physik, Technische Universität Clausthal, Germany — [3]Institut für theoretische Physik, Goethe-Universität Frankfurt am Main, Germany — [4]Centre de Physique Théorique, École polytechnique, Palaiseau, France

Rare-earth hexaborides (REB_6) are strongly correlated materials, where the strong Coulomb interaction between electrons in the rare earth's f-electron shell influence the electronic properties of the whole material decisively. REB_6 exhibit a variety of low-temperature phenomena, including antiferromagnetic ordering for most partially filled f-shells, ferromagnetic ordering in EuB_6, superconductivity for LuB_6, topological insulating behavior in SmB_6 and a complex phase diagram with Kondo behavior in CeB_6. We present results of DFT+DMFT

simulations performed on selected REB_6, in particular for the spectral function. For the DFT calculations, the Wien2k code is applied, while for the DMFT we employ the continuous-time hybridization expansion quantum Monte Carlo (CT-HYB) matrix code of the ALPSCore project. Our goal is to compare with ARPES experiments.

We gratefully acknowledge financial support by the DFG project PR298/19-1.

TT 5.6 Mon 10:45 H 3005

Magnetic anisotropy in $YbRh_6Si_4$ single crystals — •Sebastian Witt, Doan-My Tran, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

Recently, researchers have started to investigate the structural properties of rhodium-rich silicides $RERh_6Si_4$ (RE = rare earth) [1]. The new interest in these hexagonal and non-centrosymmetric compounds derives from the suppression of a ferromagnetic transition to a quantum critical point in Si-doped $CeRh_6Ge_4$. Recently, a magnetic transition at 4.5K in $YbRh_6Si_4$ polycrystals was reported.

Here, we present the single crystal growth of $YbRh_6Si_4$ with indium flux. In first measurements (susceptibility, resistivity and specific heat) we have investigated the magnetic transition around 4.5K in needle-shaped single crystals. In susceptibility and resistivity data the magnetic anisotropy for field along and perpendicular to the c-direction will be presented.

[1] D. Voßwinkel et al., Z. Naturforschung B, **72**, 11 (2017).

TT 5.7 Mon 11:00 H 3005

A Study of the Ferromagnetic and Lifshitz Phase Transitions in the Heavy-Fermion Metal $YbNi_4P_2$ by Ultrasonic Measurements — •Yeekin Tsui, Lars Postulka, Bernd Wolf, Ulrich Tutsch, Kristin Kliemt, Cornelius Krellner, and Michael Lang — Goethe-Univeristät, Physikalisches Institut SFB/TR49, D-60438 Frankfurt(M),Germany

$YbNi_4P_2$ is a stoichiometric heavy-fermion Kondo-lattice system with a Kondo temperature of 8 K [1]. This system is situated in the close vicinity of a ferromagnetic (FM) quantum-critical point (QCP) and can be tuned to the FM QCP by substituting a small amount of phosphorous by arsenic [1]. Recently, nine field-induced Lifshitz transitions (LTs) have been proposed in $YbNi_4P_2$ [2] from the results of the transport and thermodynamic measurements, revealing a complicated electronic band structure of the system. We have performed ultrasonic measurements on single crystals of $YbNi_4P_2$ to deepen the understanding of these phase transitions. We found clear features in the ultrasound velocity (v) and the attenuation (α) corresponding to crystal-electric-field and Kondo effects. However, we detected no or very small anomalies in v or α at the expected FM phase transition in the longitudinal c33 mode, reflecting a weak coupling of the corresponding symmetry strain to the magnetic structure. On the other hand, pronounced features were identified at the proposed Lifshitz transitions at roughly 0.4, 6 and 7 T clearly demonstrating the different character of these transitions.

[1] A. Steppke et al., Science 339 (2013) 933.
[2] H. Pfau et al., Physical Review Letters 119 (2017) 126402.

15 min. break.

Invited Talk TT 5.8 Mon 11:30 H 3005

Superconductivity in $YbRh_2Si_2$ — •Erwin Schuberth — Technische Universität München

Our recent experiments on $YbRh_2Si_2$ showed - aside from the well known antiferromagnetic transition at 70 mK - two new phases below 10 mK and 2 mK respectively[1]. The latter is practically coinciding with superconductivity. Evidence for these findings came from magnetic susceptibility measurements, dc as well as ac, performed at the Walther-Meissner Institut in Garching. The 2mK A-phase transition is a hybrid electronic-nuclear spin transition and it extends to fields of 23 mT where it is suppressed to below our detection limit of 800 μK. In addition, specific heat data show, that at this transition a large entropy is involved coming from the nuclear spins of the Yb isotopes. Here we present additional, unpublished results around and below this temperature up to the Quantum Critical Point at 60 mT. Also, we reanalyzed previous data on the magnetic susceptibility of $CeCu_6$ taken in Garching and Cornell in 1994 [2]. The results are very similar to those of $YbRh_2Si_2$ and it is very likely that the same mechanism holds in both systems.

[1] E. Schuberth et al., Science 351, 485 (2016)
[2] C. Jin et al., Physica B 194-196, 207-208 (1994)

TT 5.9 Mon 12:00 H 3005

Crystal field scheme of the topologically non-trivial Kondo insulator $CeRu_4Sn_6$ determined by RIXS — •Andrea Amorese[1,2], Kurt Kummer[3], Oliver Stockert[2], Andrey Prokofiev[4], Silke Paschen[4], Maurits Haverkort[5], and Andrea Severing[1,2] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [4]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [5]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

Rare earth Kondo insulators have the potential for being strongly correlated topological insulators and $CeRu_4Sn_6$ is one of the promising candidates. Unfortunately, in the presence of correlations the models employed for describing the topological insulating properties lack reliability so that information about the electronic structure must be determined experimentally. In particular, the degeneracy of the the Ce^{3+} Hund's rule ground multiplet is lifted in $CeRu_4Sn_6$ by the crystal electric field (CEF), but the CEF potential was up to now only partially characterized, due to limitations of the traditional neutron-based techniques. Resonant inelastic soft x-ray scattering (RIXS) has been recently shown to be a very powerful tool to overcome these limitations. With RIXS the ground state and excited Hund's rule multiplet are accessible and due to the resonant process the electronic excitations are pure and not overshadowed by e.g. phonons. With soft RIXS we have fully determined the CEF scheme of $CeRu_4Sn_6$.

TT 5.10 Mon 12:15 H 3005

Nuclear magnetic resonance investigation of the novel heavy fermion system $Ce_2CoAl_7Ge_4$ — •Adam P. Dioguardi[1,2], Pedro Guzman[2,3], Priscila F. S. Rosa[2], Nirmal J. Ghimire[2], Serena Eley[2], Stuart E. Brown[3], Joe D. Thompson[2], Eric D. Bauer[2], and Filip Ronning[2] — [1]IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany — [2]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Department of Physics and Astronomy, UCLA, Los Angeles, California 90095, USA

We present nuclear magnetic resonance (NMR) and nuclear quadrupole resonance (NQR) measurements performed on single crystalline $Ce_2CoAl_7Ge_4$, a member of a recently discovered family of heavy fermion materials $Ce_2MAl_7Ge_4$ (M = Co, Ir, Ni, or Pd). A clear Knight shift anomaly ($K \not\propto \chi$) is observed at coherence temperatures $T^* \sim 17.5$ K for $H_0 \parallel \hat{c}$ and 10 K for $H_0 \parallel \hat{a}$ at the ^{59}Co site, and $T^* \sim 12.5$ K at the ^{27}Al(3) site for $H_0 \parallel \hat{a}$ characteristic of the heavy fermion nature of this compound. At high temperatures the ^{59}Co NMR spin-lattice relaxation rate T_1^{-1} is dominated by spin fluctuations of the 4-f local moments with a weak metallic background. Furthermore, we find $(T_1TK)^{-1} \propto T^{-1/2}$ at the ^{59}Co site as expected for a Kondo system for $T < T^*$ and $T < T_K$. ^{59}Co NQR T_1^{-1} measurements at low temperatures indicate slowing down of spin fluctuations above the magnetic ordering temperature $T_M \sim 1.8$ K. A weak ferromagnetic character of fluctuations around $\mathbf{q} = 0$ is evidenced by an increase of χT vs T above the magnetic ordering temperature.

TT 5.11 Mon 12:30 H 3005

Optical response of Cerium-based clathrates — Farzaneh Zamani[1], •Stefan Kirchner[2], and Silke Paschen[3] — [1]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China — [3]Institute of Solid State Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria

Clathrates are a class of caged compounds that display a wide range of physical properties as a function of host-guest composition. Cerium-based type-I clathrates are of particular interest due to their unusual thermoelectric properties with potential for application[1]. The origin of the observed thermopower enhancement at comparatively high temperature in $CeBa_7Au_6Si_{40}$, however, is still a matter of debate. While Kondo scattering does occur in the system, Curie-Weiss behavior prevails down to about 1K. In order to understand the role of the rattling modes in the thermopower enhancement we address the optical response of $CeBa_7Au_6Si_{40}$. In particular, we investigate if a model of phonon-enhanced Kondo scattering can explain the differences observed [2] in the optical conductivity of $CeBa_7Au_6Si_{40}$ and its

rare-earth free reference compound.
[1] A. Prokofiev et al.,Nature Mat. **12**, 1096-1101 (2013).
[2] G. Johnstone et al., unpublished.

TT 5.12 Mon 12:45 H 3005

Crystalline electric field calculations for $CeIr_3Ge_7$ — •Jacintha Banda[1], Binod Rai[2], Emilia Morosan[2], Christoph Geibel[1], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA

$CeIr_3Ge_7$ is a metallic antiferromagnet with an extremely low Néel temperature of 0.65 K despite the absence of Kondo effect and geometrical frustration. We have solved the crystalline electric field (CEF) scheme for the well localized Ce^{3+} moment which has a trigonal point symmetry. We compared our calculations with experimental data on single crystalline samples and found an excellent agreement with one possible solution. This yields a large positive B_2^0 CEF parameter, resulting in a large CEF splitting with the first and second excited CEF levels at 374 and 1398 K respectively. A large off diagonal B_4^3 parameter leads to a strong mixing of the $\left|\pm\frac{5}{2}\right\rangle$ function into the predominantly $\left|\pm\frac{1}{2}\right\rangle$ CEF ground state. As a result, the system shows a huge XY anisotropy. The overall CEF splitting in this compound is one of the largest ever observed in a Ce system. Comparison with other compounds suggest that such large CEF splitting might be connected with the presence of 5d ligands.

TT 6: Quantum Magnets and Molecular Magnets (joint session TT/MA)

Time: Monday 9:30–13:00 Location: H 3010

TT 6.1 Mon 9:30 H 3010

Frustrated spin ladders in quasi-1D $S=\frac{1}{2}$ Heisenberg magnet balyakinite $CuTeO_3$ — •Helge Rosner[1] and Oleg Janson[2] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Deutschland — [2]Institut für Festkörperphysik, TU Wien, Österreich

Copper tellurium oxides are enjoying increasing attention as a promising playground for quantum magnetism [1]. A chemically simple compound, the natural mineral balyakinite $CuTeO_3$ features an intricate crystal structure with Cu_2O_6 dimers connected by TeO_4 tetrahedra into a 3D network. Magnetization measurements indicate a sizable spin gap which is not closed in a magnetic field of 60 T. By using DFT calculations, we show that the magnetism of balyakinite is quasi-1D, and can be described by a frustrated ladder model with four antiferromagnetic exchanges: the dominant rung exchange $J_\perp$, sizable $J_\parallel$ and weak $J'_\parallel$ that alternate along both legs, as well as the weak frustrated cross-coupling $J_\times$. Using the DFT+U estimates of the exchange integrals, we calculate the spin correlations in the ground state. Peculiarities of the magnetic excitation spectrum will be briefly discussed.
[1] M. R. Norman, arXiv:1708.05100.

TT 6.2 Mon 9:45 H 3010

Extreme field-sensitivity of the magnetic tunnelling in Fe-doped Li_3N — •Manuel Fix[1], James H. Atkinson[2], Paul C. Canfield[3,4], Enrique del Barco[2], and Anton Jesche[1] — [1]EP VI, EKM, University of Augsburg, D-86159, Germany — [2]Department of Physics, UCF, Orlando FL 32816, USA — [3]The Ames Laboratory, ISU, Ames, Iowa 50011, USA — [4]Department of Physics and Astronomy, ISU, Ames, Iowa 50011, USA

The magnetic properties of dilute $Li_2(Li_{1-x}Fe_x)N$ with $x \sim 0.001$ are dominated by the spin of single, isolated Fe atoms [1]. Below $T = 10$ K the spin-relaxation times become temperature-independent, indicating a crossover from thermal excitations to the quantum tunnelling regime.

The spin-flip probability increases tremendously in *transverse* magnetic fields, proving the resonant character of this tunnelling process. Upon application of *longitudinal* fields, on the other hand, the ground-state degeneracy is lifted and the tunnelling condition destroyed. We show time dependent magnetization measurements performed on single crystals in various longitudinal magnetic fields at temperatures $T = 2-16$ K. An increase of the relaxation time by four orders of magnitude in applied fields of only a few milliTesla reveals exceptionally sharp tunnelling resonances. This strong field dependence of the spin reversal could be employed to create stable ($\mu_0 H_z = 3$ mT) but switchable ($H_z = 0$) magnetic 'quantum bits' at elevated temperatures.
[1] A. Jesche *et al.*, Nature Comm. **5**:3333 (2014)

TT 6.3 Mon 10:00 H 3010

In- & interchain exchange constants of Li_2CuO_2: the origin of the ferromagnetic inchain ordering — •S.-L. Drechsler[1], R. Klingeler[2], W. Lorenz[2], R. Kuzian[3], L. Hozoi[1], R. Jadav[1], J. Richter[4], H. Rosner[5], U. Nitzsche[1], A. Tsirlin[6], and S. Nishimoto[1,7] — [1]IFW-Dresden, Germany — [2]Heidelberg University, Germany — [3]Inst. f. Problems of Material Science, Kiev, Ukraine — [4]MPI-PKS, Dresden, Germany — [5]MPI-CPfS, Dresden, Germany — [6]Augsburg University, Germany — [7]TU Dresden, Germany

Li_2CuO_2 takes a special place among frustrated chain compounds with edge-sharing CuO_4 units and a ferromagnetic (FM) nearest neighbor (NN) in-chain coupling J_1 due to its ideal planar CuO_2 chain structure and its well-defined 3D Neél-type ordering below $T_N \approx 9$ K of adjacent chains whose magnetic moments are aligned FM along the chains (*b*-axis). There are only frustrating AFM *interchain* couplings (IC) with adjacent chains *shifted* by half a lattice constant *b*. *No* room is left for strong unfrustrated IC in shtark contrast with a recently proposed scenario [1]. The AFM IC with dominant NNN components plays a decisive role in the stabilization of the FM alignment of the magnetic moments along b. Although weak, with 8 NNN IC it is significant enough to prevent a competing non-collinear spiral type ordering. We report realistic values of all relevant exchange constants based on two DFT and quantum chemistry calculations in full accord with a spin-wave analysis of INS, RIXS, and magnetic susceptibility $\chi(T)$ data. The large $J_1 \approx$ -230 K is ascribed to a sizable direct FM Cu-O coupling $K_{pd} \approx 100$ meV.
[1] G. Shu *et al.*, New J. Phys. **19**, 023026 (2017).

TT 6.4 Mon 10:15 H 3010

Magnetic susceptibility and high frequency EPR studies on three isostructural $Fe_2^{III}Ln_2^{III}$ complexes — •Silvia Menghi[1], Changhyun Koo[1], Yan Peng[2], Christopher Anson[2], Annie Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Karlsruhe Institut of Technology, Karlsruhe, Germany

Magnetic interactions and anisotropy of three 3d/4f heteronuclear metal-organic complexes are studied by means of high-frequency electron paramagnetic resonance (HF-EPR) and magnetic susceptibility measurements. All complexes under study exhibit isostructural tetranuclear core motifs $[(Fe_2^{III}Ln_2^{III}(\mu_3\text{-}OH)_2(teaH)_2(O_2CCPh)_6]\cdot 3MeCN$ (L=Y,Gd,Dy). The HF-EPR data show various resonance branches, each of which with finite zero field splitting. The static magnetic susceptibility data imply strong antiferromagnetic coupling of $J_{FeFe} = -6.71(4)$ cm^{-1} between the two Fe^{III} centers. The coupling between Fe and Ln was found to be weak and ferromagnetic. In order to gain quantitative insight into the anisotropy and the Fe-Dy exchange interaction, simulations have been performed using a proper hamiltonian which applies a Ising concept for the lanthanide ions.

TT 6.5 Mon 10:30 H 3010

Effect of radicals on coupling and anisotropy in mono- and dinuclear Ni(II) complexes with an azopyridine ligand — •Sven Spachmann[1], Roland Bischoff[2], Changhyun Koo[1], Hans-Jörg Krüger[2], and Rüdiger Klingeler[1,3] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Faculty of Chemistry, TU Kaiserslautern, Kaiserslautern, Germany — [3]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany

We present static magnetization and high-frequency electron paramagnetic resonance (HF-EPR) studies on metallorganic mono- and dinuclear Ni(II)-complexes with radical and non-radical azopyridine ligands. In the monomer, the radical is coupled ferromagnetically to the Ni(II) spin, thereby forming an $S = 3/2$ ground state. In the non-radical mononuclear system, anisotropy is of the easy-plane type with $D_{Ni} = 4.0$ K and $|E| = 0.32$ K.

We observe a strong effect of the radical bridge on the dimer systems: While the non-radical azopyridine-bridged Ni(II)-dimer has a

singlet ground state with a weak intradimer coupling of $J \approx 20$ K, a strong ferromagnetic coupling $J_{\mathrm{Ni-rad}} \approx -500$ K is observed in the radical azopyridine-bridged Ni(II)-dimer between the radical and the Ni(II)-ions. The antiferromagnetic Ni-Ni coupling in the radical-bridged dimer $J_{\mathrm{Ni-Ni}} = 25$ K is of the same order as without the radical. The HF-EPR and magnetization measurements confirm the $S = 5/2$ ground state and axial symmetry. We obtain $g_z = 2.126$ and $D_{5/2} = -0.844$ K, which corresponds to a single-ion anisotropy of $|D_{\mathrm{Ni}}| = 4.2$ K.

TT 6.6 Mon 10:45 H 3010

Highly dispersive magnons with spin-gap like features in the frustrated ferromagnetic chain system $Ca_2Y_2Cu_5O_{10}$ by inelastic neutron scattering — M. Matsuda[1], J. Ma[1], V.O. Garlea[1], T. Ito[2], H. Yamaguchi[2], K. Oka[2], •S.-L. Drechsler[3], R. Yadav[3], L. Hozoi[3], H. Rosner[4], R. Schumann[5], R. Kuzian[6], and S Nishimoto[3,5] — [1]Quantum Matter Division, Oak Ridge, NRL, USA — [2]Natiomal Institute of AIST, Tsukuba, Japan — [3]IFW-Dresden, Germany — [4]MPI-CPfS, Dresden, Germany — [5]TU Dresden, Germany — [6]Inst. f. Problems of Material Science, Kiev, Ukraine

We report an inelastic neutron scattering study including its theoretical description for $Ca_2Y_2Cu_5O_{10}$ and map out the full large magnetic dispersion relation extending up to 53 meV. A doubly frustrated linear Heisenberg-type spin chain model with two inchain and two diagonal antiferromagnetic (AFM) interchain couplings (IC) analyzed within linear spin-wave theory reproduces well the observed strong dispersion in chain direction and q weak one perpendicularly. The large dispersion leads to a record value of the NN intrachain coupling $| J_1 | \approx 280$ K which points to a large direct FM Cu-O coupling K_{pd} value slightly above 100 meV. Our J_1-value resolves an old puzzle of FM inchain ordering vs. an improper AFM pseudo Curie-Weiss (CW) behavior for $\chi(T)$. It yields a true FM CW-regime above 1500 K, only. The observed "gaps" at 11.5 and 28 meV stem from an interaction with a phonon mode and the synenergetic disorder influence on the CuO_2 chains by the incommensurate alternating cationic YCa-chains distorting the O positions and a specific quantum effect from the AFM IC, respectively.

TT 6.7 Mon 11:00 H 3010

Magnetism of atacamite, $Cu_2Cl(OH)_3$ — •Leonie Heinze[1], Randirley Beltran-Rodriguez[2], Gael Bastien[2], Anja U.B. Wolter[2], Manfred Reehuis[3], Jens-Uwe Hoffmann[3], Kirrily C. Rule[4], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Germany — [2]IFW Dresden, Dresden, Germany — [3]HZB, Berlin, Germany — [4]ANSTO, Kirrawee, Australia

Atacamite, $Cu_2Cl(OH)_3$, has been reported to exhibit magnetic behavior characteristic of a frustrated quantum magnet. Notably, an antiferromagnetic transition at $T_N = 9.0$ K has been observed and, further, susceptibility measurements previously carried out indicate a Curie-Weiss temperature $|\Theta_{CW}| \gg T_N$ [1,2]. So far, attempts have been undertaken to determine the symmetry of the magnetic ground state of this material by means of μSR and NMR measurements on polycrystalline material [2,3], however with contradictory results.

Starting from this given situation, we have reinvestigated the magnetic properties of atacamite [4]: Mineral single-crystals were studied by means of susceptibility and magnetization measurements along the principal crystal axes as well as elastic neutron scattering. This way, we have established the symmetry of the magnetic ground state and present new insights into the unusual magnetic properties of atacamite.

[1] X. G. Zheng, *et al.*, Solid State Commun. **130**, 107 (2004).
[2] X. G. Zheng, *et al.*, Phys. Rev. B, **71**, 174404 (2005).
[3] K. Zenmyo, *et al.*, J. Phys. Soc. Jpn., **82**, 084707 (2013).
[4] L. Heinze, *et al.*, Physica B, doi.org/10.1016/j.physb.2017.09.073 (2017).

15 min. break.

TT 6.8 Mon 11:30 H 3010

Alternating ferro- and antiferromagnetic Heisenberg chain: from dimer to Haldane limit — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We present results of a study of the $S = 1/2$ Heisenberg chain with alternating ferro- and antiferromagnetic exchange, J_2 and J_1 respectively. This system interpolates from a dimer to a Haldane chain as $j = |J_2/J_1|$ varies from 0 to ∞. Using perturbation theory (PT) and quantum Monte Carlo based on the stochastic series expansion (SSE) method, we study elementary excitations, thermodynamic properties, and the dynamic structure factor $S(\mathbf{q}, \omega)$. For $j \ll 1$ we find good agreement between PT and SSE. For arbitrary j we show that $S(\mathbf{q}, \omega)$, obtained from SSE, scales between triplons at $j \ll 1$ and a Haldane chain spectrum at $j \gg 1$. Finally, we contrast our findings for the spin gap versus j against existing literature.

TT 6.9 Mon 11:45 H 3010

Field Control of Magnonic Heat Flow — •Benjamin Köhler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Controlling such transport by means of external fields is vital for potential device design. Here we study thermal conductivity of a two dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of an external field. The latter is used to manipulated the heat flow due to spin canting.

Using nonlinear spin wave theory and a Kubo approach we evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon decay for finite fields and temperature. Semi-quantitative estimates for attainable variations of the heat conductivity in realistic materials will be presented as a function of the temperature and the external fields, suggesting interesting implications for spin caloritronic applications.

TT 6.10 Mon 12:00 H 3010

Suppression of spin-crossover by dynamic Jahn-Teller effect in C_{60}^{3-} — •Dan Liu, Naoya Iwahara, and Liviu Chibotaru — Theory of Nanomaterials Group, University of Leuven, Leuven, Belgium

In conventional spin crossover systems, the vibrational degrees of freedom enhances the entropic effect in excited high-spin terms resulting from the softening of vibrations [1]. Here, we show an opposite effect of vibration on the spin crossover taking C_{60}^{3-} as an example [2]. The vibronic states resulting from dynamical Jahn-Teller effect in C_{60}^{3-} are obtained using the numerical diagonalization of the linear $p^n \otimes 8d$ Jahn-Teller Hamiltonian with the currently established coupling parameters. It is found that the Jahn-Teller effect stabilizes the low-spin states, resulting in the violation of Hund's rule. The energy gain due to the Jahn-Teller dynamics is found to be comparable to the static Jahn-Teller stabilization. The Jahn-Teller dynamics influences the thermodynamic properties via strong variation of the density of vibronic states with energy. Thus, the large vibronic entropy in the low-spin states enhances the effective spin gap of C_{60}^{3-} quenching the spin crossover. This finding is used for the rationalization of the experimental data on the spin gaps in various fullerides.

[1] P. Gütlich, A. Hauser, and H. Spiering, Angew. Chem. Int. Ed. 33, 2024 (1994).
[2] D. Liu, N. Iwahara, and L. F. Chibotaru, arXiv:1711.00340 [cond-mat.mtrl-sci].

TT 6.11 Mon 12:15 H 3010

Andreev transport through single-molecule magnets — •Filip Pawlicki and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznań, Poland

Transport characteristics of a single molecule magnet coupled to two ferromagnetic and one superconducting lead are studied theoretically by means of the real-time diagrammatic technique. The coupling to the ferromagnets is assumed to be weak, while the coupling to the superconductor can be arbitrary. The quantities of interest include the Andreev current, differential conductance, tunnel magnetoresistance (TMR) and current cross-correlations. It is shown that the system exhibits splitting of Andreev states due to additional degrees of freedom of the molecule. The TMR and current cross-correlations are used to quantify the contribution of crossed and direct Andreev reflections to the current. We also compare our results to those obtained for a quantum dot in a similar three-terminal setup and discuss the possibility of using molecules for Cooper pair splitting.

TT 6.12 Mon 12:30 H 3010

Manifestations of a coherent Kondo lattice formed in adatoms — •Richard Korytár[1], María Moro Lagares[2], and David Serrate[3] — [1]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]Institute of Nanoscience of Aragon (INA), University of Zaragoza, Spain

In a recent experiment, chains of magnetic adatoms were constructed on a pristine metallic surface. A careful analysis by scanning-tunneling spectroscopy demonstrates that the Kondo screening overtakes magnetic interactions at all accessible chain lengths. A comparison with many-body calculations allows to address diverse real space aspects of the coherent Kondo lattice, such as: overlapping Kondo clouds, long-range mediated hybridization and Fermi surface effects. The phenomenology of the onset of heavy fermions in these systems can be discussed.

TT 6.13 Mon 12:45 H 3010

Formation of Local Magnetic Order in Atomic-Scale Ir Junctions — •Markus Ritter, Martin Keller, Torsten Pietsch, and Elke Scheer — Department of Physics, University of Konstanz, D-78467 Konstanz, Germany

The transition metals Pt, Pd, and Ir are paramagnets close to the Stoner transition of ferromagnetism. However, in reduced dimensions, such as small clusters and atomic contacts, a magnetically ordered state has been predicted [1]. In atomic contacts of the elements Pt and Pd, the emergence of local magnetic order has been experimentally confirmed recently [2, 3]. Currently there is no demonstration of such phenomena in Ir. Therefore, we investigate the magnetic properties of atomic Ir contacts and monoatomic chains [4]. The occurrence of local magnetic order is deduced from magnetoconductance (MC) and anisotropic magnetoconductance (AMC) measurements. The rich MC behavior is interpreted in the framework of a microscopic model of the local magnetic configuration and is compared to earlier findings in Pt and Pd contacts. Furthermore, in many contacts electronic transport ($\mathrm{d}I/\mathrm{d}V$) spectroscopy shows a pronounced zero-bias anomaly (ZBA) and further features, which are currently not fully understood. The ZBA is analyzed in the context of Kondo screening of the local magnetic moment in the junction.

[1] Delin, Tosatti. Phys. Rev. B **68**, 144434 (2003).
[2] Strigl et al. Nat. Commun. **6**, 6172 (2015).
[3] Strigl et al. Phys. Rev. B **94**, 144431 (2016).
[4] Thiess et al. Phys. Rev. Lett. **103**, 217201 (2009).

TT 7: Topological Semimetals I

Time: Monday 9:30–13:00 Location: A 053

TT 7.1 Mon 9:30 A 053

ARPES analysis of the $Mo_xW_{1-x}Te_2$-System — •Erik Haubold[1], Dmitry Efremov[1], Matthias Gillig[1], Boy Roman Piening[1], Saicharan Aswartham[1], Alexander Fedorov[1], Yevhen Kushnirenko[1], Thirupathaiah Setti[1], Igor Morozov[1,3], Timur Kim[2], Christian Hess[1], Bernd Büchner[1], and Sergey Borisenko[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Diamond Light Source, Didcot OX11 0DE, United Kingdom — [3]Moscow State University, Moscow 119991, Russia

WTe_2 and the corresponding sister compound $MoTe_2$ sparked a lot of interest and research as potential Weyl semimetals or in the field of Dirac and Weyl semimetals in general. Although the stoichiometric compounds as well as some intermediate doping levels have been analysed, no complete thorough investigation of the whole series has been carried out.

Recent transport data measured at IFW Dresden indicates a nonlinear behaviour of the electrical and magnetic properties when going from pure WTe_2 to $MoTe_2$. We have collected ARPES data for the whole series of materials and analysed their electronic structure to clarify whether the changes in the bandstructure can explain this.

Initial results show a significant shift of bands close to the Fermi energy resulting in a change of the size of the Fermi surfaces. We compare these results to transport data and calculations to check whether such shifts explain the nonlinearity.

TT 7.2 Mon 9:45 A 053

Effects of pressure on the Fermi surface of Cd_3As_2 — •Aleksandar Vasiljković[1], Filip Orbanić[2], Mario Novak[2], Malte Grosche[1], and Ivan Kokanović[1,2] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [2]Department of Physics, Faculty of Science, University of Zagreb, 10002 Zagreb, Croatia

Cd_3As_2 is a symmetry-protected three dimensional Dirac semimetal with high carrier mobility [1], motivating detailed investigations of the electronic structure and its evolution with applied pressures. Shubnikov-de Haas oscillations have previously been reported with frequencies of around 55T, corresponding to tiny Fermi surface pockets in a semimetallic band structure [2]. De Haas-van Alphen oscillations have also been observed with slightly smaller frequencies [2]. We have examined the Shubnikov-de Haas oscillations of the magnetoresistance in a high-quality crystal grown under different conditions over a wide range of temperature and pressure. In contrast to previous reports, we observe a significantly lower quantum oscillation frequency of 27T at ambient pressure in a direction perpendicular to c direction, which decreases significantly with increasing pressure. We also saw 35T frequency at ambient pressure in c direction. The observed SdH oscillations allow us to characterize the Fermi surface by extracting its relevant parameters.

[1] Z.Wang, et al., Physical Review B 88, 125427 (2013).
[2] A. Pariari et al., Physical Review B 91, 155139 (2015).

TT 7.3 Mon 10:00 A 053

Large Nernst power factor in polycrystalline Weyl semimetal NbP — •Satya N. Guin, Chenguang Fu, Sarah J. Watzman, Gudrun Auffermann, Nitesh Kumar, Vicky Suess, Walter Schnelle, Yan Sun, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The energy crisis has sparked a large boost in thermoelectric research, the base of which is the longitudinal thermoelectric response, the Seebeck effect. Recently, there is a growing interest in the Nernst effect (NE), the transverse thermoelectric response produced by the orthogonal thermal gradient and magnetic field. The NE is an alternate and simpler approach to conventional thermoelectrics as there is no need for both n-type or p-type legs. In parallel, Dirac and Weyl semimetals created an enormous interest due to interesting transport properties, which are gaining attention recently for NE. To date, the investigations are primarily engrossed on single crystals. However, the synthesis of large single crystals is the expensive, lengthy, and difficult process, which is unsuitable for mass production and practical applications. In contrast, polycrystalline samples are the better choice because of its ease of production. We demonstrate that polycrystalline, SPS sintered Weyl semimetal NbP show a large Nernst thermopower value of 90 μVK^{-1} and power factor of 35×10^{-4} $Wm^{-1}K^{-2}$ at 9 T. Our finding indicates the potential of polycrystalline Weyl semimetals for thermoelectrics.

TT 7.4 Mon 10:15 A 053

Surface and bulk superconductivity at ambient pressure in the Weyl semimetal TaP — •Maarten van Delft[1,2], Sergio Pezzini[1,2], Markus König[3], Andrew Mackenzie[3,4], Nigel Hussey[1,2], and Steffen Wiedmann[1,2] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen, NL — [2]Radboud University, Institute for Molecules and Materials, Nijmegen, NL — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, GER — [4]Scottish Universities Physics Alliance (SUPA), University of St. Andrews, St. Andrews, UK

Since the discovery of topological Weyl semimetal states in the compounds TaAs, TaP, NbAs and NbP, a considerable effort has been made to investigate their novel electronic properties. Of particular interest to this field is the search for a superconducting state, as such a state may host Majorana fermions. This search has led to observations of superconductivity in TaP under extreme pressure and after ion bombardment, but has hitherto failed to find a bulk superconductor at ambient pressure. We report on the observation of a superconducting state in Tantalum Phosphide (TaP) without any additional treatment to the material or under any extreme conditions. A Tc varying between 1.7 and 5.3 K for different samples was observed, both for microscopic samples processed with focused ion beam (FIB) etching as well as for an as-grown crystal. Our data show that the superconductivity present in our untreated crystal is inhomogeneous yet exists in the bulk. For samples made with FIB, we observe additionally a two-dimensional superconducting film on the sample surface.

TT 7.5 Mon 10:30 A 053

Giant anomalous Nernst effect in Weyl semimetals TaP and TaAs — •Federico Caglieris[1], Christoph Wuttke[1], Steffen Sykora[1], Vicky Süss[2], Shekhar Chandra[2], Claudia Felser[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01069 Dresden, Germany — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

The discovery of Weyl fermions in transition metal monoarsenides/phosphides without inversion symmetry represents an exceptional breakthrough in modern condensed matter physics. However, exploring the inherent nature of these quasiparticles is experimentally challenging because most of the experimental probes rely on analyzing the Fermi arc topology or investigating the elusive chiral anomaly.

In this work we experimentally investigate the thermoelectric transport of the prototypical type-I Weyl semimetals TaP and TaAs. In particular we show that both the compounds possess a giant Nernst coefficient, which tends to saturate with increasing the magnetic field. This behavior resembles what is typically addressed as anomalous Nernst effect and it has recently been interpreted as a direct consequence of the finite Berry curvature originated from the Weyl points. Our results thus promote the Nernst coefficient as an ideal bulk probe for detecting and exploring the fingerprints of emergent Weyl physics.

TT 7.6 Mon 10:45 A 053

Giant anomalous Nernst effect in Weyl semimetals TaP and TaAs - Theory — •Steffen Sykora[1], Federico Caglieris[1], Christoph Wuttke[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

In Weyl semimetals the Nernst coefficient is dominated by anomalous contributions to the electrical and thermal conductivity which originate from a specific property of the underlying system of conduction electrons, the Berry curvature. Motivated by recent experiments on the prototypical type-I Weyl semimetals TaP and TaAs we explain the measured anomalous field dependence of the Nernst coefficient in terms of a minimal model of the energy dispersion near two separated Dirac nodes. On the basis of this result we argue that our observed field dependence of the Nernst effect can straightforwardly be explained by a characteristic change of the chemical potential under variation of the external magnetic field which is applied to obtain the Nernst effect.

TT 7.7 Mon 11:00 A 053

Transport studies on the type-II Weyl semimetal candidate WTe_2 — •Matthias Gillig[1,2], Federico Caglieris[1], Boy Roman Piening[1], Igor Morozov[1,4], Saicharan Aswartham[1], Joseph Dufouleur[1], Bernd Büchner[1,2,3], and Christian Hess[1,2,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany — [4]Moscow State University, 119991 Moscow, Russia

The semimetal WTe_2 has attracted attention due to its non-saturating extremely large magnetoresistance. Furthermore, it has been the first compound to be predicted as a type-II Weyl semimetal which supposedly gives rise to new topological characteristics.

We have performed a broad spectrum of transport studies on WTe_2 single crystals. The peculiar magnetoresistance was reproduced while the Hall effect behaves normally. Likewise, the thermoelectric transport coefficients show no anomalous behavior. The thermopower is negative at high temperatures, changes sign at 50 K and develops a peak at 25 K. The Nernst signal is linear in field but shows a strong increase below 50 K. The thermal conductivity increases upon cooling with a phononic peak at 21 K. All results can explicitly be described by a simple two-band model where electron- and hole-like carriers are compensated and exhibit large mobilities.

15 min. break.

TT 7.8 Mon 11:30 A 053

Spectacular electrical transport in type-II Weyl semimetals WP_2 and MoP_2 — •Nitesh Kumar[1], Yan Sun[1], Nan Xu[2], Kaustuv Manna[1], Vicky Suess[1], Inge Leermakers[3], Tobias Foerster[4], Horst Borrmann[1], Uli Zeitler[3], Ming Shi[2], Claudia Felser[1], and Chandra Shekhar[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Paul Scherrer Institute, Switzerland — [3]High Field Magnet Laboratory, Nijmegen, Netherlands — [4]Dresden High Magnetic Field Laboratory, Dresden, Germany

Semimetals are in general less conducting compared to metals due to smaller number of charge carriers. However, recent progress in the topological Dirac and Weyl semimetals show spectacular electronic properties such as large mobilities accompanied by extremely high magnetoresistance. In particular, two closely neighbouring Weyl points of the same chirality are protected from annihilation by structural distortions or defects. Here we present the electronic properties of type-II Weyl semimetals, WP_2 and MoP_2, with robust Weyl points by transport and angle resolved and first principles calculations. Single crystals of WP_2 display an extremely low residual low-temperature resistivity of 3 nΩ cm accompanied by an enormous and highly anisotropic magnetoresistance above 200 million % at 63 T and 2.5 K [1]. A large suppression of charge carrier backscattering in WP_2 from transport measurements suggests the involvement of the novel Weyl fermions expressed in this compound.

[1] N. Kumar *et al.*, *Nature Commun.* **8**, (2017) 1642.

TT 7.9 Mon 11:45 A 053

Large anomalous Nernst effect driven by Berry curvature in Mn_3Ge — •Christoph Wuttke[1], Federico Caglieris[1], Kaustuv Manna[2], Steffen Sykora[1], Chandra Shekhar[2], Claudia Felser[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

Introducing Berry phase and curvature as properties of the electronic structure has not only started the quest for finding Weyl semimetal candidates, it was also predicted that the occurance of Weyl points in the band structure can lead to peculiar transport behaviour. We report Nernst effect measurements on the chiral antiferromagnet Mn_3Ge. A large anomalous compound dominates the magnetic field dependence of the Nernst signal and does not scale with the magnetization. Our theoretical examination shows that the anomalous behaviour is strongly influenced by the finite Berry curvature. The results show a significant sensitivity of transverse thermoelectric transport to the existence of Weyl points close to the Fermi surface.

TT 7.10 Mon 12:00 A 053

Quantum interference effects in 3D-Dirac antiperovskites — •Hiroyuki Nakamura[1], Johannes Merz[1], Eslam Khalaf[1], Pavel Ostrovsky[1], Debakanta Samal[3], and Hidenori Takagi[1,2,4] — [1]Max Planck Institute for Solid State Research, Germany — [2]Department of Physics, University of Tokyo, Japan — [3]Institute of Physics, India — [4]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

Magnetotrasport study has been carried out using epitaxial thin films of Sr_3PbO and Sr_3SnO grown by MBE. All the films showed clear 3D localization but differed in the sign of quantum interference governing the localization effect, which was associated with the location of E_F with respect to Dirac nodes. Detailed analysis of the localization effects for Dirac electrons will be presented.

TT 7.11 Mon 12:15 A 053

Correlation meets topology: quasiparticles along the Dirac nodal loop in ZrSiS — Sergio Pezzini[1], Maarten van Delft[1], Leslie Schoop[2], Bettina Lotsch[2], Antony Carrington[3], Misha Katsnelson[4], Nigel Hussey[1], and •Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), Radboud University, Nijmegen 6525 ED, NL — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, GER — [3]H. H. Wills Physics Laboratory, University of Bristol, Bristol BS8 1TL, UK — [4]Radboud University, Institute for Molecules and Materials, Nijmegen 6525 AJ, NL

ZrSiS belongs to the recently discovered family of topological Dirac materials whose electronic structure hosts Dirac-like crossing points that form a closed loop at the Fermi level. While transport measurements have shown the presence of small electron and hole pockets via the observation of low-frequency Shubnikov-de Haas oscillations, ex-

perimental evidence for the enhanced correlation effects predicted to occur in this class of semi-metals has until now been lacking. We have performed a quantum oscillation study of the nodal-loop in high magnetic fields that reveals significant enhancement in the quasi-particle mass residing near the nodal loop. Above a threshold magnetic field (B > 25 T), magnetic breakdown occurs across gaps in the loop structure with orbits that enclose different windings around its vertices. The analysis of the amplitudes of these breakdown orbits reveals an anomalous temperature dependence demonstrating the emergence of novel, correlation-driven physics in ZrSiS associated with the Dirac-like quasiparticles [1].

[1] S. Pezzini et al., Nature Physics, doi:10.1038/nphys4306 (2017).

TT 7.12 Mon 12:30 A 053

Correlation-driven electron-hole instability in nodal-line semimetal ZrSiS — •Alexander Rudenko[1,2,3], Evgeny Stepanov[1,2], Alexander Lichtenstein[4], and Mikhail Katsnelson[1] — [1]Radboud University, Nijmegen, The Netherlands — [2]Ural Federal University, Ekaterinburg, Russia — [3]Wuhan University, Wuhan, China — [4]Hamburg University, Hamburg, Germany

ZrSiS is an emerging material, which belongs to the class of 3D materials that feature a nodal line in the electronic band structure [1]. Recent experimental observations reveal an unconventional mass enhancement of quasiparticles in ZrSiS [2], which suggests the importance of electron correlation effects in this material. Here, we study many-body effects in ZrSiS using a combination of first-principles calculations and model approaches, taking the correlation effects perturbatively. We show that at moderately low temperatures ZrSiS exhibit electron-hole instability, leading to the formation of a pseudogap in the electronic spectrum. The results can be understood in terms of Coulomb-interaction-assisted electron-hole pairing reminiscent to that of a conventional superconductor.

[1] L.M. Schoop et al. Nat. Commun. 7, 11696 (2016).
[2] S. Pezzini et al. Nat. Phys. doi:10.1038/nphys4306 (2017).

TT 7.13 Mon 12:45 A 053

Optical Conductivity Studies of the half-Heusler Compounds GdPtBi, LuPtBi, YPtBi and YbPtBi — •Felix Hütt[1], Micha B. Schilling[1], Martin Dressel[1], Claudia Felser[2], and Artem V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Many Heusler and half-Heusler compounds are known for their diverse and appealing physical properties. Some of the compounds are predicted to possess non-trivial topological electronic structure. Although the non-trivial topology has already been discussed by theory for a few years, experiments so far remain pretty much behind theory.

In this contribution, we report on experimental investigations of the optical response of four different half-Heusler compounds (GdPtBi, LuPtBi, YPtBi, YbPtBi) using Fourier-transform infrared spectroscopy. Reflectivity measurements were performed over a large frequency range, 10 to 3000 meV, at different temperatures down to 10 K. From the measured reflectivity, the optical conductivity and the dielectric function were extracted via the Kramers-Kronig relations. In the talk, we compare our results with theoretical predictions for optical manifestations of possible Dirac physics in these materials.

TT 8: Topological Insulators I (joint session HL/TT)

Time: Monday 9:30–13:00 Location: A 151

TT 8.1 Mon 9:30 A 151

Model for ferromagnetic Weyl and nodal line semimetals: topological invariants, surface states, anomalous and spin Hall effect — Tomáš Rauch[1,2], Huong Nguyen-Minh[1], •Jürgen Henk[1], and Ingrid Mertig[1,3] — [1]Institute of Physics, Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Berc Materials Physics Center, Donostia–San Sebastián, Spain — [3]Max Planck Institute for Microstructure Physics, Halle, Germany

By adding a Zeeman term to the extended Dirac equation [1] we show that this equation describes not only topological insulators but also models the electronic properties of ferromagnetic Weyl and nodal line semimetals [2], both of which arise for specific parameter sets. We confirm the topological nontriviality of the nodal objects by calculating the topological invariants as well as by demonstrating the existence of characteristic topological surface states of the associated semi-infinite systems. Moreover, Weyl points and nodal lines produce notable features in the anomalous and in the spin Hall conductivity.

[1] S.-Q. Shen, W.-Y. Shan, and H.-Z. Lu, Spin **1**, 33 (2011).
[2] T. Rauch, H. Nguyen-Minh, J. Henk, and I. Mertig, Phys. Rev. B, submitted.

TT 8.2 Mon 9:45 A 151

Transport Spectroscopy of Induced Superconductivity in the three-dimensional Topological Insulator HgTe — •Jonas Wiedenmann — Experimentelle Physik III, Universität Würzburg, Am Hubland, 97074 Würzburg

Inducing superconducting pairing into the surface states of a topological insulator is predicted to lead to the emergence of mixed spin singlet/triplet superconducting correlations and Majorana bound state related physics. We studied the proximity-induced superconducting state into the topological surface states of strained bulk HgTe by Andreev reflection point-contact spectroscopy. By analyzing the conductance as a function of voltage for various temperatures, magnetic fields and gate-voltages, we find evidence, in equilibrium, for an induced order parameter in HgTe of 0.070 meV and an order parameter of the superconducting gap of niobium of 1.1 meV. To describe the full conductance curve we suggest that a charge imbalance suppresses the induced superconducting state. As a result the relevant scattering region changes depending on the applied bias voltage.

TT 8.3 Mon 10:00 A 151

Interplay between topology and disorder in a two-dimensional semi-Dirac material — P V Sriluckshmy, •Kush Saha, and Roderich Moessner — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We investigate the role of disorder in a two-dimensional semi-Dirac material characterized by a linear dispersion in one, and a parabolic dispersion in the orthogonal, direction. Using the self-consistent Born approximation, we show that disorder can drive a topological Lifshitz transition from an insulator to a semi-metal, as it generates a momentum independent off-diagonal contribution to the self-energy. Breaking time-reversal symmetry enriches the topological phase diagram with three distinct regimes– single-node trivial, two-node trivial and two-node Chern. We find that disorder can drive topological transitions from both the single- and two-node trivial to the two-node Chern regime. We further analyze these transitions in an appropriate tight-binding Hamiltonian of an anisotropic hexagonal lattice, by calculating the real-space Chern number. Additionally we compute the disorder-averaged entanglement entropy which signals both the topological Lifshitz and Chern transition as a function of the anisotropy of the hexagonal lattice. Finally, we discuss experimental aspects of our results.

TT 8.4 Mon 10:15 A 151

Optical properties of topological insulator nanoparticles — •Gleb Siroki, Derek Lee, Peter Haynes, and Vincenzo Giannini — Imperial College London, South Kensington, SW7 2AZ, London, UK

Topological insulators are materials that have metallic surface states protected by time-reversal symmetry. Such states are delocalised over the surface and are immune to non-magnetic defects and impurities.

Building on previous work [1] we have studied the interaction of light with topological insulator nanoparticles. Our main finding is that the occupied surface states can lead to charge density oscillations akin to plasmons in metallic nanoparticles. Furthermore, these oscillations can couple to phonons forming a previously unreported excitation [2]. Because the states occur at the surface a small number of them is enough to change the absorption spectrum of a particle containing many thousands of atoms. We are going to show how the effect can be adjusted by varying the particle's size and shape. Furthermore, we will discuss the robustness of the effect in the presence of disorder [3].

In conclusion, topological insulator nanoparticles can be used as a

highly-tunable building block to create a metamaterial operating in THz range. This may be interesting for plasmonics and metamaterials communities as well as researchers working on cavity electrodynamics and quantum information.

[1] Imura et al, PRB 86, 235119 (2012)
[2] Siroki et al, Nat. Comm. 7, 12375 (2016)
[3] Siroki et al, PRMaterials, 1, 024201 (2017)

TT 8.5 Mon 10:30 A 151

Multi probe transport measurements on Bi_2Te_3 thin films — •Sebastian Bauer, Stephanie Hoepken, Mandana Soleimani, Christian A. Bobisch, and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We present a detailed study of the electron transport properties of a thin Bi_2Te_3 film on Si(111). Bi_2Te_3 is a prototype system of so called three dimensional topological insulators. Such materials are insulating inside their bulk while they provide a metallic state on their surface which is protected by the materials topology [1]. The nanoscale transport field of the Bi_2Te_3 surface was studied by scanning tunneling potentiometry (STP), an extension of the scanning tunneling microscope (STM) which allows us to analyze the microscopic topography and the correlated microscopic electrochemical potential of the surface simultaneously [2]. The STP analysis shows that morphological features like step edges and grain boundaries are barriers for conduction electrons. The conductivity of step edges and grain boundaries were determined to 700 S/cm and 350 S/cm in the surface state, confirming former STP studies [3,4].

[1] M. Z. Hasan, C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010). [2] A. Bannani, C. A. Bobisch, R. Möller, Rev. Sci. Instrum. 79, 083704 (2008). [3] S. Bauer und C. A. Bobisch, Nat. Com. 7, 11381 (2016). [4] F. Lüpke et al., Nat. Com. 8, 15704 (2017).

TT 8.6 Mon 10:45 A 151

Mixed topological semimetals in two-dimensional spin-orbit ferromagnets — •Chengwang Niu[1], Jan-Philipp Hanke[1], Patrick M. Buhl[1], Hongbin Zhang[2], Gustav Bihlmayer[1], Daniel Wortmann[1], Stefan Blügel[1], and Yuriy Mokrousov[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Materials Science, Technische Universität Darmstadt, 64287 Darmstadt, Germany

Topological states of matter and ferromagnetism in two dimensions are nowadays two of the most intriguing and intensively researched fields in solid state physics. Here, we predict that diverse topological semimetallic phases can be obtained in 2D ferromagnets as a consequence of the spin-orbit driven changes in the electronic structure as the magnetization direction is varied. We show that the most natural way to classify these phases lies in analyzing either points or lines of degeneracies which occur in an extended phase space of Bloch vector and the magnetization direction. The emergence of the corresponding topological states, which we refer to as mixed Weyl semimetal and mixed nodal line semimetal, respectively, can be thereby confirmed by accessing corresponding topological invariants and edge states. We demonstrate the possible complexity of the topological phase diagram of 2D ferromagnets based on several model systems, and, using density functional theory, we identify two realistic examples exhibiting mixed Weyl semimetal and mixed nodal line semimetal phases.

This work was supported by SPP 1666 of the DFG.

TT 8.7 Mon 11:00 A 151

Microscopic theory of the surface anomalous Hall conductivity — •Tomáš Rauch[1], Thomas Olsen[2], David Vanderbilt[3], and Ivo Souza[1,4] — [1]Centro de Física de Materiales, San Sebastián, Spain — [2]Technical University of Denmark, Kongens Lyngby, Denmark — [3]Rutgers University, Piscataway, New Jersey, USA — [4]Ikerbasque Foundation, Bilbao, Spain

The dimensionless axion coupling θ describes the isotropic part of the linear magnetoelectric tensor. In a bulk crystal θ is only defined modulo 2π, and only its space-time gradients enter Maxwell's equations. At surfaces, the spatial gradient of θ gives rise to a surface anomalous Hall conductivity (AHC). In this work, we derive a microscopic expression for the AHC of an insulating surface. We find that in general it comprises not only a geometric contribution that is a property of the occupied states, but also a non-geometric "cross-gap" term that is absent from the expression for the intrinsic AHC of a free-standing film or slab. By constructing tight-binding models in a slab geometry, we numerically test our analytical results and explore the connection between the surface AHC and the bulk axion coupling. In particular, we illustrate how different insulating surfaces of the same bulk crystal can have AHCs that differ by an integer multiple of e^2/h, and that this difference resides in the geometric term alone.

15 min. break.

TT 8.8 Mon 11:30 A 151

A room-temperature and switchable Kane-Mele quantum spin Hall insulator — •Antimo Marrazzo, Marco Gibertini, Davide Campi, Nicolas Mounet, and Nicola Marzari — Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Ecole Polytechnique Federale de Lausanne, 1015, Switzerland

Fundamental research and technological applications of topological insulators are hindered by the rarity of materials exhibiting a robust topologically non-trivial phase, especially in two dimensions (2D). Here, by means of extensive first-principles calculations, we propose a novel quantum spin Hall insulator (QSHI) with a sizeable band gap of $\sim$0.5 eV at the G_0W_0 level, that is a monolayer of a naturally occurring layered mineral. This system realises the paradigmatic Kane-Mele model for QSHIs in a potentially exfoliable 2D monolayer with helical edge states that are robust even beyond room temperature and that can be manipulated exploiting a unique strong interplay between spin-orbit coupling, crystal-symmetry breaking, and dielectric response.

TT 8.9 Mon 11:45 A 151

Testing Topological Protection of Edge States in Bismuthene on SiC — •Fernando Dominguez[1], Benedikt Scharf[1], Gang Li[2], Werner Hanke[3], Ronny Thomale[3], and Ewelina Hankiewicz[1] — [1]Institute for Theoretical Physics and Astrophysics, TP4, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China — [3]Institute for Theoretical Physics and Astrophysics, TP1, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Due to its large bulk band gap, bismuthene on SiC offers intriguing new opportunities for room-temperature quantum spin Hall (QSH) applications. Although edge states have been observed in the local density of states (LDOS), there has been no experimental evidence until now that they are spin polarized and topologically protected. Here, we predict experimentally testable fingerprints of these properties originating from magnetic fields, such as changes in the LDOS and in ballistic magnetotransport due to a gap of a few meV opened at the crossing point between the QSH states. For armchair edges in particular, we find a distinct difference of behavior under out-of-plane (gap opening between the QSH states) and in-plane (no or tiny gap) fields. This unexpected robustness of armchair QSH edge states against in-plane fields can be understood from an effective low-energy model, where a helicity operator provides an additional protection of the QSH states. While we focus here on bismuthene on SiC, our main findings should also be applicable to other honeycomb-lattice-based QSH systems.

TT 8.10 Mon 12:00 A 151

High-temperature quantum oscillations of the Hall resistance in bulk Bi_2Se_3 — •Olivio Chiatti[1], Marco Busch[1], Sergio Pezzini[2], Steffen Wiedmann[2], Oliver Rader[3], Lada V. Yashina[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands — [3]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [4]Department of Chemistry, Moscow State University, 119991 Moscow, Russia

Protected topological surface states (TSS) with helically spin-polarized Dirac fermions (HSDF) are of high interest as a new state of quantum matter. Electronic bulk states in three-dimensional (3D) materials with TSS often mask the transport properties of HSDF. In recent work, the high-field Hall resistance and low-field magnetoresistance indicate that the TSS may coexist with a layered two-dimensional electronic system (2DES) [1]. Here, we demonstrate quantum oscillations of the Hall resistance for temperatures up to 50 K, in nominally undoped bulk Bi_2Se_3 with a high electron density n of about $2{\cdot}10^{19}$ cm^{-3}. From the angular and temperature dependence of the Hall resistance and the Shubnikov-de Haas oscillations we identify 3D and 2D contributions to transport. Angular resolved photoemission spectroscopy proves the

existence of TSS. We present a model for Bi_2Se_3 and suggest that the coexistence of TSS and 2D layered transport stabilizes the quantum oscillations of the Hall resistance.
[1] Chiatti *et al.*, Sci. Rep. **6**, 27483 (2016)

TT 8.11 Mon 12:15 A 151

Exploiting Topological Insulators for Majorana Devices — •Peter Schüffelgen[1], Daniel Rosenbach[1], Chuan Li[2], Michael Schleenvoigt[1], Tobias Schmitt[1], Sarah Schmitt[1], Abdur Jalil[1], Jonas Kölzer[1], Lidia Kibkalo[1], Benjamin Bennemann[1], Umut Parlak[1], Martina Luysberg[1], Gregor Mussler[1], Alexander Golubov[2], Alexander Brinkman[2], Thomas Schäpers[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500AE Enschede, The Netherlands

At the interface of s-wave superconductors (SC) and topological insulators (TI) exotic Majorana modes are predicted to occur. In this work, a novel fabrication technique is presented, which allows to construct TI-SC hybrid devices of high quality under ultra-high vacuum conditions. A stencil mask is applied to the substrate before growth of Bi-based TI thin films by means of molecular beam epitaxy. The shadow mask is used for stencil lithography of superconductive electrodes on top of the topological thin film in a second growth step. Measurements on such in-situ fabricated Josephson junctions indicate a high interface transparency. Furthermore, a missing first Shapiro step was detected in radio frequency experiments, indicating signatures of gapless Andreev bound states, so-called Majorana bound states. The presented process is applicable to a variety of new geometries, allowing fabrication of elaborated TI-SC hybrid devices, for further research on Majorana signatures.

TT 8.12 Mon 12:30 A 151

Topolectrical Edge States — •Tobias Helbig[1], Tobias Hofmann[1], Ching Hua Lee[2,3], and Ronny Thomale[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of High Performance Computing, A*STAR, Singapore, 138632 — [3]Department of Physics, National University of Singapore, Singapore, 117542

We report on the realization of one-dimensional topological states of matter within electrical circuits. At the example of the Su-Schrieffer-Heeger circuit, we elaborate how topological edge states and domain walls manifest themselves in the impedance read-out of a periodic electrical circuit. We further outline prospective generalizations and applications.

TT 8.13 Mon 12:45 A 151

Topolectrical Band Structures — •Tobias Hofmann[1], Tobias Helbig[1], Ching Hua Lee[2,3], and Ronny Thomale[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of High Performance Computing, A*STAR, Singapore, 138632 — [3]Department of Physics, National University of Singapore, Singapore, 117542

Topolectrical circuits constitute a new avenue of topological states realized in a classical environment. With them, it is possible to reproduce band structures seen in models for topological insulators (TI) where the bands correspond to impedance (or admittance) eigenvalues. Because electrical circuits are more easily accessible than TIs, they are particularly suitable for studying topological states, reaching from the simplest models to non-hermitian and other types of rather "exotic" physics. In our talk, we illustrate the explicit measurement of topological band structures in the context of topolectrical circuits.

TT 9: Quantum Dots, Quantum Wires, Point Contacts

Time: Monday 9:30–13:00 Location: HFT-FT 101

Invited Talk TT 9.1 Mon 9:30 HFT-FT 101

Unconventional Superconductivity in Quantum-Dot Systems — •Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

The fermionic nature of electrons allows for four classes of superconducting correlations with definite symmetry in spin, space and frequency. Conventional (s-wave) superconductors accommodate even-frequency singlet Cooper pairs which are odd in spin and even in space and frequency. Odd-frequency triplet correlations generically arise in superconductor-ferromagnet heterostructures. Recently, we have suggested double quantum dots (DQDs) coupled to conventional superconductors in the presence of inhomogeneous magnetic fields as a model system exhibiting all four types of unconventional pairing. When reducing spatial degrees of freedom of the system further, i.e., to a single quantum dot, only odd-triplet and conventional superconducting correlations are allowed by symmetry. With the help of a diagrammatic real-time technique, the interplay of spin symmetry and superconductivity and its signatures in electronic transport, in particular current and zero frequency shot noise has been analyzed [2]. An applied magnetic field or attached ferromagnetic leads partially or fully reduce the spin symmetry, and odd-triplet superconducting correlations are generated.
[1] B. Sothmann, S. Weiss, M. Governale, J. König, Phys. Rev. B **90**, 220501 (2014).
[2] S. Weiss and J. König, Phys. Rev. B **96**, 064529 (2017).

TT 9.2 Mon 10:00 HFT-FT 101

Phase-dependent heat transport through superconductor-quantum dot hybrids — •Mathias Kamp and Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Phase-coherent charge transport in mesoscopic systems has received a lot of attention in past decades. Although phase-dependent heat currents through Josephson junctions have been predicted [1] and observed recently [2], phase-coherent heat transport has largely been neglected so far. Here, we consider a junction consisting of a quantum dot tunnel coupled to two superconducting leads. The system combines the interplay of superconducting correlations and strong Coulomb interaction on the dot in a nonequilibrium situation. We derive a generalized master equation using a real-time diagrammatic approach and calculate the phase-dependent heat and charge current in linear and nonlinear response.
[1] K. Maki and A. Griffin, Phys. Rev. Lett. **15**, 921 (1965).
[2] F. Giazotto and M. J. Martínez-Pérez, Nature **492**, 401 (2012).

TT 9.3 Mon 10:15 HFT-FT 101

Odd-frequency superconductivity revealed by thermopower — Sun-Yong Hwang[1], Pablo Burset[2], and •Björn Sothmann[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany — [2]Department of Applied Physics, Aalto University, FIN-00076 Aalto, Finland

Conventional superconductivity is well-explained in the framework of BCS theory by the formation of spin-singlet Cooper pairs. However, other exotic types of superconductivity involving, e.g., spin-triplet pairs exist as well. In general, superconducting correlations can be characterized by a nonvanishing pair amplitude which has a definite symmetry in spin, momentum and time or frequency. While the spin and momentum symmetry have been probed experimentally for different classes of superconductivity, the odd-frequency nature of certain superconducting correlations has so far been probed only indirectly. Here, we propose the thermopower as an unambiguous way to assess odd-frequency superconductivity. This is possible since the thermoelectric coefficient given by Andreev-like processes is only finite in the presence of odd-frequency superconductivity. We illustrate our general findings with a simple example of a superconductor-quantum dot-ferromagnet hybrid.

TT 9.4 Mon 10:30 HFT-FT 101

Electron transport and thermoelectricity in quantum dot Cooper-pair splitters — •Robert Hussein[1], Sigmund Kohler[2], Wolfgang Belzig[1], Francesco Giazotto[3], Michele Governale[4], and Alessandro Braggio[3] — [1]Fachbereich Physik, Universität Konstanz, Germany — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — [3]NEST, Istituto Nanoscienze-CNR, Italy — [4]Victoria University of Wellington, New Zealand

We investigate electronic and thermoelectric transport in a Cooper-pair splitter based on a double quantum dot realized in a nanowire.

We study how the interplay between local and nonlocal tunneling processes between the superconductor and the dots influences the transport properties. For finite Coulomb interaction and in the presence of interdot tunneling, the Cooper-pair splitter may develop spatial entanglement even in the absence of the cross Andreev reflection process. We show that the spin-orbit coupling of the nanowire can be used to control the symmetry (singlet or triplet) of the entangled electron pairs. We further analize under which conditions thermoelectric induced currents may lead to nonlocal cooling of one of the normal contacts, and when they may give rise to nonlocal power generation.
[1] R. Hussein, L. Jaurigue, M. Governale, and A. Braggio, Phys. Rev. B 94, 235134 (2016).
[2] R. Hussein, A. Braggio, and M. Governale, Phys. Status Solidi B 254, 1600603 (2017).

TT 9.5 Mon 10:45 HFT-FT 101

Charge-vibration interaction in normal-superconductor quantum dots — •Gianluca Rastelli[1], Pascal Stadler[2], and Wolfgang Belzig[2] — [1]Zukunftskolleg & Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Fachbereich Physik, Universität Konstanz, Konstanz, Germany

We study the quantum transport and the nonequilibrium vibrational states of a quantum dot embedded between a normal-conducting and a superconducting lead with the charge on the quantum dot linearly coupled to a harmonic oscillator of frequency ω [1,2]. We analyze the inelastic, vibration-assisted tunneling processes in the regime $\omega < \Delta$, with the superconducting energy gap Δ, and for sharp resonant transmission through the dot. Inelastic vibration-assisted Andreev reflections as well as quasiparticle tunneling induce a strong nonequilibrium state of the oscillator. In particular, we show that ground-state cooling of the oscillator - with phonon occupation n « 1 - can be achieved simultaneously for many of the oscillator's modes of different frequencies. We discuss how the nonequilibrium vibrational state can be readily detected by the asymmetric behavior of the inelastic current peaks with respect to the gate voltage.
[1] Phys. Rev. B. 96 , 045429 (2017);
[2] Phys. Rev. Lett. 117, 197202 (2016).

TT 9.6 Mon 11:00 HFT-FT 101

Temperature effects in superconducting quantum dots — •Vladislav Pokorný[1] and Martin Žonda[2] — [1]Institute of Physics, Na Slovance 2, 18221 Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 12116 Prague, Czech Republic

We study the temperature effects in a system consisting of a single-level quantum dot with local Coulomb interaction attached to two superconducting leads and optionally a third, metallic lead. The system is described by the single-impurity Anderson model coupled to BCS superconducting baths and solved using the continuous-time, hybridization-expansion (CT-HYB) quantum Monte Carlo as well as the numerical renormalization group (NRG). We study the behavior of the subgap (Andreev-Shiba) states, the Josephson current and the fate of the zero-pi (singlet-doublet) quantum phase transition. We also show the limits of usability of the stochastic optimization method for obtaining the spectral functions from the imaginary-time CT-HYB results.

TT 9.7 Mon 11:15 HFT-FT 101

Simple transformation between symmetrically and asymmetrically coupled superconducting quantum dots — •Martin Žonda[1,2], Alžběta Kadlecová[2], and Tomáš Novotný[2] — [1]Institute of Physics, University of Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, CZ-121 16 Prague 2, Czech Republic

We will present simple, yet very powerful correspondence between the characteristics of a single-level quantum dot coupled symmetrically to two phase-biased superconducting leads with its asymmetrically coupled equivalents. Counter-intuitively, it is the symmetric setup which is the most general one and its characterization enables full description of any equivalent asymmetrically coupled system. This discovery makes it possible to utilize known results for symmetric setups in general asymmetric cases via trivial analytical relations. We will present ready-to-use conversion formulas for the $0-\pi$ phase transition boundary, on-dot quantities, and the Josephson current and illustrate them on the numerical renormalization group results. The formulas also provide an efficient tool for estimating the coupling asymmetry directly from the experimental data, which is otherwise a demanding task. We will demonstrate this by analysing recent $0-\pi$ transition measurements [1].
[1] Delagrange et al., Phys. Rev. B **93**, 195437 (2016).

15 min. break.

TT 9.8 Mon 11:45 HFT-FT 101

Fermionic reaction coordinates and their application to an autonomous Maxwell demon in the strong coupling regime — •Philipp Strasberg[1], Gernot Schaller[2], Thomas L. Schmidt[1], and Massimiliano Esposito[1] — [1]Physics and Materials Science Research unit, University of Luxembourg, Luxembourg — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany

We establish a theoretical method which goes beyond the weak coupling and Markovian approximations while remaining intuitive, using a quantum master equation in a larger Hilbert space. The method is applicable to all impurity Hamiltonians tunnel-coupled to one (or multiple) baths of free fermions. The accuracy of the method is in principle not limited by the system-bath coupling strength, but rather by the shape of the spectral density and it is especially suited to study situations far away from the wide-band limit. In analogy to the bosonic case, we call it the fermionic reaction coordinate mapping. If time permits, we will discuss as an application a thermoelectric device made of two Coulomb-coupled quantum dots. We pay particular attention to the regime where this device operates as an autonomous Maxwell demon shoveling electrons against the voltage bias thanks to information. Contrary to previous studies we do not rely on a Markovian weak coupling description. Our numerical findings reveal that in the regime of strong coupling and non-Markovianity, the Maxwell demon is often doomed to disappear except in a narrow parameter regime of small power output.

TT 9.9 Mon 12:00 HFT-FT 101

Quantum thermodynamics in strongly coupled quantum dots — •Thomas Schmidt, Massimiliano Esposito, and Patrick Haughian — Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

It has emerged over the past years that it is not straightforward to find consistent definitions of thermodynamic quantities, such as heat and entropy, in driven quantum systems which are strongly coupled to reservoirs. In order to shed light on this question, we have investigated the simplest prototypical model, namely a noninteracting resonant level model coupled to fermionic reservoirs. Using an exact solution of the fully driven quantum mechanical model, we show how to define observable thermodynamical quantities which allow the derivation of a first and second law of thermodynamics.

TT 9.10 Mon 12:15 HFT-FT 101

Shot Noise and electron pairing in integer quantum Hall interferometers — •Giovanni Andrea Frigeri[1,3], Daniel D. Scherer[2], and Bernd Rosenow[3] — [1]MPI for Mathematics in the Sciences, Leipzig, Germany — [2]Niels Bohr Institute, Copenhagen, Denmark — [3]University of Leipzig, Germany

Recently, halving of the magnetic flux period was observed experimentally for a Fabry-Perot interferometer in the integer quantum Hall regime with bulk filling factor between 2.5 and 4.5 . In addition, shot noise measurements yielded a Fano factor of two, indicating that the halving of the flux period could be interpreted in terms of electron pairing [1].

While the flux period halving has been explained by a strong Coulomb interaction between the outermost interfering edge mode and an inner non-interfering edge mode [2], an extension of the model [2] is needed to compute shot noise produced by electron partitioning in the interferometer. Specifically, we consider a model in which the number of electrons in the inner edge mode can change stochastically, affecting in this way the tunnelling probability of an interfering electron, and giving rise to an enhanced Fano factor. In addition, we calculate the interference visibility in the presence of inner edge charge fluctuations, and derive a relation between Fano factor and interference visibility.
[1] H. Choi, I. Sivan, A. Rosenblatt, M. Heiblum, V. Umansky, and D. Mahalu, Nature Comm. 6 (2015)
[2] G. A. Frigeri, D. D. Scherer, B. Rosenow, arXiv:1709.04504 (2017)

TT 9.11 Mon 12:30 HFT-FT 101

Crystallization of Levitons in the fractional quantum Hall regime — •Flavio Ronetti[1,2], Luca Vannucci[1], Dario

Ferraro[3], Jérôme Rech[2], Thibaut Jonckheere[2], Thierry Martin[2], and Maura Sassetti[1] — [1]Università di Genova and CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy. — [2]Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France. — [3]Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, I-16163 Genova, Italy

The emergence of self-organized regular patterns in optical solitons has been recently subject of intense investigation, as they promise to be exceptionally useful in quantum communication [1]. In the framework of electron quantum optics, a train of Lorentzian voltage pulses emerges as the solid state counter-part of optical solitons, namely robust ballistically propagating wave-packets carrying an integer number q of electrons called Levitons [2,3]. Using a periodic train of Levitons, we investigate the charge density backscattered off a quantum point contact in the fractional quantum Hall regime, finding a self-organized and regular pattern of peaks and valleys[4]. We demonstrate that the predicted features manifest themselves as unexpected additional dips in the well-studied Hong-Ou-Mandel noise.

[1] D. C. Daniel, et al. Nature Photonics 11, 671 (2017).
[2] J. Keeling, et al., Phys. Rev. Lett. 97, 116403 (2006).
[3] J. Dubois, et al., Nature (London) 502, 659 (2013).
[4] F. Ronetti, et al., in preparation (2017).

TT 9.12 Mon 12:45 HFT-FT 101

Fractionalization of charge in incoherent, sequential electron transport — •Roman-Pascal Riwar — JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany

The notion of a fractional charge was up until now reserved for quasiparticle excitations emerging from strongly correlated, topological quantum systems, such as Laughlin quasiparticles in the fractional quantum Hall effect or, more recently, parafermions. Here, we argue that a topological braiding transition in the full counting statistics can lead to a fractionalisation of the charge - strikingly - in fully incoherent electron transport out of equilibrium. Importantly, this effect emerges already on the level of standard sequential tunneling through quantum dots and metallic islands, making its observation experimentally accessible to a large and easily controllable class of systems. We show that the fractional charge and the underlying topological invariants can be measured by means of the detector's waiting time distribution. Based on its topology, we find that this fractional charge effect can, in spite of its very different physical origin, be regarded as a quasiclassical analogy to the fractional transport of Cooper pairs in topological Josephson junctions.

TT 10: Heusler Compounds, Semimetals and Oxides (joint session MA/TT)

Time: Monday 9:30–13:15 Location: EB 301

TT 10.1 Mon 9:30 EB 301

Epitaxial growth of compensated ferrimagnetic Heusler thin films Mn-Fe-V-Al — •Siham Ouardi, Kazuya Z. Suzuki, and Shigemi Mizukami — WPI Advanced Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Cubic Heusler compound $Mn_{1.5}FeV_{0.5}Al$ is a fully compensated half-metallic ferrimagnet with 24 valence electrons per formula unit. Here we report on epitaxial growth of the compensated ferrimagnetic Mn-Fe-V-Al Heusler films. The thin films of 30 nm thickness were grown directly on single crystalline MgO (001) substrates by using an ultra-high-vacuum magnetron sputtering technique. The Heusler structure was characterized by x-ray diffraction. The crystal structure ordering was controlled by the deposition at various substrate temperatures. Magnetometry measurements show a nearly vanishing magnetization where the anomalous Hall measurements exhibited magnetic ordering. The ferrimagnetic coupling between the different sublattices (Mn, Fe, and V) will discussed based on magnetic dichroism in angle-resolved hard X-ray photoelectron spectroscopy (MCD-HAXPES). The advantage of vanishing magnetization in combination with high spin polarization of this material thin films provides the possibility for spintronic device applications.

This work is supported by the Grant-in-Aid for Scientific Research KAKENHI (17H06513).

TT 10.2 Mon 9:45 EB 301

Polycrystalline vs Epitaxial Fe2-xMn1+xAl Heusler films with exchange bias shift — •Samer Kurdi[1], Giorgio Divitini[1], Massimo Ghidini[1,2,3], Markus Meinert[4], Marco Coïsson[5], Thomas Forrest[3], Günter Reiss[4], Sarnjeet Dhesi[3], Paola Tiberto[5], and Zoe Barber[1] — [1]University of Cambridge, UK — [2]Department of Physics, University of Parma, Italy — [3]Diamond Light Source, Oxfordshire, UK — [4]Center for Spinelectronic Materials and Devices, Bielefeld University, Germany — [5]INRIM, Torino, Italy

Magnetic recording devices are pervasive in current technology, and the development of environmentally friendly, sustainable and scalable devices based on Earth-abundant materials is a high research priority. In this study we investigate a simple, cost-effective single-layer exchange biased film for spin valves, a fundamental part of data storage systems.

We grew 200 nm polycrystalline and epitaxial Fe2-xMn1+xAl (x = -0.25, 0, 0.25) Heusler alloy films and characterized them to study the influence of Mn content on the exchange bias shift. The microstructure is shown to have a profound effect on film properties. In-situ annealing TEM studies show that the polycrystalline samples have Mn-rich and Fe-rich phases inducing a spin glass exchange bias shift of around 150 Oe at 4 K for Fe1.75Mn1.25Al. The exchange bias shift was observed at temperatures up to 12 K for the Fe1.75Mn1.25Al and up to 6 K for Fe2MnAl polycrystalline samples, whilst only the Fe1.75Mn1.25Al epitaxial film showed any bias shift (50 Oe, below 2 K). XMCD sum rule analysis of the polycrystalline samples showed different behaviour from the as-predicted perfectly ordered L21 Heusler structure.

TT 10.3 Mon 10:00 EB 301

Evolution of the interfacial perpendicular magnetic anisotropy constant of the Co_2FeAl interface upon annealing — •Andres Conca[1], Alessia Niesen[2], Guenter Reiss[2], and Burkard Hillebrands[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Center for Spintronic Materials and Devices, Physics Department, Bielefeld University, 33615 Bielefeld, Germany

We investigate a series of films with different thicknesses of the Heusler alloy Co_2FeAl in order to study the effect of annealing on the interface with a MgO layer and on the bulk magnetic properties. Our results reveal that while the perpendicular interface anisotropy constant $K_S^{\perp}$ is zero for the as-deposited samples, its value increases with annealing up to a value of 1.14 ± 0.07 mJ/m^2 for the series annealed at 320°C and of 2.0 ± 0.7 mJ/m^2 for the 450°C annealed series owing to a strong modification of the interface during the thermal treatment. This large value ensures a stabilization of a perpendicular magnetization orientation for a thickness below 1.7 nm. The data additionally shows that the in-plane biaxial anisotropy constant has a different evolution with thickness in as-deposited and annealed systems. The Gilbert damping parameter α shows an absolute minimum value of $2.8 \pm 0.1 \times 10^{-3}$. The thickness dependence is explained in terms of an inhomogeneous magnetization state generated by the interplay between the different anisotropies of the system and by the crystalline disorder.

Support by M-era.Net and HEUMEM is acknowledged.

TT 10.4 Mon 10:15 EB 301

high throughput screening for 3D spin gapless semiconductors in Heusler compounds — •qiang gao, ingo ophale, and hongbin zhang — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

In recent years, spin-gapless semiconductors (SGSs) have drawn intensive attention to the spintronics community. SGSs are half metals with the valence band maximum and conduction band minimum touching each other directly or indirectly (1). In this work, we performed high throughput screening for novel three-dimensional SGSs in quaternary Heusler compounds. Following the empirical rule, we focused on compounds with 18, 21 or 26 valence electrons (2). We have found many new Heusler compounds as candidate SGSs, with both direct and indirect touching. In particular, it is observed that spin-orbit coupling can also drive some systems into the SGS phase, resulting in possible interesting applications for future spintronic devices. (1) X.L. Wang,

Phys. Rev. Lett., **100**, 156404 (2008). (2) X.T. Wang, Z.X. Cheng, J.L. Wang, X.L. Wang, G.D. Liu, J. Mater. Chem. C, **4**, 7176-7192 (2016).

TT 10.5 Mon 10:30 EB 301

Symmetry and magnitude of intrinsic spin-orbit torques in the half-Heusler alloy PtMnSb — •Johannes Mendil[1], Jan Krieft[2], Phuong Dao[1], Can Onur Avci[1], Myriam Haydee Aguirre[3], Karsten Rott[2], Jan-Michael Schmalhorst[2], Frank Freimuth[4], Günter Reiss[2], Timo Kuschel[2], and Pietro Gambardella[1] — [1]Department of Materials, ETH Zürich — [2]CSMD, Department of Physics, Bielefeld University — [3]Universidad de Zaragoza — [4]Peter Grünberg Institut, FZ Jülich

Magnetization manipulation by spin-orbit torques (SOTs) has advanced to an active research field over the past few years and is mostly focused on conventional ferromagnets deposited on heavy metal layers where the space inversion symmetry is broken at the interface[1]. However, space inversion symmetry is intrinsically broken in non-centrosymmetric crystals [2]. We present the first observation of intrinsic SOTs in PtMnSb single layers, which is a magnetic half-Heusler alloy. It was prepared by co-sputtering [3]. Using crystallographic symmetry, we separate the observed SOTs in odd and even components with respect to magnetization inversion. We reveal corresponding effective fields that scale up to the 2nd and 3rd power of magnetization components with a distinct symmetry compared to standard field-like and damping-like SOTs. Finally, we characterize the SOTs as a function of PtMnSb thickness and discuss the possibility of using PtMnSb for magnetic switching applications. [1] Garello et al., Nat. Nanotech. 8, 587 (2013) [2] Ciccarelli et al., Nat. Phys. 12, 855 (2016) [3] Krieft, Mendil et al., Phys. Stat. Sol. (RRL) 11, 1600439 (2017)

TT 10.6 Mon 10:45 EB 301

Electrical transport in the tetragonal Heusler system Mn-Pt-Ga — •Vivek Kumar[1], Ajaya K. Nayak[2], Nitesh Kumar[1], Peter Adler[1], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Institute of Science Education and Research Bhubaneswar, Jatni, India

Nontrivial magnetic textures have attracted interest for improving desired properties in spintronic devices. Materials with non-centrosymmetric crystal structure are capable of inducing nontrivial spin structures due to the presence of Dzyaloshinskii-Moriya interaction (DMI). We have recently reported the magnetic antiskyrmions in tetragonal Heusler material $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Here, we present the effect of spin-orbit interaction in another inverse tetragonal Heusler system Mn-Pt-Ga by electrical transport measurements. The tetragonal Mn_3Ga has ferrimagnetic order where Mn atoms sit on two different magnetic sublattices. The substitution of a late transition metal in place of Mn, here Pt, leads to breaking the inversion symmetry [2]. We found an anomaly in Hall resistivity which is dominating at higher Pt substitution. The behavior of Hall resistivity cannot be scaled with magnetization. This is an indication of non-coplaner spin configurations in this system which are stabilized due to increase in DMI.
[1]A. K. Nayak *et al.*, Nature **548**, 561 (2017).
[2]S. Chadov *et al.*, Phys. Rev. B **91**, 094203 (2015).

TT 10.7 Mon 11:00 EB 301

Physical properties of the CuMnAs alloy - promising material for the antiferromagnetic spintronics — •Frantisek Maca[1], Josef Kudrnovsky[1], Vaclav Drchal[1], Karel Carva[2], Pavel Balaz[2], and Ilja Turek[2] — [1]Institute of Physics ASCR, Praha — [2]Faculty of Mathematics and Physics, Charles University, Praha

We have investigated from first principles the role of defects in the antiferromagnetic CuMnAs alloy with tetragonal structure [1]. Mn_{Cu}, Cu_{Mn}, Mn-Cu swaps, and vacancies on Mn- and Cu-sublattices are the most probable defects in this material. We have found that the electron correlations play important role in description of the phase stability.

We calculated transport properties for CuMnAs with defects of low formation energies and estimated in-plane resistivity of CuMnAs. Our numerical simulations fitted experiment very well if we assumed concentrations 3.5-5% Mn_{Cu} or Mn-Cu swaps, much larger concentrations would be needed for Cu_{Mn} defects or Mn-vacancies. We have estimated also the Neel temperature using the Monte Carlo approach, result agrees reasonably well with the experimentally observed value.

[1] F. Máca, J. Kudrnovský, V. Drchal, K. Carva, P. Baláž, and I. Turek, Phys. Rev. B **96** (2017) 094406.

15 minutes break

TT 10.8 Mon 11:30 EB 301

Improved reversibility by hydrostatic pressure in Ni-Mn based Heusler alloys — •Parul Devi[1], Luana Caron[1], Sanjay Singh[1], Alexandre Magnuu G. Carvalho[2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Laboratório Nacional de Luz Síncrotron, SáoPaulo, Brasil

Ni-Mn based Heusler alloys show first order diffusionless magnetostructural phase transition. The first order magnetostructural phase transition results in large magnetocaloric effect due to the change in both magnetic and crystal structure. The thermal or magnetic hysteresis is characteristic of first order phase transition which results in irreversibility of MCE. This irreversibility makes these materials less efficient for magnetic refrigeration. Therefore, nowadays, a lot of efforts have been made to reduce the hysteresis in these alloys [1]. In the present work, we observed a large reduction of hysteresis in off stoichiometric composition of Ni-Mn-In by hydrostatic pressure. To confirm that it is applicable to all Heusler alloys, we did it for two more different compositions of Ni-Mn based Heusler alloys. We got the decrement of hysteresis in these materials as well. However the rate of decrease in all three materials were different. Furthermore, we confirmed that the decrease in hysteresis was because of the increasingly geometric compatibility condition, recently predicted by James and co-workers [2].
[1]J. Liu *et al.*, Nature materials **11**, 620 (2012).
[2]Y. Song *et al.*, Nature Letter **502**, 85 (2013).

TT 10.9 Mon 11:45 EB 301

NMR investigations of irradiation-induced structural changes in Co_2MnSi thin films — •Franziska Hammerath[1], Mira R. D. Brandt[1], Rantej Bali[2], Kay Potzger[2], Roman Böttger[2], Rene Hübner[2], Yuya Sakuraba[3], Bernd Büchner[1], and Sabine Wurmehl[1] — [1]IFW Dresden, Institute for Solid State Research, Helmholtzstraße 20, 01069 Dresden — [2]Institute of Ion Beam Physics and Materials Research, HZDR, Bautzner Straße 400, 01328 Dresden, Germany — [3]National Institute for Materials Science (NIMS), Sengen 1-2-1, Tsukuba, Ibaraki 305-0047, Japan

Co_2MnSi is a well-known Heusler compound which is predicted to be half-metallic, i.e., possessing 100% spin-polarization and, thus, being a promising candidate material for enhancing the magneto-resistance of spin-valves [1]. Half-metallicity depends sensitively on the local chemical order, hence methods to improve the structure of Co_2MnSi towards the ideal $L2_1$ order and, thus, to achieve full spin-polarization are of huge technological relevance. On the basis of XRD measurements it has been argued that irradiation with He^+ ions induces an improvement of B2-order in Co_2MnSi thin films towards a possible formation of $L2_1$ order [2]. We investigated the structure-property relationship of He^+-irradiated Co_2MnSi alloy thin films locally by means of ^{59}Co nuclear magnetic resonance (NMR) and observed an increased disorder upon increasing the ion flux, going along with a decrease of the saturation magnetization.
[1] T. Iwase *et al.*, Appl. Phys. Express **2**, 063003 (2009).
[2] O. Gaier *et al.*, Appl. Phys. Lett. **94**, 152508 (2009).

TT 10.10 Mon 12:00 EB 301

Optical properties of pyrochlore iridates: signatures of electron correlation and spin-orbit-lattice coupling — •Alexander Boris[1], Alexander Yaresko[1], Timofei Larkin[1], Ksenia Rabinovich[1], Aleksandra Krajewska[1,2], Tomohiro Takayama[1,2], Hidenori Takagi[1,2], and Bernhard Keimer[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Stuttgart, Germany

Spectroscopic ellipsometry is used to determine the dielectric function of $A_2Ir_2O_7$ (A = In, Lu, Y) polycrystalline samples in the wide spectral range from 10 meV to 6.5 eV at temperatures from 7 K to 300 K. Comparing the spectra with the results of relativistic LSDA+U band structure calculations, we quantitatively classify pyrochlore $A_2Ir_2O_7$ as spin-orbital $J_{eff} = 1/2$ Mott insulators with the on-site Coulomb interaction $U \approx 1.5$ eV and electronic bandwidths $W = 0.3 \div 0.5$ eV. Exciton doublets with pronounced Fano line shapes were identified in $Y_2Ir_2O_7$ and $Lu_2Ir_2O_7$ upon cooling below the magnetic ordering temperatures $T_N = 150$ K and 145 K, respectively. Our results indicate considerable effects of long-range Coulomb interaction and spin-orbit-lattice coupling in the 5d pyrochlore compounds and the need for a

detailed analysis of their influence on the $J_{eff} = 1/2$ states. Newly synthesized $In_2Ir_2O_7$ does not exhibit the absorption edge and phonon anomalies below $T_N = 45$ K and thus serves as a reference.

TT 10.11 Mon 12:15 EB 301

Anisotropy of the spin-fluctuations and its impact on the symmetry of the order parameter in the unconventional Sr2RuO4 superconductor. — S. Khmelevskyi[1], B. Kim[2], D. D. F. Agterberg[3], P. Mohn[1], •I. I. Mazin[4], and C. Franchini[2] — [1]Center for Computational Materials Science, Vienna University of Technology, Vienna, Austria — [2]Center for Computational Materials Physics, Vienna University, Vienna, Austria — [3]University of Wisconsin, Milwaukee, USA. — [4]Naval Research Laboratory, Washington DC, USA.

The superconductivity (SC) in the Sr2RuO4 has attracted a considerable interest in the past two decades comparable to that in cuprates and iron pnictides. NMR experiments strongly suggested a triplet chiral order parameter, while more recent probes of strained crystals point toward singlet pairing. In this work the structure of the spin-fluctuations in the Sr2RuO4 has been investigated from first principles using the DLM formalism and Lichtenstein method. We find that IC spin-fluctuations are stabilized but several magnetic ground states with q close to the commensurate (1/3, 1/3, 0) value are degenerate. We show that the degeneration is removed by Spin-orbit coupling and a very special collinear modulated magnetic structure with periodicity 1/3 is stabilized in the mean field in the [110] direction. We show that anisotropic magnetic terms provide an energy penalty for rotating the order parameter that is several orders of magnitude too large for the accepted interpretation, thus rendering the NMR experiment completely inexplicable in terms of the conventional theory.

TT 10.12 Mon 12:30 EB 301

Magnetic shape-memory effect in $SrRuO_3$ — •Daniel Brüning[1], Stefan Kunkemöller[1], Agung Nugroho[2], Isabelle Stunault[3], Markus Braden[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Faculty of Mathematics and Natural Science, Institut Teknologi Bandung, Indonesia — [3]Institut Laue Langevin, Grenoble, France

As most perovskites, $SrRuO_3$ exhibits structural phase transitions associated with rotations of the RuO_6 octahedra. From a high temperature cubic phase it becomes tetragonal at 975 K and orthorhombic at 800 K resulting in six possible domains. Furthermore, $SrRuO_3$ orders ferromagnetically at $T_c = 160$ K with easy axis anisotropy due to spin orbit coupling. Our neutron diffraction and macroscopic measurements unambiguously show that magnetic fields rearrange structural domains, although the ferromagnetic order occurs at six times lower temperature than the structural distortion. For the field along a cubic $[110]_c$ direction, a fully detwinned crystal is obtained. Subsequent heating above T_c causes a magnetic shape-memory effect, where the initial structural domains recover, which is similar to Heusler alloys.

Kunkemöller *et al.*, arXiv:1709.05688 (2017)

Funded by the DFG via CRC 1238 Projects A02, B01, and B04.

TT 10.13 Mon 12:45 EB 301

Multicritical Lifshitz transition of the Fermi-surface in $Sr_3Ru_2O_7$ — •Joseph Betouras[1], Dmitry Efremov[1,2], Alex Shtyk[3], Andreas Rost[4], Claudio Chamon[5], and Andrew Mackenzie[4,6] — [1]Department of Physics, Loughborough University, Loughborough, UK — [2]Leibniz-Institut fur Festkorper- und Werkstoffforschung, D-01069 Dresden, Germany — [3]Department of Physics, Harvard University, Cambridge, MA 02138, USA — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, U.K. — [5]Department of Physics, Boston University, Boston, MA, 02215, USA — [6]Max Planck Institute for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden, Germany

We present a theoretical framework, supported by experimental evidence for a Lifshitz topological transition of the Fermi surface in the ultra-clean layered perovskite metal $Sr_3Ru_2O_7$ [1]. Strong power-law dependence of the density of states on energy, associated to the topological transition, in addition to other main features of the Fermi surface as well as interactions, can lead to novel physics. As a consequence, many yet unexplained properties of the thermodynamics and formation of phases of this material can be understood. In particular, we naturally explain the increase of the entropy[2] as well as the formation of spin density wave (phase A) [3]. This work provides an example of the power of Fermi surface topological transitions.

[1]S. A. Grigera, S. A. et al. Science 306, 1154 (2004).
[2] A. Rost et al., Science 325, 1360 (2009).
[3] C. Lester et al, Nature Materials 14, 373 (2014).

TT 10.14 Mon 13:00 EB 301

Study of reorientation in $NdFe_{0.5}Mn_{0.5}O_3$ — Ankita Singh[1], Anil Jain[2], Avijeet Ray[1], Vivian Nassif[3], Tulika Maitra[1], and •Vivek K. Malik[1] — [1]Department of Physics, IIT Roorkee, Roorkee, 247667, India — [2]Solid State Physics Division, Bhabha Atomic Research Center, Mumbai 400085, India — [3]Institut Laue -Langevin, 71 Avenue des Martyrs, 38000 Grenoble, cedex 9 France

In the present study, we have studied spin reorientation in $NdFe_{0.5}Mn_{0.5}O_3$ using neutron powder diffraction technique. Polycrystalline compound $NdFe_{0.5}Mn_{0.5}O_3$ was synthesized using the standard solid state reaction method. Neutron powder diffraction experiments over the temperature range of 1.5-300 K have been performed. Our neutron diffraction study shows that below the Néel temperature (T_N250 K), the magnetic structure (for the Fe/Mn spins) is a G-type antiferromagnet [corresponding to the Γ_1 representation with spins aligned along the crystallographic b direction. Below 70 K, additional peaks appear in the neutron diffraction pattern. Rietveld refinement (below 70 K) confirms a coexistence of two magnetic phases corresponding to representations Γ_1 and Γ_2. In the magnetic structure corresponding to the Γ_2 representation, Fe/Mn spins are aligned along the crystallographic c direction (with small ferromagnetic component along the crystallographic a axis). Upon cooling (below 50 K), the phase fraction of the second magnetic phase increases. At 1.5 K, magnetic structure can be described only by Γ_2 representation. An antisymmetric exchange interaction between R^{3+}-Mn^{3+}/Fe^{3+}spins might be responsible for the observed spin reorientation.

TT 11: Ferroelectric Domain Walls I (joint session KFM/TT)

Organizer: Sergey Artyukhin - Istituto Italiano di Tecnologia - Genova (Italy)

Time: Monday 9:30–12:45 Location: EMH 225

Invited Talk TT 11.1 Mon 9:30 EMH 225

Atomic-resolution imaging of electronic inversion layers at ferroelectric domain walls — •Julia Mundy[1], J. Schaab[2], Y. Kumagai[2], A. Cano[3], M. Stengel[4,5], I. Kung[6], D. Gottlob[7], H. Doganay[7], M. Holtz[8], R. Held[8], Z. Yan[2,9], E. Bourret[9], C. Schneider[7], D. Schlom[8], D. Muller[8], R. Ramesh[9,10], N. Spaldin[2], and D. Meier[2,11] — [1]Harvard University — [2]ETH Zurich — [3]Université de Bordeaux, ICMCB — [4]ICREA Institució Catalana de Recerca i Estudis Avançat — [5]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB — [6]TU Berlin — [7]Forschungszentrum Julich — [8]Cornell University — [9]Lawrence Berkeley National Laboratory — [10]UC Berkeley — [11]Norwegian University of Science and Technology

Ferroelectric domain walls hold great promise as functional two-dimensional materials because of their unusual electronic properties. Particularly intriguing are the so-called charged walls where a polarity mismatch causes local, diverging electrostatic potentials requiring charge compensation and hence a change in the electronic structure. These walls can exhibit significantly enhanced conductivity and serve as a circuit path. Here we use atomic-resolution STEM-EELS to directly probe the charge transfer at these charged ferroelectric domain walls in $ErMnO_3$. Our direct quantification of the charge transfer to the domain boundary gives insight into the the formation and eventual activation of an inversion layer that acts as the channel for the charge transport. The findings provide new insight into the domain-wall physics in ferroelectrics.

TT 11.2 Mon 10:00 EMH 225

Charged domain walls and point defect-DW interactions in hexagonal manganites — Didrik Rene Småbråten[1], Quitin Meier[2], Sandra Helen Skjaervoe[1], Thomas Tybell[1], Dennis Meier[1], and •Sverre Magnus Selbach[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Materials Theory, ETH Zurich, Zürich, Switzerland

Charged head-to-head and tail-to-tail ferroelectric domain walls (DW) in hexagonal manganites are stable because of the improper nature of the ferroelectricity in these materials, and it has been experimentally shown that their electronic properties can differ strongly from bulk. First principles studies of charged DWs are scarce and the inherent electrostatic fields make DFT calculations challenging. Here we combine density functional theory (DFT) calculations with a continuum model based on Landau theory to study the properties of charged DWs in $YMnO_3$, $InMnO_3$ and isostructural $YGaO_3$. We find excellent agreement between the micro- and macroscopic models, and show that the Mexican hat energy landscape of hexagonal maganites derived from Landau theory also emerges naturally from DFT calculations of their DWs. Head-to-head and tail-to-tail DW are structurally inequivalent due to the different local chemical bonding. We formulate a general criterion based on polarization and band gap for when charged DWs become conducting. Finally, we study interactions between DWs and oxygen interstitials and vacancies by DFT.

TT 11.3 Mon 10:15 EMH 225

Local control of chemical structure in a functional oxide — •Donald M. Evans[1], Theodor S. Holstad[1], Aleksander B. Mosberg[2], Per-Erik Vullum[2], Didrik Småbråten[1], Sverre Selbach[1], Antonius T. J. Van Helvoort[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU, Norway — [2]Department of Physics, NTNU, Norway

Since the suggestion to use ferroelectric domain walls (DWs) in nanoelectronics, there has been a great deal of research into their properties. The most obvious use of DWs with enhanced conductivity was as nano-wires. But more recently, research is moving towards using the DW as the functional element within a circuit, e.g. as a switch or diode. This approach could allow whole circuit elements to be replaced by a single sub nanometre wide object - an option with clear technological potential. Attractive as this concept is, the research is still in its embryonic stage with many unanswered questions, not least, how to connect these DW circuit elements. In this work, we demonstrate how an atomic force microscope (AFM) can be used to change the functional properties locally: that is, we can use an AFM to write conducting strips on demand with all the position and control associated with AFM techniques. This is demonstrated on a hexagonal manganite ($ErMnO_3$) and foreshadows the possibility to interconnect functional DWs into nanoscale circuits. To better understand this ability to locally control functional properties, these modified regions were analysed with both TEM, and EELS.

TT 11.4 Mon 10:30 EMH 225

Anomalous domain wall motion in Cu-Cl boracite: negative permittivity in an improper ferroelectric? — •Charlotte Cochard[1], Joseph G.M. Guy[1], Michael P. Campbell[1], Roger W. Whatmore[2], Amit Kumar[1], Raymond G.P. McQuaid[1], and Marty Gregg[1] — [1]Queen's University Belfast, Belfast UK — [2]Imperial College London, London, UK

Negative capacitance has attracted a lot of attention recently thanks to its potential to enable shorter switching time of transistors. It has been observed in systems as diverse as p-n junction, electrochemical systems, and ferroelectrics. To date, no single-phase material has been reported to exhibit negative capacitance.

In this work, we show that regions in a boracite crystal ($Cu_3B_7O_{13}Cl$) exhibit anomalous electric-field-induced movement of charged domain walls, consistent with negative permittivity. Boracites naturally display domain wall configurations, seen to be electrically active by current mapping [1]. While applying an electric field across some of these charged walls, we observed that domains with polarisation components pointing opposite to the electric field grow at the expense of domains with polarisation components aligned with the field. Thus dP/dE is negative and hence permittivity is negative. This behaviour is proposed to originate from the improper ferroelectric nature of the boracite: the elastic energy payoff, due to polarisation-strain coupling, is greater than the work done in generating increased polarisation against the applied electric field.

[1] R.G.P. McQuaid, et al. Nat. Commun. 8, 15105 (2017).

15 min break

TT 11.5 Mon 11:00 EMH 225

Interplay between point defects and domain wall mobility in improper ferroelectric $YMnO_3$ — •Didrik René Småbråten, Dennis Meier, and Sverre Magnus Selbach — Norwegian University of Science and Technology (NTNU), Trondheim, Norway

Understanding the domain wall (DW) dynamics in ferroelectrics is key to controlling and fine-tune the domain structure and hence the ferroelectric properties. The DW dynamics strongly couple to the defect chemistry in the material, where stationary dopants may act as pinning centers or mobile defects may move with the DWs. The overall aim of this study is to give chemical guidelines for how to control the domain wall mobility via defect chemistry. Improper ferroelectric $YMnO_3$ has a complex and exotic DW structure, including neutral, as well as positively and negatively charged DWs. Furthermore, the material has a large chemical flexibility being robust against donor and acceptor doping of its cation sublattices, and it is stable under both oxygen deficiency and excess. This unique flexibility makes $YMnO_3$ an ideal model system for studying the interplay between DW mobility and defect chemistry. From density functional theory (DFT) calculations we show how changes in the two cation sublattices affect the DW mobility. In addition, we study how mobile anion defects couple to the DW movement and determine if they move with or pin the DWs.

TT 11.6 Mon 11:15 EMH 225

Conducting domain wall networks in $TbMnO_3$ and $BiFeO_3$ — •Mart Salverda[1], Wilson Acevedo[2], Diego Rubi[2], Saeedeh Farokhipoor[1], and Beatriz Noheda[1] — [1]Zernike Institute for Advanced Materials, Groningen, The Netherlands — [2]CNEA and INN, Buenos Aires, Argentina

Ferroelastic domain walls in thin films of some complex oxides show a higher conductivity than the domains [1][2]. This effect is proposed to originate from the accumulation of ionic species at the domain walls due to the presence of strain gradients [2][3][4]. In a recent study [5] we propose a model that accounts for the electrical behavior measured in $TbMnO_3$ thin films using macroscopic techniques, by assuming that the structural domain walls that are present in these films [6] are conducting. From the model, the value of the sheet resistance of the domain walls has been extracted. To further investigate the validity of this approach for other materials, we perform a similar analysis on systems incorporating thin films of $BiFeO_3$ where the domain walls are already proven to be conducting. Our aim is to elucidate the intrinsic transport properties of the domain walls.

[1] J. Seidel et al., *Nature Materials* **8**, 229 (2009) [2] S. Farokhipoor and B. Noheda, *Physical Review Letters* **107**, 127604 (2011) [3] E. Salje and H. Zhang, *Phase Transitions* **82**, 452 (2009) [4] T. Rojac et al., *Nature Materials* **16**, 322 (2017) [5] W. Román et al. (in preparation) [6] S. Farokhipoor et al., *Nature* **515**, 379 (2014)

Invited Talk TT 11.7 Mon 11:30 EMH 225

Understanding the dielectric enhancement from domain walls in conventional and relaxor ferroelectrics — •Andrew Rappe — University of Pennsylvania, Philadelphia, PA, USA

The dielectric properties of ferroelectric materials are a key driver of smart materials applications. In this talk, two key aspects of anomalous dielectric enhancement will be analyzed: domain walls and relaxor ferroelectrics. A comprehensive theoretical viewpoint will be sketched that unifies these aspects, based on multi-scale materials modeling.

Incorporating quenched Coulombic disorder in ferroelectrics disrupts and changes the character of this transition; instead of a sharp transition in a small temperature range, these oxide alloys exhibit "relaxed" transitions over 100-200 K and are called "relaxor ferroelectrics." I will describe how a first-principles based multi-scale model can reveal the dynamic and statically correlated motions of ions that lead to relaxor behavior, and I will discuss their promise for next-generation piezoelectric and dielectric material systems, with emphasis on the emergent stabilization of a high density of low-angle domain walls.

I will also present molecular dynamics simulations of 90 degree domain walls (separating domains with orthogonal polarization directions) in the ferroelectric material $PbTiO_3$ to provide microscopic insights that enable the construction of a simple, universal, nucleation-and-growth-based analytical model that quantifies the dynamics of many types of domain walls in various ferroelectrics. This new model illuminates domain wall influence on the dielectric responses of conventional and relaxor ferroelectrics.

TT 11.8 Mon 12:00 EMH 225

In-situ 4D observation of ferroelectric domain wall dynamics using second-harmonic generation microscopy — •Lukas Wehmeier, Alexander Haussmann, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, 01062 Dresden, Germany

Second-harmonic generation microscopy (SHGM) allows for the three-dimensional (3D) observation of ferroelectric domain walls (DWs) across millimeter-thick bulk materials [1,2]. For example, this is of supreme value for exploring inclined and charged domain walls [1,3]. Here, we apply SHGM in order to quantify the DW dynamics in triglycine sulfate (TGS) single crystals upon the ferroelectric-to-paraelectric phase transition at the Curie temperature of $\approx 49\,^{\circ}\mathrm{C}$ [4]. In addition, we study DW dynamics that are induced by external electric fields.

We show for TGS that SHGM allows exploring such electric-field-induced and temperature-driven DW dynamics in 4D, i.e. in real-time and full 3D imaging.

[1] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014).
[2] T. Kämpfe et al., Appl. Phys. Lett. 107, 152905 (2015).
[3] C. Godau et al., ACS Nano 11, 4816 (2017).
[4] L. Wehmeier et al., Phys. Stat. Solidi RRL 11, 1700267 (2017).

TT 11.9 Mon 12:15 EMH 225

Electrical half-wave rectification at improper ferroelectric domain walls — •J. Schaab[1], S. H. Skjaervo[2], S. Krohns[3], X. Dai[1], M. Holtz[4], M. Lilienblum[1], D. A. Muller[4,5], M. Fiebig[1], S. M. Selbach[2], and D. Meier[1,2] — [1]ETH Zürich — [2]NTNU Trondheim — [3]University of Augsburg — [4]Cornell University — [5]Kavli Institute at Cornell for Nanoscale Science

Ferroelectric domain walls represent multifunctional 2D-elements that offer great potential for novel device paradigms. Improper ferroelectrics display particularly promising domain walls, which due to their unique robustness, are the ideal template for imposing the desired electronic behavior. Chemical doping, for instance, induces p- or n-type characteristics and electric fields reversibly switch between resistive and conductive domain-wall states.

Here, we demonstrate conversion of alternating current (AC) into direct current (DC) output based on neutral 180° domain walls in improper ferroelectric $ErMnO_3$. By combining scanning probe and dielectric spectroscopy, we show that the AC-to-DC conversion occurs for frequencies at which the domain walls are pegged to their equilibrium position. The practical frequency regime and magnitude of the output is controlled by the conductivity of the surrounding domains. Using density functional theory, we attribute the distinct transport behavior to oxygen defects that accumulate at the neutral walls. Our study reveals domain walls acting as 2D half-wave rectifiers, extending domain-wall-based nanoelectronics applications into the realm of AC-technology.

TT 11.10 Mon 12:30 EMH 225

Unexpected $BiFeO_3$ 71 degree domain wall vibration — •Peng Chen and Sergey Artyukhin — Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova (Italy)

Emergent phenomena excitations at domain walls are attracting enormous attention recently. Recent scanning impedance microscopy (SIM) measurements reveal AC conductance attributed to domain wall-localized phonons, that give important contributions to low-frequency dynamics in ferroic materials. In $BiFeO_3$ the polarization change across 71 degree domain walls is perpendicular to the electric field applied by the SIM tip, and therefore the DW-localized phonon should not be excited by the tip. However, the experimental observations show a violation of this intuitive picture. Here we use Landau-Ginzburg theory and first-principles calculations to address this puzzling behavior.

TT 12: Dynamics in Many-Body Systems: Interference, Equilibration and Localization I (joint session DY/TT)

Time: Monday 10:00–12:45 Location: EB 107

TT 12.1 Mon 10:00 EB 107

Post-Ehrenfest many-body quantum interferences far-out-of-equilibrium many-body systems — Steve Tomsovic[1,4], Denis Ullmo[2], Peter Schlagheck[3], •Juan-Diego Urbina[4], and Klaus Richter[4] — [1]Washington State University, USA — [2]Universite Paris Sud, France — [3]University of Liege, Belgium — [4]University of Regensburg, Germany

Many-body quantum dynamics in isolated systems far from equilibrium generate interferences beyond the Ehrenfest time where quantum and classical expectation values diverge, with recent interest in the role these interferences play in the spreading of quantum information across the many degrees of freedom[1]. We have developed a semiclassical theory which properly incorporates such quantum interference effects and showed that, for mesoscopically populated Bose-Hubbard systems, it captures post-Ehrenfest quantum phenomena very accurately even to the point to alllow for high-precision many-body spectroscopy [2].

We present here a description of this novel approach and point out how it can be used to improve the heavily used truncated Wigner method [3] by incorporating exact degenaracies of classical actions responsible of robust many-body interference effects.

[1] S. H. Shenker and D. Stanford, JHEP 3, 67 (2014).
[2] S. Tomsovic, P. Schlagheck, D. Ullmo, J. D. Urbina, and K. Richter arXiv 1711.04693 (2017).
[3] A. Sinatra, C. Lobo, and Y. Castin, J. Phys. B: Atom. Molec. Opt. Phys. 35, 3599 (2002).

TT 12.2 Mon 10:15 EB 107

Signatures of indistinguishability in bosonic many-body dynamics — Tobias Brünner[1], Gabriel Dufour[1,2], •Alberto Rodríguez[1], and Andreas Buchleitner[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, D-79104, Freiburg, Germany — [2]Freiburg Institute for Advanced Studies, Albert-Ludwigs-Universität Freiburg, Albertstraße 19, D-79104 Freiburg, Germany

Many-body interference occurs as a fundamental process during the evolution of a quantum system consisting of two or more indistinguishable particles. The (measurable) consequences of this interference, as a function of the particles' mutual indistinguishability, was studied for non-interacting photons transmitted through beam-splitter arrays. However, the role of many-body interference in the dynamics of interacting particles, e.g. cold atoms in optical lattices, had so far remained unclear. We identify a quantifier of the particles' mutual indistinguishability attuned to time-continuously evolving systems of (interacting) particles, which predicts the dynamical behaviour of observables influenced by genuine few-body interference. Our measure allows a systematic exploration of the role of many-body interference in the weakly and strongly interacting regimes.

TT 12.3 Mon 10:30 EB 107

Trajectory-based approaches for simulating nonequilibrium dynamics in open quantum systems — •Shunsuke Sato[1], Aaron Kelly[2], and Angel Rubio[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, DE — [2]Dalhousie University, Halifax, Canada

We present our recently developed trajectory-based quantum dynamics approach for treating nonequilibrium phenomena in electron-phonon systems. Based on a simple extension of mean field theory, this new approach leads to simulation scheme that uses a statistical ensemble of coupled trajectory pairs. The time-evolution of each pair is governed by the Euler-Lagrange variational principle. This method yields mean field theory in the limit that the trajectories are orthogonal, and in the limit that they completely overlap. Although trajectories are only coupled to a single partner, this method shows a substantial improvement over mean field theory in capturing quantum coherence in the nuclear dynamics as well as electron-nuclear correlation. The performance of our coupled trajectory method is particularly favourable in nonadiabatic systems, as it retains quantitative accuracy well beyond the perturbative electron-phonon coupling regimes of the spin-boson model, and the Holstein polaron model.

Furthermore, when utilized in tandem with the Nakajima-Zwanzig-

Mori generalized quantum master equation formalism, this hybrid trajectory-based master equation approach provides an attractive route forward to a fully ab initio description of relaxation processes, such as thermalization, in condensed phase systems.

TT 12.4 Mon 10:45 EB 107

Energy transport in the driven disordered XYZ chain — •Maximilian Schulz[1,2], Scott Taylor[2], Chris Hooley[2], and Antonello Scardicchio[3,4] — [1]Max Planck Institut für Physik komplexer Systeme — [2]University of St Andrews — [3]Abdus Salam ICTP — [4]INFN, Sezione di Trieste

The delocalized region preceding the many-body localization (MBL) transition is currently receiving a significant amount of attention due to apparent deviations from typical diffusive transport. The XXZ spin chain has been shown to exhibit subdiffusive spin transport at intermediate disorder strengths, and the nature of energy transport close to the MBL transition is still a matter of debate.

We present results of a combined time-evolving block decimation and exact diagonalization study of energy currents in the disordered XYZ spin chain on the delocalized side of the MBL transition. The significance of this choice of model is that its clean hydrodynamics involves only energy currents, whereas the XXZ model has both energy and spin currents. This allows us to explore the question of how the nature of the delocalized phase depends on the hydrodynamic properties of the underlying clean model.

TT 12.5 Mon 11:00 EB 107

Construction of exact constants of motion and effective models for many-body localized systems — •Marcel Goihl, Marek Gluza, Christian Krumnow, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, 14195 Berlin, Germany

One of the defining features of many-body localization is the presence of extensively many quasi-local conserved quantities. These constants of motion constitute a corner-stone to an intuitive understanding of much of the phenomenology of many-body localized systems arising from effective Hamiltonians. They may be seen as local magnetization operators smeared out by a quasi-local unitary. However, to accurately identify such constants of motion remains a challenging problem. Current numerical constructions often capture the conserved operators only approximately or trade desirable properties such as exactly commuting with the Hamiltonian against each other, restricting a conclusive understanding of many-body localization. In this talk, we use methods from the theory of quantum many-body systems out of equilibrium to establish a new approach for finding a complete set of exact constants of motion which are in addition by construction guaranteed to represent Pauli-z operators. By this we are for the first time able to construct and investigate the proposed effective Hamiltonian using exact diagonalization. Hence, our work provides an important tool expected to further boost inquiries into the breakdown of transport due to quenched disorder.

15 min. break

TT 12.6 Mon 11:30 EB 107

Non-Ergodic Dynamics in Many-Body Systems — Carlo Danieli and •Sergej Flach — Center for Theoretical Physics of Complex Systems, Institute for Basic Sciences, Daejeon, Korea

Integrable models are characterized by a set of preserved actions. Close to the limits, the nonintegrable perturbations span a coupling network in action space which can be short or long ranged. The equilibrium dynamics of a system close to such limits is sensitive to the network type. Long range networks enforce ergodicity with large but finite relaxation time scales at a finite distance to the integrable limit. Short range networks lead to a loss of ergodicity at a finite distance from the limit. We demonstrate this by choosing observables which turn conserved actions at the limit. Off the limit, and fixing their value to the proper statistical average, they define manifolds in the phase space of an ergodic and equipartitioned many-body system. A typical trajectory pierces such manifolds infinitely often as time goes to infinity. Close to the integrable limit, the dynamics yields a power-law distribution of the excursion times off the manifolds. The exponent is used as a measure of distance from a potential nonergodic regime. We analyse several cases: the Fermi Pasta Ulam chain in the limit of small energies (long range network), and the Klein-Gordon, Discrete Gross Pitaevskii and coupled rotor lattices in the limit of large energies (short range network).

TT 12.7 Mon 11:45 EB 107

memory effects in the strongly anharmonic FPUT model — •Graziano Amati[1], Hugues Meyer[2], and Tanja Schilling[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität, 79104 Freiburg, Germany — [2]Research Unit in Engineering Science, Université du Luxembourg, L-4364 Esch-sur-Alzette, Luxembourg

The Fermi-Pasta-Ulam-Tsingou (FPUT) Problem represents an intriguing challenge in Modern Physics. In its original formulation, it questions whether or not a Dynamical System can reach thermalization if a small anharmonicity is added to an integrable system, under specific out-of-equilibrium initial conditions. The problem was originally raised by the apparent lack of energy spreading between the normal modes of a one-dimensional chain of particles with a small anharmonicity, in case the energy at the initial time is given to the lowest frequencies of the system.

In the present work, we consider a one-dimensional chain of many particles with a strongly anharmonic interaction potential. The model is initialized at canonical equilibrium, and we take as a relevant variable the Fourier Transform of the density of particles for a tagged degree of freedom. The time correlation function of this observable exhibits an interesting non-ergodic behavior due to a temperature-driven 'FPU-like' dynamical localization, that corresponds to a nontrivial memory profile.

Via a novel coarse-graining technique, we are able to reconstruct the dynamics of the memory, and to show that the exhibited non-ergodicity can be rephrased via the memory kernel of the process.

TT 12.8 Mon 12:00 EB 107

Dynamical quantum phase transitions in the particle-antiparticle production of a lattice gauge theory — •Yi-Ping Huang and Markus Heyl — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

Particle-antiparticle production in the presence of a static classical electric field, known as the Schwinger mechanism, represents a central physical phenomenon in gauge theories. How the particle production is affected in the quantum limit, where the backaction onto the electric field becomes essential, remains a major challenge. In this work, we study particle-antiparticle production in the quantum quench dynamics after a strong coupling of the bare particles to dynamical gauge field in a quantum link model. We find that for a strong coupling the system experiences dynamical quantum phase transitions (DQPTs) where the vacuum persistence probability (Loschmidt echo) develops non-analytic behavior at critical times. As opposed to the Schwinger mechanism, where matter fields are suddenly coupled to a classical electric field, we observe that the dynamics of the vacuum persistence probability and therefore the DQPTs cannot be understood using the classical picture of particle production. Instead, a quantum dynamical pattern emerges from the strongly coupled matter fields and dynamical gauge fields. We discuss how these findings can be experimentally observed in quantum simulators such as trapped ions.

TT 12.9 Mon 12:15 EB 107

Critical quench dynamics of random quantum spin chains — •Gergő Roósz[1,2], Yu-Cheng Lin[3], and Ferenc Igloi[2] — [1]Technische Universität Dresden — [2]MTA Wigner RCP, Hungary — [3]Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan

By means of free fermionic techniques combined with multiple precision arithmetic we study the time evolution of the average magnetization, $\overline{m}(t)$, of the random transverse-field Ising chain after global quenches. We observe different relaxation behaviors for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow described by $\overline{m}(t) \sim \ln^a t$, and in a finite sample of length L the average magnetization saturates at a size-dependent plateau $\overline{m}_p(L) \sim L^{-b}$; here the two exponents satisfy the relation $b/a = \psi = 1/2$. Starting from a fully disordered initial state, the magnetization saturates to an asymptotic value $\overline{m}_p(L) \sim L^{-b'}$, with $b' \approx 1.5$. For both quenching protocols, finite-size scaling is satisfied in terms of the scaled variable $\ln t/L^{\psi}$. Furthermore, the distribution of long-time limiting values of the magnetization shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behavior of the magnetization is explained through semi-classical theory.

TT 12.10 Mon 12:30 EB 107

Many-Body Localization in the Central Spin Model — •Hetterich Daniel[1], Yao Norman[2], and Trauzettel Björn[1] — [1]Institut für Theoretische Physik, Universität Würzburg, D-97074 W\"urzburg, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA

The periodic Heisenberg chain model obeys signatures of many-body localization (MBL) that persist the insertion of a central spin, which interacts with all other spins of the periodic chain. To support this statement, we present numerical results for the level repulsion of eigenvalues and for the growth of entanglement entropy of subsystems. We discuss why under which conditions the central spin destroys the localized phase. Finally, we show that local observables that measure the central spin only serve as a MBL detector.

TT 13: Graphene: Electronic Properties, Structure and Substrate Interaction I (joint session O/TT)

Time: Monday 10:30–13:15 Location: MA 043

TT 13.1 Mon 10:30 MA 043

A Molecular Model System for 5-7 Defects in Graphene — •Benedikt P. Klein[1], Markus Franke[2], Claudio K. Krug[1], Stefan R. Kachel[1], Phil Rosenow[1], Francois Posseik[2], Martin Schmid[1], Reinhard J. Maurer[3], Ralf Tonner[1], Christian Kumpf[2], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Philipps-Universität Marburg, Germany — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Department of Chemistry, University of Warwick, United Kingdom

The electronic and mechanical properties of graphene are strongly influenced by the presence of defects. One important type of defect is the 5-7 motif with a 5-membered ring adjacent to a 7-membered ring. Little is known about the interaction of 5-7 defects with an underlying substrate. In this study, we have obtained insight into this interaction by using molecular model systems. As a model for the 5-7 defects we use azulene, which is a bicyclic aromatic compound with a 5- and a 7-membered ring, while naphthalene is used as a model for the regular 6-6 motif. We investigated both molecules on Cu(111) and Ag(111) using PES, NEXAFS, TPD, scanning probe and NIXSW experiments. To deepen the understanding of the occurring interactions between molecule and surface, periodic DFT calculations were performed. The more localized frontier orbitals of azulene result in a much stronger and more localized interaction with the Cu(111) surface. This leads to interfacial charge transfer in the former LUMO and substantial in-plane and out-of-plane deformations, as well as a much smaller adsorption height.

TT 13.2 Mon 10:45 MA 043

The Effect of Carbon 1s Core Hole on the Polarization Spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Our band structure calculations show a good agreement with experimental polarization spectra [1] across the carbon 1*s* edge of highly oriented pyrolytic graphite. The change of polarization characteristics upon reflection of linearly polarized synchrotron radiation as the huge rotation of polarization plane of up to 140° and the change to nearly fully circularly polarized light can be resembled good, showing best results for not full but partially core hole per excitation. The contributions from the *A* and *B* site of HOPG are discussed as well as the amount of electron removed from core state.

References: 1. C. Jansing et al, PRB **94**, 045422 (2016).

This work was supported by Czech National Foundation grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

TT 13.3 Mon 11:00 MA 043

Giant magneto-photoelectric effect at a graphene edge — •Friedemann Queisser, Jens Sonntag, Annika Kurzmann, Martin Geller, Sascha Lang, Axel Lorke, and Ralf Schützhold — Fakultät für Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

Graphene is a promising material for optical or infrared absorption, as its pseudo-relativistic energy-momentum relation allows for a broad absorption bandwidth. In [1] we studied the charge separation at a graphene edge via a strong magnetic field. Motivated by the proposed mechanism, a surprisingly high magneto-photocurrent was measured in suspended graphene [2]. The observed photo-responsitivity (100 incident photons create up to 17 particle-hole pairs) strongly exceeds the predicted value. A possible mechanism to explain the large observed current is Auger-type scattering. The strong Coulomb interaction, $\alpha_{\text{graphene}} \gg \alpha_{\text{QED}}$, together with the enlarged phase space at the graphene edge lead to a large probability per unit time for the secondary particle-hole pair creation. We discuss various aspects of Auger-type scattering at the graphene edge.

References:

[1] F. Queisser and R. Schützhold *Phys. Rev. Lett.* **111**, 046601 (2013)

[2] J. Sonntag, A. Kurzmann, M. Geller, F. Queisser, A. Lorke, R. Schützhold, *New. J. Phys.* **19** 063028 (2017)

TT 13.4 Mon 11:15 MA 043

Synthesis of two-dimensional materials using liquid metal catalysts: Instrument development for *in situ* studies — •Amirmehdi Saedi[1], Marc de Voogd[2], Arthur Sjardin[2], Gertjan van Baarle[2], and Irene Groot[1] — [1]Catalysis and Surface Chemistry, Leiden Institute of Chemistry, Leiden University, The Netherlands — [2]Leiden Probe Microscopy BV, Leiden, The Netherlands

Two-dimensional materials (2DMs), e.g. graphene, hold great promise for future applications in many technological areas. The current state-of-the-art synthesis method of these materials involves the dissociative adsorption of gas-phase precursors on a solid catalyst. This process is slow by nature, inefficient, and environmentally unfriendly. Using liquid metal catalysts (LMCats) instead of solid ones bears the prospect of a continuous production of 2DMs with unprecedented quality and production speed. The aims of this multinational collaborative project are to develop instrumentation capable of studying the ongoing chemical reactions on a LMCat, *in situ* investigations on its catalytic activity, and unraveling the growth mechanisms of 2DMs on surfaces of LMCats. Gaining this knowledge would be the key toward establishing the first efficient mass production method for 2DMs using this new technology. (Visit http://lmcat.eu/ for more info)

TT 13.5 Mon 11:30 MA 043

Effects of bi-axial strain on heterostructure of hBN and graphene — •Francesco Delodovici[1], Silvana Botti[2], and Giovanni Onida[1] — [1]Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano, Italy — [2]Institute of Condensed Matter Theory and Optics Max-Wien-Platz 1 07743 Jena Germany

I will present a theoretical/computational study of the mechanical and electric properties of an heterostructure consisting of graphene superimposed to hexagonal boron nitride (hBN) when external biaxial strain is applied.

As a preliminary case, we consider a free-standing layer of hBN under uniform biaxial strain: we predict new thermodinamically stable configurations and analyze their mechanical properties, to understand whether they could be accessible experimentally. In addition, we characterize their electrical and optical properites, to detect the emergence of radical changes in hBN properties.

Further on, we turn our attention to the effects of equi-biaxial strain on the graphene-hBN heterostructure.

We use ab-initio crystal structure prediction, and more precisely the fixed-volume minima hopping method to sample the configuration space searching for new configurations. We use density functional tight

binding methods to obtain energies and forces for structural prediction and DFT to characterize the electric properties of the new phases.

TT 13.6 Mon 11:45 MA 043

Light-field-driven currents in graphene — •Christian Heide, Takuya Higuchi, Konrad Ullmann, Heiko B. Weber, and Peter Hommelhoff — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen

Strong-field physics centres on controlling the motion of electrons by virtue of an optical electric field with attosecond (10^{-18} s) precision. Graphene is an ideal playground for extending the scope of strong-field phenomena to a conductor because of its excellent carrier mobility, much weaker screening due to a low carrier concentration compared with conventional metals and its ultrafast and broadband optical response.

We will show that one can control the residual conducting current in epitaxially grown graphene by tailoring the electric-field waveform of few-cycle laser pulses, on attosecond timescales [1]. We interpret the waveform-dependent conducting current by considering graphene as a simple two-band system, interacting with an oscillating optical field of an ultrashort laser pulse. We found a transition from the weak, perturbative nonlinear response (photon-driven) to optical-field-driven, nonperturbative electron dynamics, in which the influence of the intraband dynamics to the interband transition cannot be neglected. Inthis strong-field regime, electrons exhibit quantum-mechanical interference known as Landau-Zener-Stückelberg interference.

[1] T. Higuchi, C. Heide, K. Ullmann, H. B. Weber, and P. Hommelhoff, Light-field-driven currents in graphene, Nature 550, 224 (2017).

TT 13.7 Mon 12:00 MA 043

Can the Coulomb interaction be added to the Dirac-Weyl equation of graphene? — •Fabian Rost and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen, Germany

On the basis of an exact operator equivalence between a lattice tight binding model and a continuum description $H(\mathbf{r},\mathbf{p})$ [1], we address the question of the required form the interaction potential $V_{eff}(\mathbf{r},\mathbf{r}')$ should take in the continuum description in order to maintain operator equivalence with the tight-binding Hamiltonian in the presence of an interaction potential $V(\mathbf{r},\mathbf{r}')$. To lowest order we find the natural answer: that $V_{eff}(\mathbf{r},\mathbf{r}') = \mathbf{V}(\mathbf{r},\mathbf{r}')$ but also that this is sufficient only in the case that $V(\mathbf{r},\mathbf{r}')$ does not change on the scale of the lattice constant. Taking the example of graphene we derive the corrections to the lowest order result for the case of the Coulomb interaction.

[1] N. Ray et al., arXiv preprint arXiv:1607.00920, 2016

TT 13.8 Mon 12:15 MA 043

Optical deformations in graphene — •Reena Gupta and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Deformations in graphene slow on the scale of the lattice constant are, at lowest order, very well described by the addition of a pseudo-magnetic gauge field to the Dirac-Weyl equation [1]. Here we explore what happens when we consider slow deformations but of both possible modes that the two-atom unit cell allows, i.e., optical as well as acoustic modes. While the acoustic mode simply reproduces the well-known pseudo-magnetic gauge field, the optical mode generates both a chiral field as well as an imaginary magnetic gauge, with Hermiticity of the Hamiltonian maintained by a position dependent velocity correction. We comment on the relevance of these results to hybrid metal/graphene systems which feature strong deformation.

[1] B. Amorim et al., Physics Reports 617, 1 (2016).

TT 13.9 Mon 12:30 MA 043

Moiré ordered current loops in the graphene twist bilayer — •Dominik Weckbecker and Sam Shallcross — FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany

Moiré lattices in layered two dimensional materials possess, in the presence of a magnetic field of 1-5 Tesla, comparable structural and magnetic length scales and, as a consequence, exhibit remarkable magnetic field phenomena such as the recently observed Hofstadter butterfly [1,2].

In this contribution, we present the results of our simulations on twisted bilayer graphene nanoribbons, which were conducted using a semi-empirical tight-binding method [3].

We report novel phenomena arising from this interplay of length scales in the form of an ordered array of permanent current loops throughout a moiré generated by twisting graphene layers [3,4]. Strikingly, these current loops are found at significantly weaker fields than those required to observe the Hofstadter butterfly, and such current loops thus represent an additional low field imprint of the moiré lattice on Landau physics, and an unusual situation in which the field induced currents are found in the bulk of a material.

[1] D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976)
[2] C. R. Dean et al. , Nature 497, 598-602 (2013)
[3] W. Landgraf et al., Phys. Rev. B. 87, 075433 (2013)
[4] manuscript in preparation

TT 13.10 Mon 12:45 MA 043

A novel delocalized phase in the small angle graphene twist bilayer — •Maximilian Fleischmann, Reena Gupta, Dominik Weckbecker, and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

In this work we demonstrate that the small angle limit of the graphene twist bilayer contains, in addition to its well known localized phase [1], a novel delocalized phase accessible by applied interlayer bias. This phase differs profoundly from the large angle delocalized phase as, in contrast to the almost perfectly circular Fermi surface found at large angles, one finds almost perfectly linear Fermi lines. These may be translated into each other by a so-called nesting vector, the magnitude of which is controllable by the applied field. The finding of a phase in the twist bilayer consisting solely of one dimensional Fermi lines connected by field tunable nesting vectors, marks this system out as an unexpected playground for the study of nested Fermiology and electronic instabilities.

[1] D. Weckbecker et al., Phys. Rev. B **93**, 035452, 2016.

TT 13.11 Mon 13:00 MA 043

Electronic and geometric structure of PTCDA films adsorbed on Graphene passivated Ni(111) — •Dominik Jungkenn[1], Johannes Seidel[1], Florian Haag[1,2], Leah L. Kelly[1], Mirko Cinchetti[3], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, Erwin-Schrödinger-Str 46, 67663 Kaiserslautern — [2]Graduate School of Excellence Materials Science in Mainz, Erwin Schroedinger Straße 46, 67663 Kaiserslautern — [3]Experimentelle Physik VI, Technische Universität Dortmund, 44221 Dortmund

Organic molecules are highly intriguing materials for spintronics due to their wide range of functionalities. However, to take full advantage of these functionalities, ferromagnetic surfaces have to be passivated , either by an organic buffer layer or by an inert 2D material [1]. Along these lines, we have investigated the geometric and electronic structure as well as the hot electron dynamics of a PTCDA monolayer on a Graphene (Gr) passivated Ni(111) surface. We find the formation of long-range ordered PTCDA monolayer films on Gr/Ni(111) resembling the herringbone structure of PTCDA/Ag(111). The frontier molecular states reveal the orbital emission pattern of unperturbed PTCDA molecules suggesting, as expected, a weak coupling of the molecular layer to the Graphene sheet. [1] Cinchetti et al. Nat. Mater. 16, 507 (2017)

TT 14: Frontiers of Electronic-Structure Theory: Correlated Electron Materials I (joint session O/MM/DS/TT/CPP)

Exploring, understanding, and describing materials with strong electronic Coulomb correlations remain among the big challenges of modern condensed matter physics. Correlated materials are characterized by an extreme sensitivity to external probes such as pressure or temperature, and slight changes in composition, constraints during the growth process (e.g. by heterostructuring) or off-stoechiometries can significantly alter their properties. While the invited lectures will have a focus on correlated electron materials, the symposium will cover the general field of computational materials science and electronic-structure theory.

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Time: Monday 10:30–13:00 Location: HL 001

TT 14.1 Mon 10:30 HL 001

How Derivative Discontinuities in the Energy Yield Interatomic Steps in the Exact Kohn-Sham Potential of Density-Functional Theory — •Eli Kraisler[1], Matthew J. P. Hodgson[1], Axel Schild[2], and Eberhard K.U. Gross[1,3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [2]Laboratorium für Physikalische Chemie, ETH Zürich, Switzerland — [3]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Israel

Accurate density-functional calculations hinge on reliable approximations to the unknown exchange-correlation (xc) potential. The most popular approximations usually lack features of the exact xc potential that are important for an accurate prediction of the fundamental gap and the distribution of charge in complex systems. Two principal features in this regard are the spatially uniform shift in the potential, as the number of electrons infinitesimally surpasses an integer, and the spatial steps that form, e.g., between the atoms of stretched molecules. Although both aforementioned concepts are well-known, the exact relationship between them remained unclear. In this talk, we establish this relationship and introduce a new concept: the charge-transfer derivative discontinuity, Δ^{CT}. By numerically solving the many-electron Schrödinger equation, we extract the exact Kohn-Sham potential and directly observe its features, particularly the spatial interatomic steps. For the first time, spatial steps in the exact xc potential of a full configuration-interaction (FCI) calculation of a molecule are presented in three dimensions.

TT 14.2 Mon 10:45 HL 001

Steps in the exact Kohn-Sham potential of ensemble density-functional theory for excited states and their relation to the derivative discontinuity — •Matthew J. P. Hodgson[1], Eli Kraisler[1], Michael T. Entwistle[2], Axel Schild[3], and Eberhard K. U. Gross[1,4] — [1]MPI für Mikrostrukturphysik, D-06120 Halle, Germany — [2]Dep. of Physics, Uni. of York, Heslington, YO10 5DD, UK — [3]Lab. für Physikalische Chemie, ETH Zürich, 8093, Switzerland — [4]Fritz Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, 91904, Israel

An accurate approximation to the exchange-correlation (xc) part of the Kohn-Sham (KS) potential is essential for any density-functional calculation. Understanding the behaviour of the exact xc potential and developing improved approximations to it are crucial. The focus of calculations within density functional theory is usually on the ground state. However, knowledge of how the system responds to an excitation is important. In this talk we present the exact KS potential of an ensemble of the ground state and the first excited state of a 1D diatomic molecule. For this system, upon excitation, a small amount of charge transfers from one atom to the other. In the corresponding exact ensemble xc potential we find two plateaus: one that forms around the nucleus of the acceptor atom, associated with the derivative discontinuity of that atom, and another that forms around the donor atom and corresponds to a new phenomenon which we term the 'charge-transfer derivative discontinuity'.

TT 14.3 Mon 11:00 HL 001

Koopmans-compliant functionals: A reliable and efficient tool for the prediction of spectroscopic quantities — •Nicola Colonna[1], Ngoc Linh Nguyen[1], Andrea Ferretti[2], and Nicola Marzari[1] — [1]THEOS and MARVEL, EPFL, Lausanne, Switzerland — [2]Centro S3, CNR-Istituto Nanoscienze, Modena, Italy

Commonly used approximate density functionals produce total energies that do not exhibit the expected piecewise-linear behavior as a function of the particle number, leading to a discrepancy between total and partial electron removal/addition energies and poor predictive capabilities of ionization potentials. Koopmans-compliant functionals enforce a generalized criterion of piecewise linearity in the energy of any approximate density functional with respect to the partial removal/addition of an electron - i.e., with respect to charged excitations - from/to any orbital of the system. When used to purify approximate density functionals, Koopmans' corrections lead to orbital-density dependent functionals and potentials that are able to deliver accurate spectroscopic properties. As an example, ionization potentials of a large set of molecules (the GW100 test set), photoemission spectra of organic donors and acceptors and band gaps of 35 semiconductors and insulators are presented, showing very good agreement with experiment or higher-order theories. Being this a functional framework, the straightforward advantages are that forces and other derivatives are also readily accessible, that the computational costs are much reduced, and the numerical parameters are those typical of DFT calculations.

TT 14.4 Mon 11:15 HL 001

Selfconsitent density embedding - a new class of functionals for DFT — •Uliana Mordovina[1], Teresa E. Reinhard[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

We propose a new technique to find functionals for density functional theory (DFT) in an ab-initio fashion. This technique origins in the recently developed density-matrix embedding theory (DMET) [1]. DMET is a quantum-in-quantum embedding method, which is based on finding a projection between the high-dimensional wave function of the full system and a lower-dimensional wavefunction living in the active space of the embedded system, which is then solved exactly. In the original DMET scope, the projection is improved via optimization of the reduced one-body density matrix. We replace this optimization by a density inversion, exploiting the one-to-one mapping between electronic density and Kohn-Sham potential.

The proposed density-embedding scheme serves as functional in DFT, which, unlike in usual DFT, can be systematically improved by increasing the size of the active space.

We show convergence toward exact results for 1D systems as well as results for 2D systems.

[1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012)

TT 14.5 Mon 11:30 HL 001

Pressure dependence of the effective screened Coulomb interactions in transition metal monoxides — •Swarup Kumar Panda[1], Hong Jiang[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, France — [2]College of Chemistry and Molecular Engineering, Peking University, China — [3]Collège de France, Paris, France

In transition metal compounds, the magnitudes of the effective Coulomb interaction parameters (Hubbard U) and their pressure dependence are of utmost importance in any realistic many-body simulations for describing their pressure driven insulator-metal transition. One of the powerful methods for calculating the Hubbard U from first

principles is based on linear response theory within the constrained random-phase approximation (cRPA) [1], which provides the full U matrix including off-site elements and its frequency dependence. In this presentation, we apply this method (in its implementation into the Wien2k code [2]) to the transition metal monoxides (FeO, CoO, NiO, and CuO) [3]. Although the pressure induced changes in the bare Coulomb interactions are negligible, the effective screened U grows monotonically with increasing pressure for all of the above monoxides. Finally, I will argue that neither the pressure dependence nor the frequency dependence of U should be ignored in a reliable theoretical description of correlated oxides.

References: [1] Aryasetiawan et al., PRB 70, 195104 (2004) [2] Vaugier et al., PRB 86, 165105 (2012) [3] Panda et al., PRB 96, 045137 (2017)

TT 14.6 Mon 11:45 HL 001

Self-Interaction Corrected SCAN for Molecules: All-Electron Implementation with Numerical Atom-Centered Basis Functions — •Sheng Bi, Igor Ying Zhang, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The self-interaction error (SIE) is a well-known problem in all semilocal density-functional approximations (DFAs), including the recently proposed "strongly constrained and appropriately normed" (SCAN) functional [1]. The so-called self-consistent Fermi-orbital SIC (FSIC) algorithm proposed by Pederson *et al.* [2] shows promising potential to eliminate the self-interaction error in semilocal approximations, which has been demonstrated for the local-spin-density approximation (LSDA) in a study of molecules.

We present an all-electron implementation of the self-consistent FSIC approach on the SCAN method [1]. Beside a systematic benchmark with respect to a selected molecular test set, we examine the performance of FSIC-SCAN in predicting the geometry of Pentacene, which is a well-documented challenge for standard semilocal DFAs [3]. Finally, we briefly discuss our ongoing work concerned with the implementation of the all-electron FSIC-SCAN approach for solids.

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew, *Phys. Rev. Lett.* **115**, 036402 (2015).
[2] M. R. Pederson and T. Baruah, *Advances In Atomic, Molecular, and Optical Physics* **64**, 153 (2015).
[3] M. R. Pederson, T. Baruah, D. you Kao, and L. Basurto, *The Journal of Chemical Physics* **144**, 164117 (2016).

TT 14.7 Mon 12:00 HL 001

Progress in Fermi-Löwdin orbital self-interaction correction to DFT — •Torsten Hahn[1], Sebastian Schwalbe[1], Simon Liebing[1], Mark Pederson[2], and Jens Kortus[1] — [1]TU Freiberg, Institute for Theoretical Physics, Germany — [2]Johns Hopkins University, Department of Chemistry, USA

The accuracy of density functional theory (DFT) calculations is limited by the so called self-interaction error [1]. The recently proposed Fermi-Löwdin orbital based method [2,3,4] for self-interaction correction (FLO-SIC) is a unitary invariant and size extensive approach to overcome this error. We present the current state of the method and discuss the performance of FLO-SIC DFT applied to atoms and molecules in combination with different exchange-correlation functionals. In addition, this method delivers a description of the chemical bonding as intuitive as Lewis theory that may bridge the gap between DFT and chemical intuition.

[1] J. P. Perdew, A. Zunger, Phys. Rev. B 23, 5048 (1981)
[2] M. R. Pederson et al., J. Chem. Phys., vol. 140, 121103 (2014)
[3] M. R. Pederson, J. Chem. Phys., vol. 142, 064112 (2015)
[4] T. Hahn et. al., J. Chem. Phys., vol- 143, 224104 (2015)

TT 14.8 Mon 12:15 HL 001

First-principles modeling of mixed-valence compounds from extended Hubbard-corrected functionals — •Matteo Cococcioni and Nicola Marzari — Theory and Simulations of Materials and MARVEL, EPFL, Lausanne, Switzerland

Modeling the electronic properties of mixed valence compounds is central to developing many materials of technological relevance. Unfortunately, most approximate implementations of density functional theory (DFT) fail in capturing the localization of valence electrons on low dispersion states (e.g., of d or f kind) and mis-represent many properties of these systems. Quantitatively predictive first-principles calculations thus require, for these systems, the use of corrective functionals able to improve the description of electronic localization. Using the results of a recent study on materials for cathodes of Li-ion batteries this work shows how an extended Hubbard correction to DFT functionals, including on-site (U) and inter-site (V) interactions (named DFT+U+V) improves considerably on simpler approximations for electronic, magnetic and structural properties and correctly describes localized states even in presence of significant inter-site hybridization. The work also demonstrates that evaluating the effective interaction parameters (U and V) consistently with the electronic and crystal structures, and treating them as material-specific quantities, improves the prediction of thermodynamic quantities and of average voltages. Finally, a novel method to compute these interactions from density-functional perturbation theory is shown to guarantee unprecedented efficiency, accuracy and convergence control.

TT 14.9 Mon 12:30 HL 001

A Kohn-Sham type construction on a lattice with the exact kinetic energy density — •Iris Theophilou[1], Michael Ruggenthaler[1], Florian Buchholz[1], Florian Eich[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In this presentation we explore a possible formulation of ground state Density Functional Theory by introducing the kinetic energy density as basic quantity in addition to the density. We presently restrict this formulation to the lattice case, and show that for a few site Hubbard interacting model it is numerically feasible to find an equivalent non-interacting system that yields the same density and kinetic energy density. By finding such a non-interacting system we mean here finding the local/on site potential and the non-local site dependent hopping that will give the target density and kinetic energy density. Our hope is that by including the kinetic energy density we will facilitate the functional construction and also put into grounds already existing approximations based on this quantity.

TT 14.10 Mon 12:45 HL 001

Small-Polaron Formation in Polymorphs of Ga_2O_3 and TiO_2 — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin 14195, Germany

Transparent oxides are key materials for new devices in photovoltaics and electronics. One important factor influencing the behavior of charge carriers in these materials is the interaction with polar phonon modes. We focus on materials with strong electron-phonon coupling, where small polarons are formed. Although, density-functional theory (DFT) is often used for calculating polaron properties, there are two challenges: Sensitivity of the calculated properties to the errors in exchange-correlation treatment, and finite-size effects in supercell calculations. We have developed an approach [1] to address these issues. The polaron properties are obtained using a modified neutral potential-energy surface from DFT [2]. Based on Pekar′s model [3], we correct for the proper elastic long-range behavior of the polaron in a supercell. With this approach, the influence of the crystal structure on the polaron properties is investigated for rutile and anatase TiO_2, and for the monoclinic β– and orthorhombic ε–Ga_2O_3. We find that in rutile TiO_2 only small electron polarons are stable, while only small hole polarons are found in anatase. On the contrary, small hole polarons exist in both Ga_2O_3 polymorphs but have significantly different binding energies.

[1] S. Kokott, arXiv:1710.03722 (2017)
[2] B. Sadigh et al., Phys. Rev. B **92**, 75202 (2015)
[3] S. I. Pekar, Zh. Eksp. Teor. Fiz. **16** 335 (1946)

TT 15: Dual-Method Approaches to Quantum Many-Body Systems I

To make an impact on possible applications, theoretical approaches for correlated many-body systems must allow for studying more realistic models and lead to more accurate predictions as compared to what is achievable nowadays. This requires, on the one hand, the development of specialized tools which are mathematically and/or algorithmically demanding. On the other hand, an emergent promising approach to make significant progress beyond toy-model understanding of many-body physics is the combined use of two or more complementary methods. The demand for such type of approaches is growing. The two session of contributed talks will provide an overview of recent successes in such dual-(multi-)method approaches involving analytical as well as numerical tools, and will indicate prospects for future directions.

Compilation: Volker Meden, RWTH Aachen; Stefan Wessel, RWTH Aachen

Time: Monday 15:00–18:45 Location: H 0104

TT 15.1 Mon 15:00 H 0104

Combining diagrammatic Monte-Carlo with large-N field theory — •Gunnar Möller — School of Physical Sciences, University of Kent, Canterbury, UK

We explore a new avenue for quantitative investigations of strongly interacting systems by combining large-N fermionic theories with stochastic sampling of high order Feynman graphs.

Our work focuses on the unitary Fermi gas as a blueprint example for a strongly interacting system of fermions without a small expansion parameter in the Hamiltonian. The unitary Fermi gas is realised experimentally in cold atomic gases of two-species fermions interacting via a Feshbach resonance [1]. Previous work has established a diagrammatic Monte-Carlo (diagMC) approach [2] but it has left uncertainties about the convergence properties of the interaction expansion [3,4]. Here, we re-examine the problem by introducing a small parameter via a large-N generalisation [5,6], to which we then apply diagMC. Formally, this yields an expansion around the mean-field superconducting theory, whose properties are recovered in the $N \to \infty$ limit. We benchmark the approach by examining density distributions and the contact parameter against prior approaches.

[1] W. Zwerger, Springer (2012).
[2] Van Houcke, K. et al., Nat Phys 8, 366 (2012); and arXiv:1305.3901 (2013).
[3] Kozik, E., Ferrero & Georges, PRL 114, 156402 (2015)
[4] Rossi, R., Werner, F., Prokof'ev, N. V. & Svistunov, B., Phys. Rev. B 93, 161102 (2016).
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[6] Nikolić, P. & Sachdev, S. Phys. Rev. A 75, 033608 (2007).

TT 15.2 Mon 15:15 H 0104

Parquet equations for the 2D Hubbard model using channel decomposition — •Christian Eckhardt[1], Giulio Schober[1], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [2]JARA-FIT, Jülich Aachen Research Alliance - Fundamentals of Future Information Technology, Germany

The parquet equations are a set of self consistent equations for the effective interaction vertex of an interacting many-fermion system. The application of the parquet equations in bulk models is, however, complicated by the complex emergent momentum and frequency structure of the vertex. Here we show how techniques for the treatment of the momentum dependence, that were developed in the context of the functional renormalization group, can be applied to the parquet equations. We present solutions using this technique for the half-filled Hubbard model on the square lattice and discuss ways to include the frequency dependence of the vertices.

TT 15.3 Mon 15:30 H 0104

New approach towards conceptual and numerical extensions of cluster dynamical mean-field theory — •Marcel Klett, Sabine Andergassen, and Philipp Hansmann — Institut für Theoretische Physik, Universität Tübingen, 72076 Tübingen

The dynamical mean-field theory (DMFT) provides the exact solution of a quantum many-body Hamiltonian in the limit of infinite spatial dimensions. The accurate (and non-perturbative) description of all local correlations allows to describe the Mott-Hubbard metal-to-insulator transition in three-dimensional bulk systems. At the same time, the mean-field nature with respect to the spatial degrees of freedom implies that all non-local spatial correlation effects are neglected in DMFT. These can be included in cluster extensions which have been introduced both in real and momentum space [1,2]. Here we propose an idea to improve upon typical re-periodization problems of real space cluster DMFT and discuss the transformation of the Hubbard model between lattice orbital and so-called ligand orbital basis sets.

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TT 15.4 Mon 15:45 H 0104

Functional RG investigation of the antiferromagnetic phase diagram of the three dimensional Hubbard model — •Jannis Ehrlich[1,2], Carsten Honerkamp[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany

The phase diagram of the three dimensional Hubbard model shows a phase transition to an antiferromagnetic ground state for repulsive interactions. While the Néel temperature can be obtained by Hartree Fock and the Heisenberg model for the limit of weak and strong interactions respectively, the intermediate range of interactions is subject of recent investigations.

We use the recently developed truncated unity functional renormalization group (TUfRG) approach, which has been used successfully to study the phase diagram of the extended 2D Hubbard model. This approach enables us to study this model on a fine momentum grid in an unbiased form, i.e. including the particle-particle and both particle-hole channels. We compare the resulting Néel temperature curve to those from previous studies using DΓA, DCA, QMC and dual fermion approaches.

TT 15.5 Mon 16:00 H 0104

A nonequilibrium DMFT+FLEX formalism for dynamics of d-wave superconductivity — •Sharareh Sayyad[1], Naoto Tsuji[2], Abolhassan Vaezi[3], Massimo Capone[4,5], Martin Eckstein[6], and Hideo Aoki[7,8,9] — [1]Institute for Solid State Physics, University of Tokyo, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan — [2]RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan — [3]Department of Physics, Stanford University, Stanford, CA 94305, USA — [4]International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy — [5]CNR-IOM Democritos, Via Bonomea 265, I-34136 Trieste, Italy — [6]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany — [7]Department of Physics, ETH Zürich, 8093 Zürich, Switzerland — [8]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8568, Japan — [9]Department of Physics, University of Tokyo, Tokyo 113-0033,Japan

For studying nonequilibrium dynamics of d-wave superconductors, we have constructed a nonequilibrium DMFT+FLEX method with a novel full-SU(2) slave-boson impurity-solver. An advantage of the method is that it can treat multiple phases on an equal footing for the Hubbard model on bipartite lattices. With the method, we expect to deal with the competition between antiferromagnetic and superconducting phases and to shed some light on the pseudogap physics with a slave-particle decomposition.

TT 15.6 Mon 16:15 H 0104

Lattice susceptibility calculations via a generalized CT-Hyb

QMC DMFT solver — •Julian Musshoff[1,2], Amin Kiani[1], and Eva Pavarini[1,3] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]JARA-HPC, RWTH Aachen University, Aachen, Germany

Linear-response functions are essential for comparing theory to experiments, and yet for strongly correlated systems their calculation is very challenging. The state-of-the-art technique for real materials is based on the dynamical mean-field (DMFT) approach and the local-vertex approximation. The bottleneck of this method is the calculation of local susceptibilities. Here we present an efficient scheme based on the massively-parallel general implementation of the continuous-time quantum Monte Carlo impurity solver of Ref. [1]. We use both the Legendre polynomial representation and a recently proposed numerical basis [2], and compare efficiency. To calculate lattice susceptibilities we solve the Bethe-Salpeter equation. We present results for the static and dynamical response functions of representative systems: $La_{2-x}Sr_xCuO_4$ and several orbitally ordered materials.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, Phys. Rev. B **87**, (2013) 195141
[2] H. Shinaoka, J. Otsuki, M. Ohzeki, K. Yoshimi, Phys. Rev. B **96**, (2017) 035147

TT 15.7 Mon 16:30 H 0104

Effective models for correlated systems: effects of basis orthogonalization — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Setting up a many-body Hamiltonian requires choosing an orbital basis. Starting from atomic orbitals we have to deal with the non-orthogonality of the basis functions on different sites. We demonstrate the effects arising from orthogonalization on the example of the Hubbard dimer. First we study the change in hopping matrix elements with the bond length for the hydrogen molecule ion. Then we analyze the change in Coulomb matrix elements for the hydrogen molecule. In particular, we investigate how orthogonalization changes the on-site interaction as well as the direct and the exchange contributions to the long-range Coulomb terms. Finally, we discuss how the Coulomb tensor transforms under general (i.e. non-unitary) basis changes.

15 min. break.

TT 15.8 Mon 17:00 H 0104

Non-equilibrium dynamics of correlated materials: perturbation theory approach. — •Viktor Valmispild[1,2], Evgeny Gorelov[3], Nagamalleswara Dasari[4], Martin Eckstein[4], and Alexander Lichtenstein[1,2] — [1]Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [4]Department of Physics, University of Erlangen-Nurnberg, 91058 Erlangen, Germany

We study the single-band Hubbard model on a infnite-dimensional and finite 2D square lattices in the presence of a large spatially uniform electric field. We study the model out of equilibrium using the Keldysh formalism and perturbation theory in the Coulomb interaction U. *Thus using time dependent dynamical mean-field theory and different impurity solvers: second order perturbation theory (SOPT) and fluctuation exchange approximation (FLEX) we investigate the behavior of the total energy of the system, double occupancy and spectral function as a function of time, strength of an external electric field and on-site Coulomb repulsion U.

TT 15.9 Mon 17:15 H 0104

Logarithmic corrections to the dynamical correlation functions of one-dimensional fermion systems with impurities — •Polina Matveeva[1], Dominik Strassel[1,2], Sebastian Eggert[1], and Imke Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [2]Competence Center for High Performance Computing, Fraunhofer ITWM, 67663 Kaiserslautern, Germany

Dynamical correlation functions are central objects in neutron scattering and photoemission spectroscopy experiments. They provide us with important information about the interactions and the spectrum of elementary excitations in strongly correlated systems. In one-dimensional gapless systems the correlation functions decay like power laws, with multiplicative logarithmic corrections from marginal operators. We study this corrections for general one-dimensional electron systems and the Heisenberg spin chain in the presence of impurities using bosonization. We obtain different multiplicative logarithmic corrections for the correlation functions in the boundary and bulk limits. Our results are supplemented by numerical Quantum Monte Carlo data. Finally, we discuss implications on the local density of states in the 1D-Hubbard model where previous numerical results revealed unexpectedly strong finite size corrections due to the marginal operator in the spin channel.

TT 15.10 Mon 17:30 H 0104

The dynamic structure factor in impurity-doped spin chains — •Kevin Jägering[1], Annabelle Bohrdt[2], Sebastian Eggert[1], and Imke Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [2]Department of physics and Institute for Advanced Study, Technische Universität München, 85748 Garching, Germany

The effects of impurities in spin-1/2 Heisenberg chains are recently experiencing a renewed interest due to experimental realizations in solid state systems and ultra-cold gases. The impurities effectively cut the chains into finite segments with a discrete spectrum and characteristic correlations, which have a distinct effect on the dynamic structure factor. Using bosonization and the numerical Density Matrix Renormalization Group we provide detailed quantitative predictions for the momentum and energy resolved structure factor in doped systems. Due to the impurities, spectral weight is shifted away from the antiferromagnetic wave-vector $k = \pi$ into regions which normally have no spectral weight in the thermodynamic limit. The effect can be quantitatively described in terms of scaling functions, which are derived from a recurrence relation based on bosonization. We present length-averaged and kintegrated results in terms of the doping concentration.

TT 15.11 Mon 17:45 H 0104

Influence of phonon-assisted tunneling on the thermoelectric transport through molecular quantum dots — •Andisheh Khedri[1,2], Theo Costi[2], and Volker Meden[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA–Fundamentals of Future Information Technology, 52056 Aachen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Research Center Jülich, 52425 Jülich, Germany

We investigate the effect of vibrational degrees of freedom on the thermoelectric transport through a single level quantum dot described by the spinless Anderson-Holstein impurity model. To study the effects of strong electron-phonon coupling in the linear response regime, we use the nonperturbative numerical renormalization group approach. We also compare our results, at weak to intermediate coupling, with those obtained by employing the functional renormalization group method, finding good agreement in this parameter regime. When applying a gate voltage at finite temperatures, the inelastic scattering processes, induced by phonon-assisted tunneling, result in an interesting interplay between electrical and thermal transport. We explore different parameter regimes and identify situations for which the thermoelectric power as well as the dimensionless figure of merit are significantly enhanced. By applying the functional renormalization group on the Keldysh contour, we further study the nonlinear thermoelectric transport in scenarios, in which the vibrating molecule is coupled to reservoirs held at different temperatures and chemical potentials.

TT 15.12 Mon 18:00 H 0104

Functional Renormalization Group Approach to Transport through a Kondo Quantum Dot — •Jan Diekmann and Severin G. Jakobs — Institute for Theory of Statistical Physics, RWTH Aachen University, 52056 Aachen, Germany

We study nonequilibrium properties of the Kondo model. For this we use the 1PI functional renormalization group (fRG), and work in Keldysh formalism. We choose a drone-fermion representation for the impurity spin.

As a first step we reproduce the leading logarithmic approximation in the weak-coupling regime ($T \gg T_K$) known as Poor Man's Scaling (PMS), which is an equilibrium result. Within fRG the employed approximation scheme emerges in a very natural way, and a clear interpretation of the flowing quantities is given as amplitudes of the renormalized 1PI vertex functions.

We devise a more sophisticated fRG approximation scheme as a direct extension of the one used to reproduce the PMS result. In particular we take frequency dependence and the self energy of the spin back

into account. With this we seek to describe the nonequilibrium case and to check whether the approach is suitable to describe the crossover to the strong-coupling regime.

A long term goal is to investigate the relation between different RG approaches to the nonequilibrium Kondo problem.

TT 15.13 Mon 18:15 H 0104

New hierarchical quantum master equation approach based on an interaction expansion: A first implementation for an Anderson impurity — •Jakob Bätge[1,2] and Rainer Härtle[1,2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen — [2]Institute of Physics, University of Freiburg

The description of transport through open quantum systems is important for the quantum information processing or molecular electronics. Physical systems of interest are, for example, several coupled qubits or the voltage profile along a molecule. As the amount of possible states of quantum systems increases exponentially with the number of degrees of freedom, the numerical effort for exact techniques typically increases exponentially with system size. The exact treatment of large systems might open the view on new physical effects. The numerically exact hierarchical quantum master equation approach (HQME)[1-3] is based on a systematically improvable hybridization expansion and predicts the time-evolution of the quantum system. Due to its time-local formulation stationary state properties can be studied. Here we present an extension of the HQME, which includes an additional expansion in the many-body interaction. The new approach focuses on the low-particle reduced density matrices and hence shows a power law dependence on system size. The newly extended HQME is still a numerically exact approach. A first implementation for the well studied Anderson impurity model shows the usefulness of the new method.

[1] J. Jin *et al.*, JCP **128**, 234703 (2008)
[2] R. Härtle *et al.*, PRB **88**, 235426 (2013)
[3] R. Härtle *et al.*, PRB **92**, 085430 (2015)

TT 15.14 Mon 18:30 H 0104

Auxiliary master equation approach within stochastic wave functions — •Delia Fugger, Max Sorantin, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, Austria

The auxiliary master equation approach AMEA [1,2] allows us to assess the time evolution and, in particular, the steady state properties of quantum impurities and small molecules in as well as out of equilibrium. It is based on a mapping of the physical system to an auxiliary open quantum system, whose dynamics is determined by a Lindblad master equation. In this talk I will present results obtained from a scheme to address the resulting Lindblad equation based on the stochastic evolution of the wave function [3-6]. A set of wave functions sampling the density operator is propagated by piecewise deterministic time evolutions, which are interrupted by stochastic jump processes [6]. This implementation aims at extending the capabilities of the AMEA approach as well as making it more efficient.

[1] E. Arrigoni *etal.*, PRL **110**, 086403 (2013)
[2] A. Dorda *etal.*, PRB **89**, 165105 (2014) + PRB **92**, 125145 (2015)
[3] J. Dalibard *etal.*, PRL **68**, 580 (1992)
[4] K. Mølmer *etal.*, J. Opt. Soc. Am. B **10**, 524 (1993)
[5] H.-P. Breuer *etal.*, PRA **56**, 2334 (1997)
[6] B. Kappler, PhD thesis, University of Freiburg (1998)

TT 16: Superconductivity: Properties and Electronic Structure II

Time: Monday 15:00–17:30 Location: H 0110

TT 16.1 Mon 15:00 H 0110

Resistivity in the Vicinity of a Van Hove Singularity: Sr_2RuO_4 Under Uniaxial Pressure — •Mark E. Barber[1,2], Alexandra S. Gibbs[2,3], Yoshiteru Maeno[4], Andrew P. Mackenzie[1,2], and Clifford W. Hicks[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance (SUPA), University of St. Andrews, United Kingdom — [3]ISIS Facility, Rutherford Appleton Laboratory, United Kingdom — [4]Department of Physics, Kyoto University, Japan

Sr_2RuO_4 is an unconventional superconductor with a well characterised Fermi liquid normal state. One of its three conduction bands is known to be in close proximity to a Van Hove singularity. We have previously shown that the application of uniaxial pressure causes T_c to pass through a strong peak at a uniaxial compression of 0.6 %, and at which T_c is more than double its value in the unstrained lattice. DFT calculations provide strong evidence that this peak coincides with tuning the Van Hove singularity to the Fermi level. Here, we present data on the normal-state resistivity as Sr_2RuO_4 is tuned through this peak and analyse the temperature dependence, which also appears to be consistent with a Van Hove singularity. In particular, the low-temperature resistivity also passes through a pronounced peak - arguably a surprise because the singularity affects only small sections of one Fermi surface - and at the peak its temperature dependence deviates strongly from the Fermi liquid T^2 dependence.

TT 16.2 Mon 15:15 H 0110

Muon spin relaxation studies of Sr_2RuO_4 under uniaxial pressure — •Shreenanda Ghosh[1], Rajib Sarkar[1], Vadim Grinenko[1], Jean-Christophe Orain[2], Hubertus Luetkens[2], Joonbum Park[3], Clifford Hicks[3], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland — [3]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We present transverse field muon spin relaxation data on the unconventional superconductor Sr_2RuO_4 under uni axial pressure. Results from previous μSR studies on unstressed Sr_2RuO_4 indicate a spontaneous magnetization in the superconducting state [1], that has been associated with a time reversal symmetry breaking order parameter, $p_x \pm ip_y$. The superconducting T_c of Sr_2RuO_4 has been shown experimentally to be sensitive to uni axial pressure [2], so for more information about the complex superconducting order parameter, we investigate pressurized Sr_2RuO_4 by μSR. For this purpose, we have developed a dedicated device, which offers in situ uni axial strain tuning via piezoelectric stacks.[5]

[1] G.M.Luke et al., Nature, 394, 558 (1998).
[2] J.R.Kirtley et al., Phys.Rev.B, 76, 014526 (2007).
[3] C.W.Hicks et al., Science, 344, 283 (2014)
[4] Steppke et al. Science 355,6321(2017)
[5] C.Hicks et al.accepted in Conference proceedings of μSR 2017

TT 16.3 Mon 15:30 H 0110

Heat Capacity Measurements of Sr_2RuO_4 Under Uniaxial Stress — •You-Sheng Li[1,2], Alexandra Gibbs[3], Naoki Kikugawa[5], Dmitry Sokolov[1], Yoshiteru Maeno[4], Andrew P. Mackenzie[1,2], Clifford W. Hicks[1], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St. Andrews, School of Physics and Astronomy, United Kingdom — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan — [5]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba, Ibaraki 305-0003, Japan

We present heat capacity measurements on the superconductor Sr_2RuO_4 under uniaxial stress. Under uniaxial stress, the degeneracy of the components p_x and p_y of the proposed superconducting order parameter $p_x \pm ip_y$ should be lifted, resulting in two heat capacity jumps. We have now measured four samples of varying quality, including one where, thanks to high sample quality and careful mounting, the transitions remain very sharp as strain is applied. In measurements up to the peak in Tc (at 3.6 K and a compression of 0.6%), no splitting is observed at any strain. We discuss whether this null result can still be consistent with a hypothesis of $p_x \pm ip_y$ superconductivity.

TT 16.4 Mon 15:45 H 0110

Mixed-pairing superconductivity in $5d$ Mott insulators with antisymmetric exchange — Mohammad-Hossein Zare[1], Mehdi Biderang[2], and •Alireza Akbari[2] — [1]Department of Physics, Qom University of Technology, Qom, Iran — [2]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea

Currently, remarkable attentions have been attracted to exotic physics

driven by the interplay of the spin-orbit coupling and electronic correlations. Particularly, in 5d transition metals, neither the spin-orbit coupling nor the Coulomb interaction can merely lead to the insulating behavior. We study the symmetry of the potential superconducting order parameter in $5d$ Mott insulators with an eye to hole doped Sr_2IrO_4. Using a mean-field method, a mixed singlet-triplet superconductivity, $d+p$, is observed due to the antisymmetric exchange originating from a quasi-spin-orbit-coupling. Our calculation of ribbon geometry shows possible existence of the topologically protected edge states, because of nodal structure of the superconducting gap. These edge modes are spin polarized and emerge as zero-energy flat bands, supporting symmetry protected Majorana state, verified by evaluation of winding number and $\mathbb{Z}_2$ topological invariant. At the end, a possible experimental approach for observation of these edge states and determination of the superconducting gap symmetry are discussed based on the quasi-particle interference (QPI) technique.
[1] Phys. Rev. B 96, 205156 (2017)

TT 16.5 Mon 16:00 H 0110

Vortex dynamics in driven Type-II Superconductor heterostructures — •Björn Niedzielski and Jamal Berakdar — Martin-Luther Universität Halle-Wittenberg, Halle, Germany

Superconductors exhibit a variety of intriguing phenomena in the presence of magnetic fields. For example, type-II Superconductors respond to an external field by generating vortices of magnetic flux. Our aim is to control the motion of these flux lines as well as to understand their nature in confined geometries and in the proximity of ferromagnetic or multiferroic order. Along this direction we will present simulations obtained from solving the time-dependent Ginzburg-Landau-Equations and discuss the behavior of the simulated systems. The role of material parameters, external magnetic fields and currents will be discussed. We will also show how the shape of the sample influences the dynamics of the superconducting order parameter.

15 min. break.

TT 16.6 Mon 16:30 H 0110

Experimental test of an alternative electrodynamic theory of superconductors by means of scanning tunnelling and force microscopy — Sungmin Kim[1,4], Johannes Schwenk[1,2], Julian Berwanger[3], •Angelo Peronio[3], Steven R. Blankenship[1], William G. Cullen[1], Young Kuk[4], Franz J. Giessibl[3], and Joseph A. Stroscio[1] — [1]NIST, Gaithersburg, Maryland — [2]University of Maryland, College Park, Maryland — [3]University of Regensburg, Germany — [4]Seoul National University, Korea

In the traditional theoretical description of superconductivity, a static electric field cannot penetrate a superconductor, since screening occurs like in a normal metal. This can be traced back to the fact that the London equations [1], the phenomenological equations describing the electrodynamics of superconductors, are derived within the Coulomb gauge. J. E. Hirsch proposes to use the Lorenz gauge instead [2], deriving a consistent solution where the electric field penetrates the superconductor up to the London penetration depth.

If a superconductor screens electric fields differently from a normal metal, the electrostatic interaction between a scanning probe tip and a superconductive sample should change when the latter becomes superconductive. We report on experiments to test Hirsch's hypothesis, performed on aluminium samples in a combined STM/AFM microscope operated in ultra-high vacuum at mK temperatures.
[1] F. London, Superfluids Vol. I, Wiley (1950)
[2] J. E. Hirsch, Physica C 508, 21 (2015)

TT 16.7 Mon 16:45 H 0110

Fabrication of electrospun BSCCO nanowire networks with reduced preparation temperature — •Michael Koblischka[1], XianLin Zeng[1], Fabian Laurent[1], Thomas Karwoth[1], Anjela Koblischka-Veneva[1], Uwe Hartmann[1], Crosby Chang[2], Thomas Hauet[2], Praveen Kumar[3], and Oliver Eibl[3] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Institut Jean Lamour, UMR CNRS-Université de Lorraine, 54506 Vandoevre-lès-Nancy, France — [3]Institute of Applied Physics, University of Tübingen, 72076 Tübingen, Germany

$Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) nanowire networks [1] were fabricated by electrospinning. A thermal treatment is required to obtain the final crystal structure, however, if the preparation temperature is too high, the nanowire structure may completely collapse. Therefore, Li acetate was added in various amounts to the starting composition. This enabled us to produce the desired Bi-2212 phase already at 750 °C instead of 840 °C. X-ray and TEM analysis proved that the resulting nanowires were single-phase Bi-2212. After electrospinning, the resulting samples form fabric-like networks, and the nanowire structure survived. The nanowires exhibit a polycrystalline structure with grain sizes of 20-50 nm, an average wire diameter of 100 nm and a length of up to several micrometers. The nanowire network samples were characterized by magnetic and electric measurements in fields up to 7 T. This work is part of DFG-project Ko2323/8.
[1] M.R.Koblischka et al., AIP Adv. 6, 035115 (2016).

TT 16.8 Mon 17:00 H 0110

Electrospun BSCCO donut-shaped superconducting rings — •XianLin Zeng, Fabian Laurent, Michael Koblischka, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany

By means of electrospinning, $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) nanowire networks were fabricated. Using the as-spun polymer nanowires, we were able to create donut-shaped superconducting rings via mechanical treatment. These samples were heat-treated at 840 °C to form the superconducting phase and to remove the polymer. On the donut-shaped nanowire samples, we performed magnetization measurements in a PPMS magnetometer in fields up to 7 T to investigate their behavior concerning trapping of magnetic fields and persistent currents flowing in the remanent state after application of magnetic fields. Using a Hall probe, we measured the local field, Bi, inside the rings at various temperatures and fields. Our results show that these donut-shaped rings can act as magnetic shields at low temperatures.

This work is part of DFG-project Ko2323/8.

TT 16.9 Mon 17:15 H 0110

Experimental evidences of a possible superconducting transition above room temperature in natural graphite crystals — •Christian Eike Precker[1], Pablo David Esquinazi[1], Markus Stiller[1], José Luis Barzola Quiquia[1], and Ana Melva Champi Farfan[2] — [1]Felix-Bloch-Institut, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany. — [2]CCNH, Universidade Federal do ABC, São Paulo, Brazil

By use of the four-terminal sensing method and high resolution electrical transport measurement, natural graphite samples from Brazil and Sri Lanka mines were measured. Temperature dependent resistance *R(T)* measurements shows a step-like transition at $T \sim 350$ K. Further experiments were performed, like magnetization and time dependence *R(T)* after a field change, showing a magnetic irreversibility, i.e. trapped flux and flux creep and partial magnetic flux expulsion. All before mentioned experimental results suggest the existence of granular superconductivity below 350 K. X-rays diffraction measurements proved the existence of rhombohedral graphite phase in all measured samples, suggesting the presence of interfaces formed between the rhombohedral and Bernal phase as responsible for the high-temperature superconductivity, as predicted by theoretical calculations. The measured remanence in the magnetoresistance is due to pinned fluxons produced through superconducting currents. The current path of a graphite sample in remanence state has been measured using magnetic force microscopy. The current path vanished at the same critical temperature measured with the resistance.

TT 17: Superconductivity: Qubits II

Time: Monday 15:00–17:00 Location: H 2053

TT 17.1 Mon 15:00 H 2053

Effective Evolution of a Driven Qubit Beyond the Rotating Wave Approximation — •Daniel Zeuch[1], Fabian Hassler[2], and David P. DiVincenzo[1,2] — [1]Peter Gruenberg Institut, Forschungszentrum Juelich, Juelich, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, Aachen, Germany

Decreasing the duration of quantum gates requires high-amplitude pulses. In the high-amplitude regime one needs to take into account effects beyond those captured by the rotating wave approximation. Such effects include rapid oscillations on the time scale of $1/\omega$, where ω is the qubit frequency, making it difficult to accurately describe the state evolution. For constant-amplitude pulses there is an effective Hamiltonian which describes shifts of the resonance frequency, known as the Bloch-Siegert shift [1], and of the Rabi frequency. For the case of time-dependent amplitudes of the order of the qubit frequency, we employ the Magnus expansion [2] to analytically determine an effective Hamiltonian which depends on time only through the amplitude. The time evolution due to our effective Hamiltonian is a family of rotating-frame trajectories, each of which agrees at periodic points in time with the actual state trajectory. We expect that using such effective Hamiltonians will reduce computational resources when designing pulse shapes.

[1] F. Bloch and A. Siegert, Physical Review **57**, 522 (1940).
[2] R. R. Ernst, G. Bodenhausen, A. Wokaun, Clarendon Press, Oxford (1987)

TT 17.2 Mon 15:15 H 2053

FPGA-based Quantum Feedback for Superconducting Qubits — •Richard Gebauer[1,2], Nick Karcher[1], Martin Weides[2], Oliver Sander[1], Alexey V. Ustinov[2], and Marc Weber[1] — [1]Institut für Prozessdatenverarbeitung und Elektronik, KIT — [2]Physikalisches Institut, KIT

A typical measurement setup for superconducting qubits consists of arbitrary waveform generators, signal recorders and vector network analyzers. Although sufficient for simple experiments, its applicability is limited due to long data communication delays, poor scalability and static pulse sequences. A faster and more flexible solution for qubit readout and control is FPGA-based custom hardware. It not only dramatically reduces costs and space requirements but also simplifies measurements and enables customized control schemes like quantum feedback where a low response time is critical.

We implemented an FPGA design for experiments with superconducting qubits which also enables fast feedback loops to control qubits depending on their measured state. Thus, it provides the basis for experiments and algorithms like quantum error correction or active reset. While typically the signal-to-noise ratio is improved by averaging, feedback loops require single shot measurements. Therefore, we employ a Josephson parametric amplifier with its superior noise characteristics. In the current state of development, we demonstrate arbitrary qubit rotations around X and Y axis. Furthermore, we can perform all standard measurements for qubit characterization using an FPGA and will present first results on implementing quantum feedback.

TT 17.3 Mon 15:30 H 2053

Bistability, chaos and chaos-to-hyperchaos transition in a few-qubit chain. — •Alexandre Zagoskin and Alexander Balanov — Department of Physics, Loughborough University, Loughborough, UK

Based on numerical simulations, we predict that an externally driven chain of a few qubits with dissipation will demonstrate transitions between several stable regimes and chaotic behaviour due to bistability, similar to the behaviour predicted for Rydberg atoms. The system also demonstrates a transition from chaotic to hyperchaotic behaviour as the number of qubits changes from 4 to 5. We argue that the transition is determined by the dimensionality of the Hilbert pace of the system and can be observed in a system of realistic superconducting qubits.

TT 17.4 Mon 15:45 H 2053

Coherent Revival of Ramsey Oscillations in the Fluxonium Qubit Coupled to a bath of Harmonic Oscillators — •Farshad Foroughi[1], Mattia Mantovani[2], Remy Dassonneville[1], Luca Planat[1], Javier Puertas[1], Sebastien Leger[1], Etienne Dumur[4], Yuriy Krupko[1], Wolfgang Belzig[2], Cecile Naud[1], Olivier Buisson[1], Nicolas Roch[1], Frank Hekking[1], Gianluca Rastelli[2,3], and Wiebke Guichard[1] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France. — [2]Fachbereich Physik, Universität Konstanz, Konstanz, D-78457 , Germany. — [3]Zukunftskolleg, Universität Konstanz, D-78457, Konstanz, Germany — [4]The institute for Molecular Engineering, University of Chicago, Chicago, IL, United States.

We studied different fluxonium qubits in 2D and 3D cavity-structures and reached the state of the art for coherence and relaxation times. We observed a systematic increase of the relaxation time both in 3D and 2D at the optimal point of the qubit, when quasi-particle tunneling is strongly reduced. We aim to realize a 2D fluxoniums coupled to few on-chip lumped element resonators. We use a fast flux line to control the coupling between the fluxonium qubit and the resonators. We have studied theoretically the emerging spin-boson Hamiltonian for this particular circuit with the perspective of measuring revival effects in the coherent oscillations of the qubit. We started to implement measurements, revealing the effect on the qubit dynamics of a dissipative bath formed by a discrete set of harmonic oscillators.

TT 17.5 Mon 16:00 H 2053

Nonreciprocal scattering of two superconducting qubits coupled to a waveguide — •Andres Rosario Hamann[1], Clemens Mueller[1], Markus Jerger[1], Joshua Combes[1], Maximilian Zanner[2], Martin Weides[2], Thomas M. Stace[1], and Arkady Fedorov[1] — [1]ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, St Lucia QLD 4072, Australia — [2]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Recent theoretical studies of a pair of atoms in a 1D waveguide show that the system responds asymmetrically to incident fields from opposing directions at low powers. In this work we present an experimental implementation of this nonreciprocal system by using two superconducting transmon-like qubits embedded in a copper waveguide. We show that the asymmetry arises from the formation of a quasi-dark-state of the two atoms, which saturates at extremely low powers. The nonlinear saturability of the system explicitly breaks the assumptions of the Lorentz reciprocity theorem. Two external coils provide control over the flux threading the transmons, thus allowing us to individually tune their transition frequencies and to change the effective coupling between the incident fields and the quasi-dark-state.

TT 17.6 Mon 16:15 H 2053

Simple Impedance Response Formulas for the Dispersive Interaction Rates in the Effective Hamiltonians of Low Anharmonicity Superconducting Qubits — •Firat Solgun[1], David DiVincenzo[2,3], and Jay Gambetta[1] — [1]IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA — [2]Institute for Quantum Information, RWTH Aachen, Germany — [3]Peter Grünberg Institute: Theoretical Nanoelectronics, Research Center Jülich, Germany

For superconducting quantum processors consisting of low anharmonicity qubits such as transmons we give a complete microwave description of the system in the qubit subspace. We assume that the qubits are dispersively coupled to a distributed microwave structure such that the detunings of the qubits from the internal modes of the microwave structure are stronger than their couplings. We define qubit ports across the terminals of the Josephson junctions and drive ports where transmission lines carrying drive signals reach the chip and we obtain the multiport impedance response of the linear passive part of the system between the ports. We then relate interaction parameters in between qubits and between the qubits and the environment to the entries of this multiport impedance function: in particular we show that the exchange coupling rate J between qubits is related in a simple way to the off-diagonal entry connecting the qubit ports. Our treatment takes into account all the modes (possibly infinite) that might be present in the distributed electromagnetic structure and provides an efficient method for the modeling and analysis of the circuits.

TT 17.7 Mon 16:30 H 2053

Tunable ohmic environment using Josephson junction chains — •Gianluca Rastelli[1] and Ioan M. Pop[2] — [1]Zukunftskolleg & Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

We analyse a scheme to implement a tunable resistance using a double chain of Josephson junctions. The two parallel chains are formed by N dc-SQUIDs, acting as linear and tunable inductance L. The chains are coupled capacitively through a capacitance C much larger than the capacitance of the individual dc-SQUID. The system sustains electromagnetic modes forming a large but discrete set of damped harmonic oscillators. This set yields an impedance Z, that is a smooth and continuous function versus frequency. Moreover, the system can be connected to an external measurement setup, and the dissipation can be continuously monitored. We show that, by varying L, the double chain can operate as tunable ohmic resistance in a frequency band spanning several GHz, with a resistance that can exceed the quantum resistance. We argue that the circuit complexity is within reach using current Josephson junction technology.

TT 17.8 Mon 16:45 H 2053

Quantum Process Tomography of a Quantum Memory — •Michael Renger[1,2], Edwar Xie[1,2,3], Frank Deppe[1,2,3], Peter Eder[1,2,3], Michael Fischer[1,2,3], Stefan Pogorzalek[1,2], Kirill G. Fedorov[1,2], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In order to realize a quantum memory, a memory protocol for a superconducting qubit coupled to a 3D cavity resonator is realized with a Z fidelity of 85%. By exploiting the multimode structure of the 3D cavity, we combine readout and storage capability in a single device, thereby significantly enhancing scalability. With the goal of accurately characterizing the information loss during the protocol, the overall process fidelity has to be measured. To this end, we perform quantum process tomography on our quantum memory system. The protocol consists of four pulses with a total length of 240ns. The qubit density matrix is reconstructed with standard quantum state tomography for a suitable set of qubit states. The comparison of the measured outcome with the theoretical value gives us knowledge about the process matrix χ. We present tomography data and compare the quantum process fidelity to the Z fidelity.

The authors acknowledge support from DFG through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria and the IMPRS 'Quantum Science and Technology'.

TT 18: f-Electron Systems and Heavy Fermions II

Time: Monday 15:00–17:30 Location: H 3005

TT 18.1 Mon 15:00 H 3005

Thermodynamics of heavy fermions with crystal-field excitations and lattice coherence — •Farzaneh Zamani[1], Stefan Kirchner[2], and Johann Kroha[1,2] — [1]Physikalisches Institut and BCTP, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, China

Heavy-fermion (HF) compounds exhibit an interplay of various phenomena, including Kondo effect, lattice coherence and crystal-field (CF) splitting. It is crucial to understand the corresponding features in the thermodynamics of heavy-fermion metals, e.g., in order to separate their energy scales from quantum critical scales. However, a complete understanding has been hampered by the fact that the CF-split angular-momentum multiplets of the rare-earth ions induce multiple spectral resonances near the Fermi energy (CF satellites), which are of Kondo-like many-body origin. Thus, not only their occupation number is thermally activated, but also their spectral weight depends on temperature, leading to complex thermodynamic behavior. We clarify the many-body nature of the CF excitations. We develop the Dynamical Mean-Field Theory for the multi-orbital, CF-split Anderson lattice model, using the self-consistent slave particle technique as an impurity solver, accurate down to well below the Kondo scale. We employ a novel gauge fixing technique for fixing the U(1) gauge of the slave particle fields which enables a highly accurate calculation of the free energy and its thermodynamic derivatives. Thermodynamic and spectroscopic results for both, the multi-orbital Anderson lattice and the single-impurity case, are presented.

TT 18.2 Mon 15:15 H 3005

Kondo insulators vs. transition metal-based narrow-gap semiconductors — •Jan M. Tomczak — Institute of Solid State Physics, TU Wien, Austria

Kondo insulators display a pronounced temperature dependence in their experimental observables: An insulating low-temperature regime with an activated magnetic susceptibility gives way—above a coherence temperature—to metallic conduction and Curie-Weiss behaviour. Empirically, this crossover is strikingly akin to that found in some correlated narrow-gap semiconductors, such as FeSi and $FeSb_2$, which are based on transition metals. Here, we present realistic many-body calculations for the prototypical Kondo insulator $Ce_3Bi_4Pt_3$[1] and compare them to our previous results for FeSi[2]. We discuss simulated transport properties, as well as photoemission and optical spectra. Further, we propose a microscopic distinction between the physics of both compounds from the perspective of dynamical mean-field theory. This work was supported by the Austrian Science Fund (FWF) through project P 30213-N36.

[1] JMT, Topical Review for J. Phys.: Condens. Matter (submitted),
[2] JMT, K. Haule, G. Kotliar, PNAS 109, 3243 (2012)

TT 18.3 Mon 15:30 H 3005

Kondo-lattice ferromagnets and their peculiar order along the magnetically hard axis — •Daniel Hafner[1], Binod Rai[2], Jacintha Banda[1], Kristin Kliemt[3], Cornelius Krellner[3], Jörg Sichelschmidt[1], Christoph Geibel[1], Emilia Morosan[2], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, D-01187 Dresden, Germany — [2]Physics and Astronomy Department, Rice University, Houston, Texas 77005, USA — [3]Physikalisches Institut, Johann Wolfgang Goethe-Universität, D-60438 Frankfurt am Main, Germany

We show that ferromagnetism in Ce- and Yb- based Kondo-lattice systems often aligns along the magnetically hard axis. This counter-intuitive phenomenon was believed to be a rare case, but our comparative study suggests that this is rather the common case in these materials. We discuss possible theoretical scenarios by analyzing differences and similarities between all these systems. Differences appear in properties such as Curie temperatures T_C, crystalline structures, size of the ordered magnetic moment and crystal electric field ground state. Similarities lie in a usual Kondo temperature T_K of a few Kelvin, a comparable magnetic anisotropy and a non mean-field like transition in specific heat, hinting at an important role of fluctuations.

TT 18.4 Mon 15:45 H 3005

Tracking incommensurate magnetism with Slave Boson Mean Field Theory — •David Riegler[1], Michael Klett[1], Seulgi Ok[2], Titus Neupert[2], Peter Wölfle[3], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, University of Würzburg, Germany — [2]Department of Physics, University of Zurich, Switzerland — [3]Institute for Theory of Condensed Matter and Institute for Nanotechnology, Karlsruhe Institute of Technology, Germany

Accounting for strong correlations is one of the most challenging problems in solid state physics, and has given rise to the development of a plethora of different methodological approaches. Among them, the slave boson mean field formalism has been shown to successfully describe strongly correlated electron systems such as heavy fermion physics and quantum impurity models. While DMFT is another popular method of use within the scope of these systems, the slave boson mean field method can be applied to problems beyond the reach of DMFT, and such provide an interesting complementary view. In particular, this applies to models with large Hilbert spaces, and especially the investigation of incommensurate magnetic order where the magnetic unit cell would be too large to describe it within any cluster DMFT framework. Therefore, slave boson mean field is well suited to fill a niche in contemporary methods of condensed matter physics. This talk intends to elaborate on the method of spin rotation invariant

slave boson mean field theory including fluctuations around the saddle point, and its applications to the periodic Anderson model as well as the topological Kondo insulator SmB_6.

TT 18.5 Mon 16:00 H 3005

Partial Kondo screening in a frustrated Kondo lattice model — •Toshihiro Sato[1], Fakher F. Assaad[1], and Tarun Grover[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, University of California at San Diego, USA

We study a half-filled Kondo lattice model on the honeycomb lattice with geometrical frustration. The geometrical frustration adds a new competing energy scale in the Doniach phase diagram which conventionally accounts only for the competition between the RKKY interaction and the Kondo screening. Using a negative-sign-free auxiliary field quantum Monte Carlo approach, we map out the phase diagram in the presence of geometrical frustration. In addition to the conventional Kondo insulator and the anti-ferromagnetically ordered state, we provide evidence for a novel 'partial Kondo screened' phase. In this phase, the spins are selectively screened so as to alleviate frustration, and the lattice rotation symmetry is broken nematically [1].
[1] T. Sato, F. F. Assaad, T. Grover, arXiv:1711.03116 (2017)

TT 18.6 Mon 16:15 H 3005

3D topological Kondo insulators: surface band structure and space charge screening — •soroush arabi[1], francisco meirinhos[1], and johann kroha[1,2] — [1]Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China

Topological Kondo insulators (TKIs) are a new class of topological insulators, emerging through the interplay of strong correlations and spin-orbit coupling. In TKIs, the bulk is a narrow band insulator due to the appearance of a localised Kondo resonance near the Fermi level and its hybridisation with the conduction band. Additionally, the strong spin-orbit coupling of the localised moments generates a nonlocal hybridisation between the local moments and the conduction band, which results in a topologically nontrivial band structure and gapless surface states [1]. In this work, we study TKIs in a slab geometry and address the problems of space charges and screening near the surfaces. The strong Kondo correlations in the 4f orbitals are treated by a layer-dependent slave boson mean field (SBMF) theory, while the Coulomb repulsion in the conduction band is described by Hartree-Fock (HF) approximation. We solve the coupled SBMF+HF theory self-consistently and thereby analyse the perseverance of topological surface states.

15 min. break.

TT 18.7 Mon 16:45 H 3005

Bulk sensitive probe of $5f$ occupation and charge density in URu_2Si_2 and $URu_{1.7}Fe_{1.3}Si_2$ — •Martin Sundermann[1,2,3], Andrea Amorese[1,2], Hasan Yavaş[3], Pieter Glatzel[4], Maurits W. Haverkort[5], Brian Maple[6], Liu Hao Tjeng[2], and Andrea Severing[1,2] — [1]University of Cologne, Institute of Physics II, Cologne, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]PETRA III, Deutsches Elektronen- Synchrotron (DESY), Hamburg, Germany — [4]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [5]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany — [6]University of California, San Diego, La Jolla, California, USA

URu_2Si_2 goes into a nonmagnetic hidden order (HO) phase at 17.7 K and becomes superconducting below 1.5K. The order parameter of the second-order phase transition into the HO phase in URu_2Si_2 is still a mystery, despite 30 years of research. Interestingly, with applied pressure ($p \geq 0.7$GPa) the HO is replaced with antiferromagnetic order with large ordered moments of $0.4\mu_B$. This phase can also be reached by substitution of Fe on the Ru site. In the Fe substituted samples the ordered moment is even larger. Here we have addressed the questions whether the $5f$ occupation and/or the ground state wave function change with Fe substitution. We will present high energy resolution fluorescence detection M-edge and non-resonant inelastic x-ray scattering O-edge data of $URu_{1.7}Fe_{0.3}Si_2$ and compare these with results of URu_2Si_2.

TT 18.8 Mon 17:00 H 3005

High magnetic field studies on $U_2Rh_3Si_5$ — •Nico Steinki[1], Stefan Süllow[1], Marcelo Jaime[2], Franziska Weickert[2], Neil Harrison[2], Hiroshi Amitsuka[3], Michal Vališka[4], and Vladimir Sechovsky[4] — [1]IPKM, TU Braunschweig, Germany — [2]NHMFL, LANL, Los Alamos, USA, — [3]Hokkaido University, Sapporo, Japan — [4]Charles University, Prague, Czech Republic

Together with UO_2, the intermetallic $U_2Rh_3Si_5$ is a prime example of a $5f$ material exhibiting a first order magnetic phase transition [1-3]. As demonstrated by means of thermodynamic, electronic transport and neutron scattering techniques, this monoclinic system undergoes a structural transition without changing the crystallographic symmetry at $T_N = 25.6$ K. It is accompanied by one into a canted antiferromagnetically ordered state with large magnetic moments ($\mu_{ord} \sim 2.4\mu_B$), together with apparent modifications of the Fermi surface. So far, experiments have been limited to magnetic fields < 30 T, and which has hindered a better understanding of the microscopic mechanism of the phase transition in $U_2Rh_3Si_5$. Moreover, previous experiments seem to indicate that for B||a axis there is a phase boundary in the range $\sim$ 40 T. As well, the question about attaining full ferromagnetic polarization along the b axis has not been settled. Hence, in this situation we have performed high field (65 T) magnetization and magnetostriction to map out the magnetic phase diagram.
[1] B. Becker et al., Phys. Rev. Lett. **78** (1997) 1347.
[2] T. Takeuchi et al., J.A. Mydosh, Phys. Rev. B **56** (1997) 10778.
[3] R. Feyerherm et al., Phys. Rev. B **56** (1997) 13693.

TT 18.9 Mon 17:15 H 3005

Theoretical Modeling of Resonant X-Ray Emission Spectra at the Actinide $M_{4,5}$ Edges — •Jindrich Kolorenc — Institute of Physics, The Czech Academy of Sciences, Prague, Czech Republic

I discuss a theoretical description of the resonant x-ray emission spectra (RXES) that is based on the Anderson impurity model. The parameters of the model are determined from material-specific LDA+DMFT calculations. Recently, this approach was shown [1] to accurately reproduce the L-edge RXES measured in lanthanides [2]. Here, the method is extended to the M-edge spectra in actinide compounds.

The same theoretical approach applies also to the x-ray absorption spectra measured in the high-energy-resolution fluorescence-detection mode (HERFD-XAS) [3]. As an example, I investigate the origin of large variations observed among the M-edge HERFD-XAS spectra of several uranium compounds where uranium atoms are in the same oxidation state. For instance, both UO_3 and torbentite have U atoms in the U(VI) state, but the shape of their x-ray absorption spectra differs quite substantially [4,5].
[1] J. Kolorenč, Physica B (2017), DOI: 10.1016/j.physb.2017.08.069
[2] J. A. Bradley *et al.*, Phys. Rev. B **85**, 100102 (2012).
[3] K. Hämäläinen *et al.*, Phys. Rev. Lett. **67**, 2850 (1991).
[4] Y. Podkovyrina *et al.*, J. Phys.: Conf. Ser. **712**, 012092 (2016).
[5] K. O. Kvashnina, Y. O. Kvashnin, S. M. Butorin, J. Electron. Spectrosc. Relat. Phenom. **194**, 27 (2014).

TT 19: Frustrated Magnets - Spin Liquids - Theory

Time: Monday 15:00–18:15 Location: H 3010

TT 19.1 Mon 15:00 H 3010

Thermal transport of the Kitaev spin ladder in a magnetic field — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

The Kitaev spin ladder (KSL) is a minimum quasi one-dimensional (1D) representative of the celebrated two-dimensional Kitaev model on the Honeycomb lattice. The frustration caused by the compass interactions leads to fractionalization which combined with the spatial confinement of 1D leads to localization in the absence of disorder and consequently to vanishing dc transport coefficients. Furthermore, the KSL exhibits an interesting phase diagram with gapless, as well as trivial and topological gapped phases. In this work, we present results for the thermodynamical as well as for the thermal transport properties of the Kitaev spin ladder in the presence of a magnetic field, which gives rise to finite dc transport coefficients. We provide results at finite temperatures for a wide range of the magnetic field's strength, from the insulating to the diffusive regime, and for different sets of Kitaev couplings, starting from gapless or gapful phases in KSL's phase diagram. We primarily rely on numerical techniques, namely exact diagonalization and the quantum typicality but we also provide comparison with an effective fermionic model, valid for weak magnetic fields.

TT 19.2 Mon 15:15 H 3010

Thermal conductivity of a two-dimensional $\mathbb{Z}_2$ spin liquid — •Angelo Pidatella[1], Alexandros Metavitsiadis[2], and Wolfram Brenig[2] — [1]Institute for Theoretical Physics, Technical University of Dresden — [2]Institute for Theoretical Physics, Technical University of Braunschweig

We study the dynamical thermal conductivity of the two-dimensional Kitaev spin model on the honeycomb lattice. Mapping to Majorana particles, the transport properties are described in terms of itinerant matter fermions interacting with a localized $\mathbb{Z}_2$ gauge field. Analyzing isotropic as well as anisotropic cases, in order to incorporate both, gapless and gapful phases of the Kitaev model, we discuss our findings for the thermodynamic properties and the transport coefficients, at finite temperature and frequency. Our analysis is based on complementary calculations of the current correlation function, comprising exact diagonalization by means of a complete summation over all gauge sectors, as well as a phenomenological mean-field treatment of thermal gauge fluctuations, valid over a wide range of temperatures. We find the system to be a dissipative heat conductor in the isotropic case. Results for the anisotropic cases will also be discussed.

TT 19.3 Mon 15:30 H 3010

Global phase diagram for the extended Kitaev – Heisenberg model via cluster mean field theory — •Dorota Gotfryd[1,2], Juraj Rusnacko[3,4], and Jiri Chaloupka[3,4] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Lojasiewicza 11, PL-30348 Krakow, Poland — [3]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic — [4]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlarska 2, CZ-61137 Brno, Czech Republic

We present the global phase diagram for the extended Kitaev – Heisenberg model [1-4] obtained via cluster mean field theory (CMFT) [5]. We use (a) linearized and (b) full self – consistent CMFT to determine most of the magnetically ordered (Neel, FM, zigzag, stripy, vortex) and disordered (spin liquid) regions in the phase diagram. As the final outcome CMFT gives us the magnetic ordered moment direction and value for each phase. We conclude with the comparison of the characteristics of the ordered moment for CMFT, other methods and the experimental findings.

[1] J.G. Rau et al., Phys. Rev. Lett.112, 077204 (2014).
[2] J.G. Rau et al., arXiv: 1408.4811, (2014).
[3] J. Chaloupka et al., Phys. Rev. B, 92, 024413 (2015).
[4] J. Chaloupka et al., Phys. Rev. B, 94, 064435 (2016).
[5] D. Gotfryd et al., Phys. Rev. B, 95, 024426 (2017).

TT 19.4 Mon 15:45 H 3010

Existence of spin-liquid states in the Kitaev-Heisenberg ladder — •Cliò Efthimia Agrapidis[1], Jeroen van den Brink[1,2], and Satoshi Nishimoto[1,2] — [1]IFW Dresden, Dresden, Germany — [2]Technical University Dresden, Dresden, Germany

It is widely accepted that the Kitaev-Heisenberg (KH) model on a honeycomb lattice is a good minimal model for some candidate spin liquid materials (e.g. α-$RuCl_3$). Though the KH hamiltonian has been studied in 2D, systematic analysis including finite-size scaling is still lacking due to numerical difficulties. Whereas very precise analysis is possible for 1D and quasi-1D KH systems

We study the KH ladder using the exact diagonalization and density matrix renormalization group techniques. We present its phase diagram as a function of an angle parameter ϕ, having defined the Kitaev interaction as $\sin\phi$ and the Heisenberg one as $\cos\phi$. Remarkably, we find that the phase diagram has a resemblance to the one suggested for the same model on the honeycomb lattice [1], showing the same phases, namely spin-singlet (or Néel), zig-zag, ferromagnetic, stripy and two spin liquid states.

We also present some results in the presence of magnetic field and discuss the spin-liquid properties.

[1] J. Chaloupka, G. Jackeli, G. Khaliullin, PRL **110** 097204 (2013)

TT 19.5 Mon 16:00 H 3010

Majorana zero modes in the Kitaev honeycomb model — •Daniel Otten, Ananda Roy, and Fabian Hassler — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Kitaev's honeycomb model is a quantum spin liquid that gives rise to an emergent static $\mathbb{Z}_2$ gauge field coupled to Majorana fermions. In presence of an applied external magnetic field, the system is, dependent on the choice of interaction strength, in a gapped, non-abelian phase. In this phase, the vortex excitations of the emergent $\mathbb{Z}_2$ gauge field have Majorana zero modes bound to them. We investigate the properties of these Majorana zero modes. Using Jordan-Wigner transformation, we map the effective Hamiltonian to that of a chiral p-wave superconductor. We analytically calculate the wave functions of the Majorana zero modes in the continuum limit and the energy splitting that arises when two vortices approach each other. Furthermore, to understand the implications of the zero modes in the original spin model, we calculate the spin-spin correlator and the dynamical structure factor in presence of these vortices. These results are relevant for possible experimental observations and characterizations of the Majorana zero modes in systems that are dominated by the interaction of the Kitaev honeycomb model.

TT 19.6 Mon 16:15 H 3010

Probing α-$RuCl_3$ beyond magnetic order: Effects of temperature and magnetic field — •David Kaib[1], Stephen Winter[1], Kira Riedl[1], Radu Coldea[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [2]Clarendon Laboratory, University of Oxford

Recent studies have brought α-$RuCl_3$ to the forefront of experimental searches for materials realizing Kitaev spin-liquid physics. This material exhibits strongly anisotropic exchange interactions afforded by the spin-orbit coupling of the 4d Ru centers. Under strong scrutiny is the nature of the unconventional continuum of magnetic excitations [1, 2], as well as reported unconventional paramagnetic states that emerge at finite temperature [3] and finite magnetic field [4] after suppression of magnetic order. Using exact diagonalization calculations of an ab-initio guided spin model complemented by semi-classical analysis, we find a very rich evolution of the spin dynamics and the stabilization of a quantum paramagnetic state as the zigzag order is suppressed [5].

[1] A. Banerjee et al., Science **356**, 1055-1059 (2017).
[2] S. M. Winter et al., Nature Communications **8**, 1152 (2017).
[3] S.-H. Do et al., Nature Physics **13**, 1079-1084 (2017).
[4] Z. Wang et al., arXiv: 1706.06157 (2017).
[5] S. M. Winter et al., arXiv:1707.08144 (2017).

TT 19.7 Mon 16:30 H 3010

Lattice disorder and spin-orbital behaviour in $Ba_3CuSb_2O_9$ — •Andrew Smerald[1,2] and Frederic Mila[1] — [1]Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — [2]Max Planck Institute for Solid State Research,

Heisenbergstraße 1, 70569 Stuttgart, Germany

The material $Ba_3CuSb_2O_9$ has elicited attention recently due to the proposal that it realises a spin-orbital liquid state. One difficulty in understanding this behaviour comes from the fact that the lattice structure of the Cu^{2+} ions is disordered. In order to better understand the lattice we study a model of charged Sb^{5+}-Cu^{2+} dumbbells living on a triangular lattice. We find a complicated 'branch' lattice with correlated disorder of the dumbbells. Starting from this lattice structure we speculate on the possible spin-orbital state, proposing a state with delocalised orphan spins.

15 min. break.

TT 19.8 Mon 17:00 H 3010

Doping a 2d Mott insulator - Study of a quantum dimer model — •Sebastian Huber[1], Johannes Feldmeier[1], Fabian Grusdt[2], and Matthias Punk[1] — [1]Arnold Sommerfeld Center, Ludwig-Maximilians University, 80333 Munich, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Experiments with quantum gas microscopes have started to explore the antiferromagnetic phase of the Fermi-Hubbard model and effects of doping with holes away from half filling [1]. We show in this talk that the read-out of the two-particle reduced density matrix enables to distinguish magnetically ordered and interesting topologically ordered spin-liquid phases, which might occur in the Hubbard model close to half filling. Fractionalized Fermi liquids (FL*) [2] are a promising candidate for this parameter regime. The generalized quantum dimer model introduced in Ref. [3] is an effective lattice realization of such an FL* with a Hilbert space spanned by configurations of fermionic and bosonic short-range bound states. We compute the corresponding electron spectral functions using exact diagonalization on lattices of size 6x6 to verify the existence of a pseudogap.

[1] A. Mazurenko, C. Chiu et al., Nature 545, 7655 (2017)
[2] T. Senthil, S. Sachdev and M. Vojta, PRL 90, 21 (2003)
[3] M. Punk, A. Allais and S. Sachdev, PNAS 112, 31 (2015)

TT 19.9 Mon 17:15 H 3010

Negative sign free auxiliary field algorithm for frustrated Kondo systems — •Johannes S Hofmann[1], Fakher F Assaad[1], and Tarun Grover[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of California at San Diego, La Jolla, CA 92093, USA

The absence of negative sign problem in quantum Monte Carlo simulations of spin and fermion systems has different origins. Worldline based algorithms for spins require positivity of matrix elements whereas auxiliary field approaches for fermions depend on symmetries such as particle-hole. For negative-sign-free spin and fermionic systems, we show that one can formulate a negative-sign-free auxiliary field quantum Monte Carlo algorithm that allows Kondo coupling of fermions with the spins.

In this talk we will present preliminary results on the Kondo coupling between local moments participating in a $\mathbb{Z}_2$ spin liquid (based on Balents-Fisher-Girvin model) and conduction electrons on a honeycomb lattice. Our setup allows us to address the question of the relevance of the Kondo coupling at the quantum critical point corresponding to the destruction of the spin-liquid.

TT 19.10 Mon 17:30 H 3010

Fractionalized Fermi liquids and exotic superconductivity in the Kitaev Kondo lattice — •Urban F. P. Seifert[1], Tobias Meng[1], and Matthias Vojta[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, Technische Universität Dresden, 01062 Dresden, Germany

Fractionalized Fermi liquids (FL*) have been introduced as non-Fermi-liquid metallic phases, characterized by coexisting electron-like charge carriers and local moments which itself form a fractionalized spin liquid. Here we investigate a Kondo lattice model on the honeycomb lattice with compass interactions among the local moments, a concrete model hosting FL* phases based on Kitaev's $\mathbb{Z}_2$ spin liquid. We characterize the FL* phases via perturbation theory, and we employ a Majorana-fermion mean-field theory to map out the full phase diagram. Most remarkably we find triplet superconducting phases which mask the quantum phase transition between fractionalized and conventional Fermi liquid phases. Their pairing structure is inherited from the Kitaev spin liquid, i.e., superconductivity is driven by Majorana glue.

TT 19.11 Mon 17:45 H 3010

Looking at an antiferromagnet from a spin-liquid point of view — •Marc Daniel Schulz — TU Dortmund, Germany

The $\mathbb{Z}_2$ topological phase in the quantum dimer model on the Kagome-lattice is a candidate for the description of the low-energy physics of the anti-ferromagnetic Heisenberg model on the same lattice. We study the extend of the topological phase by interpolating between the exactly solvable parent Hamiltonian of the topological phase and an effective low-energy description of the Heisenberg model in terms of a quantum-dimer Hamiltonian. Therefore, we perform a perturbative treatment of the low-energy excitations in the topological phase including free and interacting quasi-particles. We find a phase transition driven by the condensation of bound states formed of topological excitations. The condensed phase corresponds to a valence bond solid and is characterized by a spontaneously broken rotational symmetry and a unit cell containing six sites.

TT 19.12 Mon 18:00 H 3010

Jammed spin liquid in the bond-disordered kagome Heisenberg antiferromagnet — •Thomas Bilitewski[1], Mike Zhitomirsky[2], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Universite Grenoble Alpes, CEA, INAC-Pheliqs, 38000 Grenoble, France

We study a class of disordered continuous classical spin systems including the kagome Heisenberg magnet. While each term in its local Hamiltonian can be independently minimised, we find discrete degenerate ground states whose number grows exponentially with system size. These states do not exhibit zero-energy 'excitations' characteristic of highly frustrated magnets but instead are local minima of the energy landscape, albeit with an anomalously soft excitation spectrum. This represents a spin liquid version of the phenomenon of jamming familiar from granular media and structural glasses. Correlations of this jammed spin liquid, which upon increasing the disorder strength gives way to a conventional spin glass, may be algebraic (Coulomb-type) or exponential.

TT 20: Topological Semimetals II

Time: Monday 15:00–18:45 Location: A 053

TT 20.1 Mon 15:00 A 053

Topological band crossings in hexagonal materials — •Andreas P. Schnyder — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, topological nodal-line semimetals have become a topic of very active research, driven by the discovery of several new nodal-line materials. In this talk, I present a complete classification of all possible non-symmorphic nodal lines in hexagonal materials with strong spin-orbit coupling. The analysis is based on (i) the algebraic relations obeyed by the symmetry operators and (ii) the compatibility relations between irreducible representations at different high-symmetry points of the Brillouin zone. I present a number of existing materials where these non-symmorphic nodal lines are realized and discuss their DFT band structures. Based on these material examples, I discuss the surface states that are associated with the topological band crossings.

TT 20.2 Mon 15:15 A 053

Realizing double Dirac particles in the presence of electronic interactions — •Giorgio Sangiovanni[1], Domenico Di Sante[1], Andreas Hausoel[1], Paolo Barone[2], Jan Tomczak[3], and Ronny Thomale[1] — [1]Institut fuer Theoretische Physik und Astrophysik, Universitaet Wuerzburg — [2]Consiglio Nazionale delle Ricerche, l'Aquila (Italy) — [3]TU Wien (Austria)

Double Dirac fermions have recently been identified as possible quasiparticles hosted by three-dimensional crystals with particular nonsymmorphic point-group symmetries. Applying a combined approach of ab initio methods and dynamical mean-field theory, we investigate how interactions and double Dirac band topology conspire to form the electronic quantum state of Bi_2CuO_4. We derive a downfolded eight-band model of the pristine material at low energies around the Fermi level. By tuning the model parameters from the free band structure to the realistic strongly correlated regime, we find a persistence of the double Dirac dispersion until its constituting time-reversal symmetry is broken due to the onset of magnetic ordering at the Mott transition. Our calculations suggest that the double Dirac fermions in Bi_2CuO_4 can be restored by experimentally accessible hydrostatic pressures. In light of the growing attention to the topological quantum chemistry approach, our results on Bi_2CuO_4 show how many-body effects must be included beyond the static mean-field level for reliable predictions on new materials.

[1] Phys. Rev. B 96, 121106(R) (2017)

TT 20.3 Mon 15:30 A 053

Drumhead surface states in topological Dirac semimetal — •Andreas Leonhardt[1], Andreas Schnyder[1], Mehdi Biderang[2], Nimisha Raghuvanshi[2], and Alireza Akbari[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Gyeongbuk 790-784, Korea

Dirac nodal line semimetals (DNLSMs) host a symmetry protected band crossing along a line in the BZ. The non-trivial Berry phase of the bulk within the nodal ring leads to localized drumhead surface states (DSSs) in the interior of the projection of the line node onto the surface BZ. Promising candidates to study the physics of DNLSMs are the compounds CaAg(P/As) and $TlTaSe_2$, which provide different SOC strengths and mechanisms.

Quasi particle interference (QPI) is dominated by surface states and provides a possibility to investigate the dispersion and spin polarization of the drumhead surface states. We present spin resolved QPI patterns from an effective low energy tight binding model for the most promising candidates of nodal line semimetals, together with a symmetry analysis of the resulting patterns with respect to the spin polarization of the DSSs, with a focus on the influence of SOC onto the line node and the surface states.

Furthermore, we investigate the effect of the non-trivial topology on non-linear optical response phenomena, where the Berry connection and curvature directly appear in terms of quadratic or higher order in the electric field.

TT 20.4 Mon 15:45 A 053

Three dimensional Dirac semimetal canditate $PtBi_2$ — •Boy Roman Piening[1], Thirupathaiah Setti[1,2], Christian Blum[1], Yevhen Kushnirenko[1], Alexander Yaresko[3], Sergey Borisenko[1], Saicharan Aswartham[1], and Bernd Büchner[1,4] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Indian Institute of Science, Bangalore, Karnataka, 560012, India — [3]Max-Planck-institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

From band structure calculations the pyrite-type cubic $PtBi_2$ has been predicted to be a three-dimensional Dirac semimetal, which is supported by experimental studies showing anomalous transport properties such as a non saturating extremely large linear magnetoresistance (XMR). Until now only the trigonal $PtBi_2$ was investigated in respect to electronic structure by ARPES revealing promising linearly dispersive Dirac states. We synthesized cm-sized cubic and trigonal $PtBi_2$ single crystals by selfflux method using different ratios of Pt to Bi in appropriate temperature regions in order to control the phase. For comparison trigonal $PtBi_2$ were grown with a mirror furnace leading to a several cm-long single crystal. Transport measurements, X-ray diffraction and Energy-dispersive spectroscopy confirm the high quality of the crystals which makes them suitable for further investigation. For the first time it was possible to measure the cubic $PtBi_2$ with ARPES.

TT 20.5 Mon 16:00 A 053

Planar Hall effect in half Heusler Weyl semimetal GdPtBi — Nitesh Kumar, Claudia Felser, and •Chandra Shekhar — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Weyl and Dirac Fermions semimetals exhibits exotic transport properties for example high carrier mobility, large positive transverse magnetoresistance, low charge carrier density, low effective mass *etc.* However, among the very few available tools to characterize Weyl semimetals through electrical transport, negative magnetoresistance is most commonly used. Considering shortcomings of this method, new tools to characterize chiral anomaly in Weyl semimetals are desirable. We employ planar Hall effect as an effective technique in half Heusler Weyl semimetal GdPtBi to study chiral anomaly. This compound exhibits a large value of 1.5 mΩcm planar Hall resistivity at 2 K and in 9 T [1]. Our analysis reveals that the observed amplitude is dominated by Berry curvature and chiral anomaly contributions. Through the angle dependent transport studies we establish that GdPtBi with relatively small orbital magnetoresistance is an ideal candidate to observe large planar Hall effect.

[1] N. Kumar, C. Felser and C. Shekhar, *arXiv*:1711.04133, 2017.

TT 20.6 Mon 16:15 A 053

An optical investigation of the strong spin-orbital coupled magnetic semimetal $YbMnBi_2$ — •Alexander Yaresko[1], Dipanjan Chaudhuri[2], Bing Cheng[2], N. Peter Armitage[2], Quinn D. Gibson[3], and Robert J. Cava[3] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Department of Physics and Astronomy, The Johns Hopkins University, Baltimore, MD 21218, USA — [3]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA

Strong spin-orbit coupling can result in ground states with non-trivial topological properties. The situation is even richer in magnetic systems where the magnetic ordering can potentially have strong influence over the electronic band structure. The class of $AMnBi_2$ (A = Sr, Ca) compounds are important in this context as they are known to host massive Dirac fermions with strongly anisotropic dispersion, which is believed to be due to the interplay between strong SOC and magnetic degrees of freedom. We report the optical conductivity of $YbMnBi_2$, a newly discovered member of this family and a proposed Weyl semi-metal candidate with broken time reversal symmetry. Comparing experimental and theoretical optical spectra we show that the complex conductivity can be interpreted as the sum of an intra-band Drude response and inter-band transitions. We find signatures of a gapped Dirac dispersion, common in other members of $AMnBi_2$ family or compounds with similar 2D network of Bi atoms.

TT 20.7 Mon 16:30 A 053

Generic Coexistence of Fermi Arcs and Dirac Cones on the Surface of Time-Reversal Invariant Weyl Semimetals —

•Alexander Lau[1], Klaus Koepernik[2], Jeroen van den Brink[2], and Carmine Ortix[3] — [1]Kavli Institute of Nanoscience, TU Delft, Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Institute for Theoretical Physics, Utrecht University, Netherlands

The hallmark of Weyl semimetals is the existence of open constant-energy contours on their surface, the so-called Fermi arcs, connecting Weyl points. Here, we show that for time-reversal symmetric realizations of Weyl semimetals these Fermi arcs in many cases coexist with closed Fermi pockets originating from surface Dirac cones pinned to time-reversal invariant momenta. The existence of Fermi pockets is required for certain Fermi-arc connectivities due to additional restrictions imposed by the six $\mathbb{Z}_2$ topological invariants characterizing a generic time-reversal invariant Weyl semimetal. We show that a change of the Fermi-arc connectivity generally leads to a different topology of the surface Fermi surface, and identify the half-Heusler compound LaPtBi under in-plane compressive strain as a material that realizes this surface Lifshitz transition.

15 min. break.

TT 20.8 Mon 17:00 A 053

Weyl semimetals with single Weyl nodes, and the fate of their chiral anomaly — •Tobias Meng and Jan Carl Budich — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Weyl semimetals are defined by the presence of isolated points in the Brillouin zone at which a conduction and a valence band touch. The so-called Nielsen-Ninomiya-theorem requires these points (the "Weyl nodes") to appear in pairs. This theorem, however, is only valid for interactions of sufficiently short range. In this talk, I discuss that long-range interactions can break the Nielsen-Ninomiya-theorem, and illustrate this point by an explicit construction of an interacting tight-binding model that contains only a single Weyl node. I will then demonstrate that the chiral magnetic effect remains intact for arbitrary interactions in such a single node Weyl semimetal. In particular, already an infinitesimal magnetic field restores a pair of chiral Landau levels of opposite chirality.

TT 20.9 Mon 17:15 A 053

Quantum anomalies in strained Weyl semimetals — Sthitadhi Roy[1], •Jan Behrends[1], Michael Kolodrubetz[2], Jens H. Bardarson[3], Nathan Goldman[4], Adolfo G. Grushin[2,5], and Roni Ilan[6] — [1]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [2]Department of Physics, University of California, Berkeley, California 94720, USA — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden — [4]Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium — [5]Institut Néel, CNRS and Université Grenoble Alpes, F-38042 Grenoble, France — [6]Raymond and Beverly Sackler School of Physics and Astronomy, Tel-Aviv University, Tel-Aviv 69978, Israel

The chiral anomaly gives the topological response of Weyl semimetals to an external perturbation, insensitive to local details of the Hamiltonian. The recent identification of strain as axial fields in these materials gives rise to other anomalies, known from high-energy theory. However, these anomalies driven by axial fields are not necessary gauge-invariant or charge-conserving; in fact, two different formulations exist, realizing just one of these conditions. In this work, we propose a way to resolve this ambiguity, supported by a lattice model that provides an intuitive picture. We identify experimental signatures and argue about their stability in presence of disorder.

TT 20.10 Mon 17:30 A 053

Creating and Controlling Weyl Fermions, Nexus Points, and Nodal Lines in the Magnetic Anti-perovskite Eu_3PbO — •Moritz M. Hirschmann[1], Alexandra S. Gibbs[2], Vahideh Abdolazimi[1], Alexander Yaresko[1], Hidenori Takagi[1,3,4], Andreas W. Rost[1,3], and Andreas P. Schnyder[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]ISIS Pulsed Neutron Facility, Didcot, United Kingdom — [3]FMQ, Universität Stuttgart, Germany — [4]Department of Physics, The University of Tokyo, Japan

Anti-perovskite materials A_3EO, where A denotes an alkaline earth metal, while E stands for Pb or Sn, exhibit low-energy electronic properties that are described by three-dimensional Dirac fermions, which are gapped out by spin-orbit coupling [1,2]. If A is replaced by the rare-earth element europium then magnetic order is expected due to the electron spin moment as confirmed by magnetization measurements. Neutron diffraction leads us to the conclusion that different magnetic phases appear. We studied the effect of magnetism on the electronic properties of Eu_3PbO. From DFT calculations the resulting splitting has been extracted and implemented into a tight-binding model to capture the physics close to the Fermi energy. We present the creation of Weyl points, Nexus points, and nodal lines and give their topological invariants. For the different magnetic phases we derived the respective surface states and anomalous Hall responses.

[1] T. H. Hsieh, J. Liu, L. Fu. Phys. Rev. B, 90 (2014) 08111.
[2] D. Samal, H. Nakamura, H. Takagi. APL Mater. 4 (7), 2016.

TT 20.11 Mon 17:45 A 053

Andreev reflection in time-reversal symmetric Weyl semimetals — •Jens Schulenborg[1], Uli Zuelicke[2], and Michele Governale[2] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]School of Physical and Chemical Sciences and Alan MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University Of Wellington, New Zealand

The study of the unusual chiral properties of Weyl fermions in Weyl semimetals (WSM) has attracted enormous attention in the past decade. Most recently, reports[1,2] on simple WSM band structures with only the minimum number of Weyl nodes suggest that it might become possible to exploit the nontrivial spin-momentum locking directly through ballistic scattering. This can be useful for spectroscopy or spin-dependent quantum optics with electrons.

To explore this perspective, we theoretically study elastic Andreev reflection in a minimal model of a time-reversal symmetric WSM, at an interface between a normal and superconducting region with s-wave pairing. We show that without interface-related spin-mixing, the subgap reflection processes at the four Weyl cones completely decouple. This arguably simplest form of Andreev scattering in a time-reversal symmetric WSM can be described by a 3D analogue of graphene, with the key difference that the pseudospin becomes an effective, yet in principle accessible spin.

[1] K. Koepernik et al., Phys. Rev. B 93, 201101 (2016)
[2] I. Belopolski et al., Nat. Commun. 8, 942 (2017)

TT 20.12 Mon 18:00 A 053

Ballistic edge states in Bismuth nanowires revealed by SQUID interferometry — •Anil Murani — Laboratoire de Physique des Solides, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay Cedex, France — Quantronics Group, Service de Physique de l'État Condensé (CNRS UMR 3680), IRAMIS, CEA-Saclay, 91191 Gif-sur-Yvette, France

Topological insulators are materials that have electronic states lying at their edges, which are protected against backscattering by time reversal symmetry. Bismuth, a semi-metal with strong spin-orbit coupling, was predicted to be topological in the case of a bilayer thick crystal. We showed numerically that edge states still exists in Bi nanowires, and experimentally demonstrated the existence of edge conduction channels as well as their ballisticity in a recent work, by embedding the nanowire into an asymetric SQUID. The goal of the present study is to go one step further and to answer quantitatively about the topological protection against backscattering as well as the lifetime of the metastable Andreev bound states that can be formed in these topological SNS junction. This is done by inductively coupling the NS loop to a multimode superconducting resonator, with eigenfrequencies ranging from 300 MHz up to 6 GHz, and measuring the magnetic flux dependent absorbtion at the vicinity of each of these frequencies. The resulting phase dependent absorbtion spectrum is measured for different temperatures and can be analyzed using a simple low energy model taking into account two Andreev bound states that nearly anticross, in agreement with a topological protection.

TT 20.13 Mon 18:15 A 053

Breakdown of the chiral anomaly in Weyl semimetals in a strong magnetic field — •Pilkwang Kim, Ji Hoon Ryoo, and Cheol-Hwan Park — Department of Physics, Seoul National University, Seoul 08826, Korea

A Weyl semimetal is a three-dimensional material whose low-energy quasiparticles are the chiral fermions described by the Weyl equation. One of the most intriguing phenomena of Weyl semimetals is the chiral anomaly, which is the nonconservation of the chiral charge in the

presence of parallel electric and magnetic fields and has been understood as an imbalance between the occupations of the zeroth Landau levels with the opposite chiralities [1]. In this presentation, we report the breakdown of the chiral anomaly in Weyl semimetals in a strong magnetic field [2]. From first-principle calculations, we demonstrate that a sizable energy gap opens up due to the mixing of the zeroth Landau levels with opposite chiralities if an applied magnetic field is sufficiently strong. Our results provide a theoretical framework for understanding a wide range of phenomena related to the chiral anomaly in topological semimetals, such as magnetotransport, thermoelectric responses, and plasmons.

[1] H. B. Nielsen, M. Ninomiya, Phys. Lett. B 130 (1983) 389.
[2] P. Kim, J. H. Ryoo, C.-H. Park, arXiv 1707.01103 (2017).

TT 20.14 Mon 18:30 A 053

Quantum oscillations in Weyl-II semimetals near magnetic breakdown — •Fabian Lambert[1], Johannes Knolle[2], and Ilya Eremin[1] — [1]Ruhr-Universität Bochum — [2]Imperial College London

The band structure of a type-II Weyl semimetal has pairs of electron and hole pockets that coexist over a range of energies and touch at a topologically protected conical point. While it is known, that in this case tunneling effects will lead to what is called a magnetic breakdown, the existence of these pairs of pockets at the Fermi energy also has an impact on the quantum oscillations associated with the topological Fermi arcs that exist on the surface of these materials. We analyze the quantum oscillations for a tight-binding model describing both Weyl I and Weyl II semimetals concentrating on the large field regime. The surface Fermi arcs coxisting with bulk electron and hole pockets lead to new experimental signatures of the quantum oscillations, which will be crucial for their experimental identification.

TT 21: Topological Insulators II (joint session HL/TT)

Time: Monday 15:00–17:30 Location: A 151

TT 21.1 Mon 15:00 A 151

Advanced MBE techniques for improved Bi2Se3 thin film growth — •Sarah Schmitt, Peter Schüffelgen, Abdur Jalil, Michael Schleenvoigt, Tobias Schmitt, Jonas Kölzer, Daniel Rosenbach, Thomas Schäpers, Gregor Mussler, and Detlev Grützmacher — Peter Grünberg Institut, Forschungszentrum Jülich & JARA Jülich-Aachen Research Alliance, D-52425 Jülich, Germany

Topological Insulators (TIs) are semiconductors with an inverted bulk band gap, but topologically protected states at their surface. The surface states exhibit promising features, useful for example for spintronic and quantum computing applications. In this study, we focus on the binary 3D TI Bi2Se3, which is unique due to its large bulk band gap and its freestanding Dirac point that lies in between valence and conduction band. However, binary compounds suffer from high back ground doping due to crystal defects in the bulk. To reduce defects in Bi2Se3, the quality of the thin films grown by molecular beam epitaxy (MBE) on Si(111) has been optimized. By varying the Bi, Se and substrate temperature as well as using InP as alternative substrate. The best conditions for low roughness, homogeneous domains and reduction of defects were investigated.

For transport measurements Hall bar structures were designed. To avoid defect formation during device fabrication, electrodes were deposited in-situ via stencil lithography. Still in-situ, the stencil mask was removed and the thin film capped with a thin dielectric layer to conserve the sample before taking it to ambient conditions. This technique allows the access to clean ultra-thin TI films by means of MBE.

TT 21.2 Mon 15:15 A 151

Interplay of Chiral and Helical states in a Quantum Spin Hall Insulator Lateral Junction — •M. R. Calvo[1,2,5], F. de Juan[2], R. Ilan[2], E. J. Fox[3], A. J. Bestwick[3], P. Leubner[4], J. Wang[3], C. Ames[4], S. C. Zhang[3], H. Buhmann[4], L. W. Molenkamp[3], and D. Goldhaber-Gordon[4] — [1]CIC Nanogune, San Sebastián, Spain — [2]Unversity of California, Berkeley, USA — [3]Stanford University, Stanford, USA — [4]Wuerzburg University, Wuerzburg, Germany — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

We study the electronic transport across an electrostatically gated lateral junction in a HgTe quantum well, a canonical 2D topological insulator, with and without an applied magnetic field. We control the carrier density inside and outside a junction region independently and hence tune the number and nature of 1D edge modes propagating in each of those regions. Outside the bulk gap, the magnetic field drives the system to the quantum Hall regime, and chiral states propagate at the edge. In this regime, we observe fractional plateaus that reflect the equilibration between 1D chiral modes across the junction. As the carrier density approaches zero in the central region and at moderate fields, we observe oscillations in the resistance that we attribute to Fabry-Perot interference in the helical states, enabled by the broken time reversal symmetry. At higher fields, those oscillations disappear, in agreement with the expected absence of helical states when band inversion is lifted.

TT 21.3 Mon 15:30 A 151

Topological transport in dimer chains — •Sina Böhling[1], Georg Engelhardt[1], Gernot Schaller[1], and Gloria Platero[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

In many fields, dimer chains have aroused great interest - not least because of the emergence of topologically protected edge states, localized to the two ends of the chain and promising lossless long-range transfer of particles. [1] Our work provides insight into properties of a dimer chain that is subject to dissipation. Applying an exact Green's function formalism applicable for any coupling strength, we investigate transport properties of a finite Su-Schrieffer-Heeger model, a paradigmatic model for a one-dimensional topological insulator, which is coupled to fermionic reservoirs at its ends.

For long chains, we observe that current and noise strongly decrease in the topologically non-trivial phase. This can be understood as a topological fingerprint, namely the occupation of edge states which are stronger coupled to the reservoirs than the conducting modes but do hardly contribute to the transmission. We show how to exploit this behavior to dissipatively prepare an edge state, while all other modes are practically unoccupied. Moreover, we discuss thermodynamic properties of the system by subjecting it to both, a potential and a thermal gradient, and discover regimes where the chain serves either as a heat engine or as a refrigerator.

[1] Bello, Creffield, Platero, Scientific Reports 6, 22562 (2016)

TT 21.4 Mon 15:45 A 151

Direct -1 to $+1$ Hall conductivity transitions in HgTe quantum wells — •Wouter Beugeling[1,2,3], Jan Böttcher[2], Christoph Brüne[1,4], Andreas Budewitz[1], Hartmut Buhmann[1], Ewelina M. Hankiewicz[2], Cristiane Morais Smith[5], and Laurens W. Molenkamp[1] — [1]Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany — [2]Institut für Theoretische Physik und Astrophysik (TP4), Universität Würzburg, Würzburg, Germany — [3]Lehrstuhl für Theoretische Physik I/II, Technische Universität Dortmund, Dortmund, Germany — [4]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway — [5]Institute for Theoretical Physics, Utrecht University, Utrecht, The Netherlands

Mercury telluride (HgTe) quantum wells have been one of the primary platforms for realization of topological states, due to its 'inverted' band structure. Typically, transport measurements of HgTe quantum well samples in a magnetic field show Hall quantization. The quantum spin Hall effect manifests itself as a special type of 'zero conductivity' Landau plateau.

We present remarkable transport measurement results, where the zero-conductivity plateau is absent, and where the Hall conductivity jumps from $-e^2/h$ to e^2/h directly. We provide a theoretical explanation, connecting this exotic transition to the 'second inversion', i.e., between the first electron (E1) and second heavy-hole (H2) subbands. We also discuss the effect of the exchange interaction induced by manganese (Mn) doping.

TT 21.5 Mon 16:00 A 151

Parallel conduction channels in topological insulator thin

films: Determination of conductance through bulk, interface and surface states — •Sven Just[1,2], Felix Lüpke[1,2], Peter Schüffelgen[1,2], Tristan Heider[1,2], Vasily Cherepanov[1,2], Gregor Mussler[1,2], Lukasz Plucinski[1,2], Detlev Grützmacher[1,2], Claus M. Schneider[1,2], F. Stefan Tautz[1,2], and Bert Voigtländer[1,2] — [1]JARA-FIT, Forschungszentrum Jülich, Germany — [2]Peter Grünberg Institute (PGI-3, PGI-6, PGI-9), Forschungszentrum Jülich, Germany

Topological insulator (TI) thin films can exhibit multiple parallel conduction channels for current transport. Beside the topological protected surface states (TSS) on top and bottom side of the film there can be more parasitic channels, i.e. the interior (bulk) of the not perfectly insulating TI film, the interface layer and the substrate. It is a crucial task to determine and minimize the influence of these parasitic parallel channels on the total current transport for taking advantage of the special TI properties in electronic devices. By using gate-dependent surface-sensitive four-probe measurements performed with a multi-tip STM and ARPES measurements in combination with theoretical calculations of the near-surface band-bending in the TI thin film, it is possible to disentangle the contributions of the different parallel conduction channels and to determine the conductivities of the interface reconstruction and the film bulk, as well as the charge carrier densities and mobilities of the top and bottom TSS for TI materials grown by van-der-Waals epitaxy, e.g. the ternary system $(Bi_{0.53}Sb_{0.47})_2Te_3$.

15 min. break.

TT 21.6 Mon 16:30 A 151

Quantum interference phenomena in selectively grown topological insulator nanoribbons — •Jonas Kölzer[1], Daniel Rosenbach[1], Tobias Schmitt[1], Christian Weyrich[1], Peter Schüffelgen[1], Michael Schleenvoigt[1], Sarah Schmitt[1], Abdur Rehman Jalil[1], Gregor Mussler[1], Vincent Sacksteder[2], Detelev Grützmacher[1], and Thomas Schäpers[1] — [1]PGI-9, Forschungzentrum Jülich and JARA-FIT, Germany — [2]Royal Holloway University of London, United Kingdom

Quantum topology offers a lot of intriguing physical phenomena and has a huge potential to realize robust quantum computing. Selectively deposited nano devices grown by means of molecular beam epitaxy (MBE) are a first step towards scalable topological insulator (TI) quantum computation.

In order to probe the evidence of topologically protected surface states, magneto conductance measurements are performed. In detail we studied quantum interference effects in the magneto conductance on selectively grown TI nanoribbons at low temperatures. From the conductance modulations we could trace distinct electron paths using FFT analysis in angular dependent measurements. Temperature dependent measurements reveal the quantum nature of the oscillations observed, since they vanish for increasing temperatures.

The next step in characterizing the material system will be to selectively grow Aharonov-Bohm ring structures to characterize quantum oscillations inside the van der Waals layer system.

TT 21.7 Mon 16:45 A 151

THz conductivity of charge puddles in the topological insulator BSTS — •Yu Mukai, Suqin He, Zhiwei Wang, Markus Grüninger, Yoichi Ando, and Paul H. M. van Loosdrecht — II, Physikalisches Institut, Universität zu Köln, Cologne, Germany

Strong Coulomb disorder in the compensation doped topological insulator $BiSbTeSe_2$ (BSTS) leads, at low temperatures, to the formation of charge puddles and consequently a non-monotonic temperature dependence of mid-infrared optical conductivity [1]. In contrast, the DC conductivity shows a monotonous decrease with temperature, as expected for an insulator [1]. To experimentally reconcile these observations we performed time domain THz spectroscopy on BSTS over the wide frequency range of 0.3 - 6 THz, thereby largely filling the gap between the DC and mid-infrared experiments. We present the temperature dependence of the conductivity spectrum in this energy range and discuss contributions from the charge puddles and thermally activated free carriers.

[1] Borgwardt et al., Phys. Rev. B 93, 245149 (2016).

TT 21.8 Mon 17:00 A 151

Topological design applied to the control of acoustic phonons — •Martin Esmann, Omar Ortiz, Fabrice R. Lamberti, Pascale Senellart, Aristide Lemaitre, and Daniel Lanzillotti-Kimura — CNRS Centre de Nanosciences et de Nanotechnologies (C2N), 91460 Marcoussis, France

The control and manipulation of acoustic phonons in the GHz-THz range appears as a new resource in the engineering of nanodevices. Here, we introduce the use of spatial mode symmetries of Bloch modes in a semiconductor superlattice to confine and control the propagation of phonons. We generate confined topological modes that are described by topological invariants and a topological transition upon band gap inversion [1]. This topological interface state between two finite size superlattices of different topology is a concept readily extendable to 3D in micropillars [2,3].

We experimentally evidence such a topologically confined nanophononic interface state in a planar structure both by coherent phonon generation (pump-probe) measurements and high resolution Raman scattering spectroscopy. Nanophononic topological interface states like the ones presented here could be at the base of developing single phonon sources, phononic sensors and phonon lasers, whose optical counterparts all led to key advances in applied photonics.

[1] M. Xiao et al., Phys. Rev. X 4, 021017 (2014).
[2] F. R. Lamberti et al., Opt. Express 25, 24437-24447 (2017).
[3] M. Esmann et al., submitted (2017).

TT 21.9 Mon 17:15 A 151

Low-dimensional topological Josephson junctions on selectively grown topological insulator nanoribbons — •Tobias W. Schmitt[1], Daniel Rosenbach[1], Peter Schüffelgen[1], Michael Schleenvoigt[1], Abdur R. Jalil[1], Chuan Li[2], Gregor Mussler[1], Stefan Trellenkamp[1], Alexander Brinkman[2], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich & JARA-FIT, 52425 Jülich, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

At the interface of a topological insulator and a s-wave superconductor, exotic Majorana modes are predicted to arise. In lateral topological Josephson junctions comprised of two superconducting leads on top of a topological insulator thin film, possible Majorana assisted transport is expected to occur in addition to conventional Andreev bound states. The latter superimpose the indications of Majorana excitations in Shapiro response measurements and make their detection more difficult. As the number of conventional Andreev bound states depends on the total number of conducting modes, their impact can be reduced in low-dimensional Josephson junctions. In our recent work, we focus on the realization of low-dimensional topological Josephson junctions by (I) selectively depositing TI nanoribbons of reduced width and (II) increasing of the Fermi wavelength by adjusting the Fermi level to the Dirac point of the linear disperse surface states. Such junctions have been prepared and characterized electrically at low temperatures, including their Fraunhofer diffraction pattern and their Shapiro response.

TT 22: Superconductivity: Topological Defects in Superconductors and Magnets (joint session TT/MA)

Time: Monday 15:00–17:45 Location: HFT-FT 101

TT 22.1 Mon 15:00 HFT-FT 101

Topological domain walls in helimagnets — •Laura Köhler[1], Peggy Schönherr[2], Jan Müller[3], Naoya Kanazawa[4], Yoshinori Tokura[4,5], Achim Rosch[3], Dennis Meier[6], and Markus Garst[1] — [1]Institut für Theoretische Physik, TU Dresden, Dresden, Germany — [2]Department of Materials, ETH Zürich, Zürich, Switzerland — [3]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany — [4]Department of Applied Physics, University of Tokyo, Tokyo, Japan — [5]RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan — [6]Department of Materials Science and Engineering, NTNU, Trondheim, Norway

The Dzyaloshinskii-Moriya interaction in chiral magnets stabilizes a magnetic helix with a wavelength set by the spin-orbit coupling. We study domain walls of helimagnetic order both theoretically and experimentally using micromagnetic simulations and magnetic force microscopy studies on surfaces of FeGe. We find that such domain walls are distinctly different from those in ferromagnets and rather similar to grain boundaries of liquid crystals. Three types of domain walls are realized depending on the relative domain orientation: a curvature wall, a zig-zag disclination wall and a dislocation wall. Disclinations are vortex defects in the helix axis orientation, and they can be combined to form dislocations. We discuss the topological skyrmion charge associated with these dislocations which can be finite. This leads to an emergent electrodynamics and thus a coupling to spin currents as well as to a contribution to the topological Hall effect.
[1] P. Schönherr et al. arXiv1704.06288 (2017).

TT 22.2 Mon 15:15 HFT-FT 101

Nanoscale imaging of magnetic topological defects in helimagnetic FeGe — •Peggy Schönherr[1], Jan Müller[2], Laura Köhler[3], Achim Rosch[2], Naoya Kanazawa[4], Yoshi Tokura[4,5], Manfred Fiebig[1], Markus Garst[3], and Dennis Meier[6] — [1]ETH Zürich, Switzerland — [2]Universität zu Köln, Germany — [3]Technische Universität Dresden, Germany — [4]University of Tokyo, Japan — [5]Riken, Japan — [6]NTNU Trondheim, Norway

Complex spin textures, like helical spin spirals with a fixed wavelength, can occur due to chiral magnetic interactions. Chiral magnets are a striking nanoscopic analog to liquid crystals, possessing lamellar phases and ordered topological defects. Defects are of great importance as they strongly influence order and mobility of the spin system. Here, we present magnetic force microscopy measurements in combination with micromagnetic simulations, discussing the dynamics and interactions of 1D and 2D objects with non-trivial topology in the helimagnetic phase of FeGe. We show that the local magnetization dynamics are strongly influenced by depinning and subsequent motion of edge dislocations (1D). Their motion is part of a slow relaxation process, having profound impact on the formation of the helical ground state. Other 1D objects that play an important role for the micromagnetism are so-called π disclinations, which can form chains and build domain walls that are distinctly different from classical antiferro- and ferromagnetic domain walls. Thus, our microscopy data reveal a new multitude of magnetic nano-objects with non-trivial topology going beyond the previously discussed skyrmions.

TT 22.3 Mon 15:30 HFT-FT 101

Mechanisms of nucleation of chiral bobbers in helical magnets — Fengshan Zheng[1,2], •Filipp N. Rybakov[3], Aleksandr B. Borisov[4], Dongsheng Song[5], Shasha Wang[6,7], Zi-An Li[8], Haifeng Du[6,7], Nikolai S. Kiselev[2], Jan Caron[1,2], András Kovács[1,2], Mingliang Tian[6,7], Yuheng Zhang[6,7], Stefan Blügel[2], and Rafal E. Dunin-Borkowski[1,2] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [3]Department of Physics, KTH-Royal Institute of Technology, Stockholm, Sweden — [4]M.N. Miheev Institute of Metal Physics, Ekaterinburg, Russia — [5]National Center for Electron Microscopy in Beijing, Tsinghua University, China — [6]High Magnetic Field Laboratory, Hefei, China — [7]Collaborative Innovation Center of Advanced Microstructures, Nanjing University, China — [8]Institute of Physics, Beijing, China

Magnetic chiral bobbers are stable particlelike states that represent a skyrmion texture combined with Bloch point [1]. Recently they were discovered experimentally in B20-type FeGe compound [2]. Here we present the detailed description on different mechanisms of nucleation of chiral bobbers which were revealed theoretically and then confirmed in experiments with FeGe specimens. The discussed mechanisms represent general phenomena and can be applied to a variety of other chiral magnetic compounds.
[1] F.N. Rybakov et al. PRL **115**, 117201 (2015).
[2] F. Zheng et al. arXiv:1706.04654 (2017).

TT 22.4 Mon 15:45 HFT-FT 101

Skyrmion optical creation/annihilation in a chiral magnet — •Gabriele Berruto[1], Ivan Madan[1], Yoshie Murooka[1], Giovanni Maria Vanacore[1], Enrico Pomarico[1], Damien McGrouther[2], Yoshihiko Togawa[2], Heinrik Rønnow[1], and Fabrizio Carbone[1] — [1]Institute of Physics, EPFL, Lausanne, Switzerland — [2]SUPA, University of Glasgow, United Kingdom

We show that single light pulses of different duration and color can create and annihilate skyrmions for a broad range of parameters in the magnetic phase diagram of a 50 nm-thick slab of FeGe, a prototypical chiral magnet. Using a combination of camera-rate and ns pump-probe cryo-Lorentz Transmission Electron Microscopy, we directly resolve the spatio-temporal evolution of the magnetization ensuing (fs and ns) optical excitation. When we excite optically the skyrmion lattice, its structural parameters are not modified, only the magnetization being affected: it transiently decreases, and recovers to the initial value over long (μs) time scales, reflecting the important role of the cooling rate of the system. Contrary to previously reported cases in different systems, in our experiment the skyrmions are not created via a transient demagnetized (paramagnetic) state. The laser pulses transiently heat the system, driving it into a region of the phase diagram where the appearance of skyrmions is strongly favored, but still staying far below the Curie temperature. The system then supercools down to base temperature, and skyrmions remain frozen into their (meta)stable state. The skyrmion topological charge is injected from geometric edges, defects, and magnetic boundaries.

TT 22.5 Mon 16:00 HFT-FT 101

Coupling of magnetic flux quanta to tunable domain structures in superconductor/ferromagnet bilayers with varying Dzyaloshinskii-Moriya interaction — •Palermo Xavier[1], Samokhvalov Alexei[3], Collin Sophie[1], Bouzehouane Karim[1], Santamaria Jacobo[1], Sander Anke[1], Reyren Nicolas[1], Cros Vincent[1], Buzdin Alexander[2], and Villegas Javier E.[1] — [1]Unité Mixte de Physique CNRS-Thales, Palaiseau, France — [2]Laboratoire Ondes et Matière d'Aquitaine (LOMA), Talence, France — [3]N.Novgorod, Russia

We study magneto-transport in hybrids combining superconducting films with magnetic multilayers in which varying the stacking sequence (e.g. Co/Pt vs. Ir/Co/Pt) allows tailoring the interfacial Dzyaloshinskii-Moriya interaction, and the characteristics of the magnetic domain structure. The magnetoresistance in the superconducting state shows a strong hysteresis, which is observed during the magnetization reversal and closely follows the reversal details. This behavior is in stark contrast with that expected for a plain superconducting film, and is strongly dependent on the size and morphology of the domain structure (presence of wormlike or skyrmion structures). The results can be understood in terms of mutual interaction between flux quanta and the local magnetization, which modifies vortex nucleation and mobility, and possibly the magnetic structure in the ferromagnets.

Work supported by the ERC grant N 64710 and French ANR grant ANR-15-CE24- 0008-01

TT 22.6 Mon 16:15 HFT-FT 101

Interactions between superconductor-ferromagnet thin films — •Annika Stellhorn[1], Anirban Sarkar[1], Emmanuel Kentzinger[1], Sonja Schröder[1], Grigol Abuladze[1], Markus Waschk[1], Patrick Schöffmann[2], Zhendong Fu[2], Vitaliy Pipich[2], and Thomas Brückel[1,2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich GERMANY —

[2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at MLZ, Lichtenbergstr. 1, 85748 Garching Germany

Interactions at superconductor-ferromagnet (S/F) interfaces have been studied on a prototype Nb (S)/ FePd (F) system. Our goal is to understand the proximity effects of FePd with different strength of perpendicular magnetic anisotropy (PMA) and magnetic domain texture on the superconducting Nb layer. Proximity effects at S/F interfaces with an inhomogeneous magnetic field texture result in various effects, like domain-wall superconductivity and long-ranged triplet cooper pairs in the F-layer, making them good candidates for superconducting spintronics. Epitaxial heterostructures of Nb/FePd are prepared on MgO (001) substrate using Molecular Beam Epitaxy. Magnetic Force Microscopy images of FePd grown by shuttered growth reveal a striped domain structure. Macroscopic magnetization measurements show weak PMA. However, co-deposition of FePd at varying temperatures results in different strength of PMA. Grazing-Incidence-Small-Angle-Neutron-Scattering reveals the depth profile of the magnetization in the heterostructure.

15 min. break.

TT 22.7 Mon 16:45 HFT-FT 101

Giant non-local vortex motion in WC nanowires grown by Ga+ focused ion beam deposition — •Rosa Córdoba[1,2], José María De Teresa[1,2,3], Ricardo Ibarra[2,3], Isabel Guillamón[4], Hermann Suderow[4], Sebastián Vieira[4], and Javier Sesé[2,3] — [1]Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC-UZ, Spain — [2]Departamento de Física de la Materia Condensada, Universidad de Zaragoza, Spain — [3]Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragón, UZ — [4]Departamento de Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain

In this contribution, we propose an unconventional route to transfer vortices as single particles through long distances (in the micrometers range), within WC nanowires (50 nm in width), taking profit of current-induced non-local vortex motion [1]. By reducing the lateral dimensions of wires near superconducting coherence length of the material, we measured a giant non-local electrical signal which is 40 times higher than those reported for wider wires of other superconductors. Comparing the non-local electrical signal in WC wires of different dimensions, we found that the signal for 50 nm-wide WC nanowires is nearly two orders of magnitude higher than for the 200 nm-wide WC ones. The measured giant non-local signal in the former strongly confirms that the vortex line is more rigid than the vortex lattice in wider wires due to its quasi-1D character and its confinement potential that prevents the transversal vortex displacements.

[1] R. Córdoba et al. manuscript submitted to Applied Physics Letters.

TT 22.8 Mon 17:00 HFT-FT 101

Unusual critical state and vortex commensurability in cuprate superconductors with regular topological defects — •Wolfgang Lang[1], Georg Zechner[1], Kristijan L. Mletschnig[1], Florian Jausner[1], Meirzhan Dosmailov[2], Marius A. Bodea[2], and Johannes D. Pedarnig[2] — [1]University of Vienna, Faculty of Physics, Wien, Austria — [2]Johannes-Kepler-University Linz, Institute of Applied Physics, Linz, Austria

The interaction of vortices with artificial defects in a superconductor is a vibrant topic in experimental and theoretical research, but also important for its prospects of technical applications. The advantage of a higher operation temperature in $YBa_2Cu_3O_{7-\delta}$ (YBCO) is opposed by the demand for advanced nanopatterning methods. To this end, YBCO thin films are irradiated with He^+ ions by shadow projection through a Si stencil mask to create a square array of columnar defect regions of 180 nm diameter and 300 nm lattice constant. Peaks of the critical current as a function of the applied magnetic field reveal the commensurate trapping of vortices in domains near the edges of the sample. Upon ramping an external magnetic field, an unconventional critical state emerges that is characterized by a pronounced hysteresis and different positions of the critical current peaks in virgin and field-saturated down-sweep curves, respectively. Interestingly, the distances of the various peaks in a sweep remain constant and correspond exactly to the matching field. The observations are interpreted as a nonuniform, terrace-like critical state, in which individual domains are occupied by a fixed number of vortices per pinning site.

TT 22.9 Mon 17:15 HFT-FT 101

Vortex motion and change inside the superconducting phase of the ferromagnetic superconductor UCoGe — •Beilun Wu[1], Dai Aoki[2,3], and Jean-Pascal Brison[2] — [1]Universidad Autonoma de Madrid, Spain — [2]CEA/University of Grenoble Alps, France — [3]Tohoku University, Japan

Ferromagnetic superconductors can show equal spin pairing superconductivity, in form, for example, of a p-wave pair wave function. Among the different candidates, the U-based single crystalline systems stand out because of the real coexistence between the superconducting and ferromagnetic order, and their numerous interesting properties, such as the unusual upper critical field and the field-induced re-entrant superconductivity. Recent measurements show that superconductive pairing is remarkably sensitive to the external magnetic field. However, it is unknown if the magnetic field induces strong difference in the pairing interaction in different parts of the phase diagram. Here we address this issue by a combined study of thermal and electrical transport in UCoGe, under magnetic field up to 15T. We observe that the resistive transition width considerably sharpens in the high field region. In addition, it lies at a lower temperature than the bulk transition observed in the thermal conductance. This shows strongly enhanced vortex mobility in this high field region, in which a freezing transition from a vortex liquid to a glass-like or solid lattice might occur. Meanwhile a sudden change in thermal conductivity is observed inside the superconducting phase. Altogether these results suggest a field-induced change in the superconducting phase. *supported by ERC Pnicteyes

TT 22.10 Mon 17:30 HFT-FT 101

Domain formation in the type-II/1 superconductor niobium — •Alexander Backs[1,2], Tommy Reimann[1,2], Michael Schulz[1,2], Vitaliy Pipich[1,3], Sebastian Mühlbauer[1], and Peter Böni[2] — [1]Heinz Maier-Leibnitz Zentrum, Garching, Germany — [2]Physik-Department E21, Technische Universität München, Garching, Germany — [3]Jülich Center for Neutron Research, Jülich, Germany

In type-II/1 superconductors, an attractive interaction between single magnetic vortices leads to the formation of a magnetic domain structure, denoted intermediate mixed state (IMS). The IMS is made up of flux free domains and regions containing a vortex lattice (VL) [1].

We have studied the nucleation and morphology of the IMS in the type-II/1 s-wave superconductor niobium [1] [2] with a combination of small and ultra small angle neutron scattering and neutron grating interferometry to gain information about the VL, the IMS domains and their spatial distribution, respectively. In the case of strong pinning, the magnetic structure changes from a homogeneous VL into clustered domains upon field cooling. This phase separation sets in below the freezing transition of the VL, thereby demonstrating how vortex pinning can be overcome on a local scale while macroscopically retaining it. The IMS scattering function shows strong similarities to the model of spinodal decomposition where the usual time dependence is implicit in the cooling process.

[1] E. H. Brandt and M. P. Das, Journal of Superconductivity and Novel Magnetism 24, 57 (2011)
[2] T. Reimann et al., Nat. Commun.6, 8813 (2015)
[3] T. Reimann et al., Phys. Rev. B 96, 144506 (2017)

TT 23: Graphene: Adsorption, Intercalation and Doping I (joint session O/TT)

Time: Monday 15:00–16:30 Location: MA 043

TT 23.1 Mon 15:00 MA 043

Intercalation of epitaxial graphene: possible mechanisms — •Mikolaj Lewandowski[1], Ewa Madej[2], Zygmunt Milosz[1], Dorota Wilgocka-Slezak[2], Michal Hermanowicz[3], Nika Spiridis[2], Jozef Korecki[2], Stefan Jurga[1], and Feliks Stobiecki[1] — [1]NanoBioMedical Centre, Adam Mickiewicz University, Umultowska 85, 61-614 Poznan, Poland — [2]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, 30-239 Krakow, Poland — [3]Institute of Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznan, Poland

Intercalation of epitaxial graphene (EG) with atoms of various elements may modify EG's structure and electronic properties, which is related both to the weakening of the graphene-support interaction, as well as the interaction of graphene with the intercalated material. We used scanning tunneling microscopy (STM), low energy electron microscopy (LEEM) and low energy electron diffraction (LEED) to study the mechanisms of intercalation of epitaxial graphene (EG) grown on Ru(0001) by thermal decomposition of ethylene (C_2H_4). The results revealed direct influence of graphene's preparation method on its structure and the intercalation mechanisms. The experimental results were supported by theoretical ab initio calculations.

Acknowledgment: The work was financially supported by the National Science Centre of Poland (OPUS project No. 2014/15/B/ST3/02927).

TT 23.2 Mon 15:15 MA 043

Modification of the graphene/SiC(0001) interface by intercalation of antimony — •Susanne Wolff[1], Florian Speck[1], Martina Wanke[1], Felix Timmermann[2], Manfred Albrecht[2], and Thomas Seyller[1] — [1]Professur für Technische Physik, TU Chemnitz, Reichenhainer Str. 70, D-09126 Chemnitz, Germany — [2]Lehrstuhl für Experimentalphysik IV, Universität Augsburg, Universitätsstr. 1 Nord, D-86159 Augsburg, Germany

Sublimation growth of graphene on SiC(0001) in argon atmosphere is a well-established method for the preparation of graphene. The first grown carbon layer is partially covalently bound to the Si atoms of the substrate. This so-called buffer layer lacks the electronic properties of graphene. A decoupling of the buffer layer from the SiC substrate can be achieved by intercalation, resulting in quasi-freestanding graphene, with electronic properties tuned by the choice of the intercalant.

We use x-ray photoelectron spectroscopy and angle-resolved photoelectron spectroscopy to investigate the intercalation of antimony. Antimony was deposited on the buffer layer by molecular beam epitaxy. Subsequent annealing in argon at atmospheric pressure results in an intercalation of metallic and oxidized antimony. A pre-intercalation annealing in argon enables an intercalation of metallic antimony only, resulting in a moderate n-type doping of the quasi-freestanding graphene.

TT 23.3 Mon 15:30 MA 043

Sulfur intercalation underneath single-layer graphene on Ru(0001) — •Lars Buss[1], Moritz Ewert[1,2], Jens Falta[1,2], and Jan Ingo Flege[1,2] — [1]Institute for Solid State Physics, University of Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany

The strong binding of epitaxially grown single-layer graphene to a wide range of transition metals has detrimental influence on its electronic properties. However, by lifting the interlayer coupling, e. g., via intercalation routes, its unique electronic properties can be restored. We have investigated the interaction of sulfur with single-layer graphene grown on Ru(0001) by ethylene exposure under UHV conditions with *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). At elevated temperature and under dimethyl disulfide background pressure, we observe that sulfur intercalates through the open edges of the graphene islands and proceeds along the substrate steps. Prolonged exposure to sulfur is also seen to induce cracking of the graphene islands perpendicular to the substrate steps, consistent with substantial relief of tensile strain after successful sulfur insertion underneath the graphene. This interpretation is backed by μLEED patterns collected from single graphene islands that consist of an incoherent superposition of the LEED patterns observed individually for pure graphene as well as pure sulfur adsorption on the clean Ru surface, indicating that the graphene layer is virtually decoupled from the substrate.

TT 23.4 Mon 15:45 MA 043

Photoemission study of the intercalation of transition metals underneath graphene on silicon carbide — •Richard Hönig, Philipp Espeter, Peter Roese, Karim Shamout, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Strasse 4a, 44227 Dortmund, Germany

Silicon carbide (SiC) is among the most promising substrates on the route to real-life graphene (G) applications. While the basic properties of G/SiC were well elucidated during the past decade, present research is focused on G/SiC as a building block of multilayer systems. In our study we analyze the interaction of G/SiC with magnetic transition metals in order to explore the potential for spintronic applications. Here, cobalt and nickel are most interesting due to a well-matched lattice constant.

The 6H-SiC(0001) samples are prepared by annealing in argon gas at atmospheric pressure leading to large-area growth. Then the sample is covered with thin transition metal films with thicknesses up to a few nanometers. Our main characterization methods are threshold photoemission electron microscopy (PEEM) and synchrotron based photoelectron spectroscopy (PES).

We performed a film thickness and temperature dependent study for Co on G/SiC and will present series of PEEM images acquired during in-situ sample annealing. Furthermore, on the basis of PES spectra we discuss the electronic structure of our sample system. Finally, we are looking forward to present first PEEM images of this sample system acquired with circularly polarized soft x-rays.

TT 23.5 Mon 16:00 MA 043

Decoupling of the graphene/ferromagnet interface by gold intercalation: Effect on optical constants — •Christine Jansing[1], Hans-Christoph Mertins[1], Markus Gilbert[1], Maxim Krivenkov[2], Andrei Varykhalov[2], Oliver Rader[2], Andreas Gaupp[2], Andrey Sokolov[2], Hud Wahab[3], Heiko Timmers[3], Dominik Legut[4], and Peter M. Oppeneer[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic — [5]Department of Physics and Astronomy, Uppsala University, S-75120 Uppsala, Sweden

X-ray absorption and reflectance spectroscopy of linearly polarized synchrotron radiation across the carbon 1s edge of graphene/Co/W and graphene/Ni/W is utilized to investigate the effect of gold intercalation on the complex optical constants of these systems. The p_z-orbitals of graphene hybridize strongly with the $3d$ states of the ferromagnetic substrate. Hybridization effects can be reduced by intercalation of gold which also leads to a change in the optical constants. A complete set of optical constants was determined, describing the π*- and σ*- resonances of graphene. The absorption index k was directly deduced from the measured absorption spectra whereas the refractive index n has been extracted from k via a Kramers-Kronig transformation. Based on these optical constants reflection spectra have been simulated that are in good agreement with our experimental data.

TT 23.6 Mon 16:15 MA 043

Graphene protected surface state on Ir(111) with adsorbed lithium — •Predrag Lazic[1] and Petar Pervan[2] — [1]Rudjer Boskovic Institute, Zagreb, Croatia — [2]Institute of Physics, Zagreb, Croatia

It is well known that electronic surface states get strongly perturbed upon the chemical adsorption of very small amount of adsorbates. Adsorption of lithium atoms on Ir(111) is no expection to that rule. Iridium surface state get strongly perturbed and is practically eradicated - it can not be seen as a sharp peak in the ARPES measurement. However, if the graphene is added on top of Ir/Li system the iridum surface state magically reapears. We present a combined experimental and theoretical study of the described system. Using the density funcional theory calculations for large unit cells with disordered lithium atoms geometries on the (111) surface of iridium we were able to re-

produce the results of the ARPES measurements -showing clearly that the surface state signal is strongly suppresed when lithium is adsorbed, while it is almost unchanged when lithium is intercalated (i.e. with graphene on top of it). Looking at the projected density of states we constructed a rather simple model explaining this behavior which seems to be general.

TT 24: Graphene: Adsorption, Intercalation and Doping II (joint session O/TT)

Time: Monday 16:45–18:15 Location: MA 043

TT 24.1 Mon 16:45 MA 043

Initial investigation of the coexistence of different structural conformations, obtained via high temperature deposition of PbPc on epitaxial graphene grown on 6H-SiC(0001) — •Chitran Ghosal[1,2], Samir Mammadov[1], Martina Wanke[1], Florian Speck[1], Thomas Seyller[1], and Christoph Tegenkamp[2] — [1]Professorship of Technical Physics, Institute of Physics, TU-Chemnitz — [2]Professorship of Solid Surfaces Analysis, Institute of Physics, TU-Chemnitz

Epitaxial deposition is one of the well documented ways of doping of graphene[1]. Therefore, it is crucial to be able to study the different possible structural configurations that can be obtained via the deposition techniques.

This study deals with the analysis of different periodic structures obtained via the deposition of PbPc on epitaxial graphene, which was grown on 6H-SiC(0001) surfaces. The graphene was characterized by LEED and high resolution XPS measurements as well as STM. PbPc molecules were deposited afterwards at high temperatures of around 330degC and densely packed molecular films were grown under UHV conditions. Fourier analysis of large scale STM images revealed the coexistence of two non-orthogonal lattice structures (1.2nm X 1.6nm) and (1.35nm X 1.4nm) forming different islands separated by grain boundaries in between. The variability of the structures underlines the weak interaction of the PbPc molecules with the substrate.

[1] I. Gierz, C. Riedl, U. Starke, C. R. Ast, and K. Kern, Nano Lett. 8, 4603 (2008).

TT 24.2 Mon 17:00 MA 043

Investigation of PbPc self-assembly on graphene: Atomic resolution and spectroscopy data — •Nhung Nguyen[1,2], Ha Nguyen[1], and Christoph Tegenkamp[1] — [1]TU Chemnitz — [2]Duy Tan University, Vietnam

Shuttlecock-like lead-Phthalocyanine (PbPc) with its two equivalent stable up- and down states corresponding to ON/OFF switch is used for high density data storage of three- orders-magnitude capability higher than the present high density storage materials capability [1]. In addition, absorption of organic molecules on graphene surface due to the charge transfer mechanism between them is one of the promising methods to break the symmetries in graphene, localize the electronic states toward open a bandgap, which makes graphene useful as a nanoelectronics material [2]. Here the self-assembly of PbPc on one monolayer graphene/SiC surface is investigated by means of scanning tunneling microscopy and spectroscopy (STM/STS) in ultra-high vacuum. Due to the weak molecule-substrate interaction as well as the thermodynamic stability, shuttlecock PbPc molecules are only deposited with Pb atom pointing upward (face-up) into the first monolayer, but face-up or face-down states appear randomly on the second layer. The occupied and unoccupied orbitals of PbPc on graphene are distinguished intuitively. The influences of surface coverage, substrate temperature and substrate properties (buffer layer and quasi-free-standing graphene substrates) on self-assembly of PbPc will be discussed. [1] Phys Chem Chem Phys., 2015, 17,23651. [2] PhysRevB., 2009, 80, 033404.

TT 24.3 Mon 17:15 MA 043

Physical adsorption on graphene: from ultra-long ranged attraction to full screening of weakly interacting substrates — •Alberto Ambrosetti and Pier Luigi Silvestrelli — via Marzolo 8, 35131 Padova, Italy

The Lifshitz-Zaremba-Kohn (LZK) theory is commonly regarded as the correct large-distance limit for the van der Waals (vdW) interactions between adsorbates and solid substrates. However, recent experiments are challenging the universality of the LZK theory over a broad spectrum of nanoscale materials. By overcoming the conventional *local* permittivity approximation, here we demonstrate that physical adsorption on graphene and other low-dimensional materials can exhibit highly non-trivial features. Substrate-adsorbate vdW interactions can be extremely long-ranged and externally tunable. Moreover, graphene can effectively screen weakly interacting supporting substrates, emerging as an effective tool for the experimental modulation of adsorption processes.

TT 24.4 Mon 17:30 MA 043

Advances in ultra-low energy ion implantation of low dimensional materials — •Hans Hofsäss and Manuel Auge — II. Physikalisches Institut, Universität Göttingen, Germany

Doping of 2D materials by ion implantation has unique requirements regarding ion energy, ion energy spread, ion beam optics, sample preparation and sample electrical conductivity. Efficient incorporation of low energy ions into 2D lattices requires energies well below 50 eV. We use a 30 keV mass selected ion beam, guided through differential pumping stages and homogenized by a beam sweep. The beam is then decelerated in a UHV-chamber down to energies as low as 10 eV onto an area of 1 cm^2 up to 2.5 cm^2. Up to now ion sources are available for B, C, N ,F, P, S, Mn, Se, W and Au ions. Ion sources for elements Al, Fe, As and rare earth elements are under development. The implanted areal concentration and elemental composition are verified with in-situ Auger spectroscopy and more quantitative with Rutherford backscattering by implanting into amorphous carbon films as test samples. The detection limit is below $1*10^{14}$ ions/cm^2 for heavier elements. Implanted B can be analyzed with the $^{11}B(p,2\alpha)\alpha$ nuclear reaction with a detection limit of about $1*10^{14}$ B/cm^2. Challenges for ULE ion implantation such as non-flat substrates, charging of substrates, cleaning of surfaces and lateral controlled implantation will be briefly discussed. Some examples for doped graphene and MoS_2 are presented

TT 24.5 Mon 17:45 MA 043

growth of fe3o4 nanorod arrays on graphene sheets for application in electromagnetic absorption fields — •huanming zhang[1], min zhou[1], yang xu[1], shipu xu[1], yujin chen[2], and yong lei[1] — [1]Institute für Physics & IMN MacroNano (ZIK), Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Key Laboratory of In-Fiber Integrated Optics, Ministry of Education, College of Science, Harbin Engineering University, 150001 Harbin, China

A facial strategy is developed to fabricate a three-dimensional (3D) Fe3O4 nanorod array/graphene architecture, in which Fe3O4 nanorods with a length and diameter of about 600 and 100 nm, respectively, are grown on both surfaces of the graphene sheets. The measured electromagnetic parameters show that the 3D architecture exhibits excellent electromagnetic wave-absorption properties, that is, more than 99*% of electromagnetic wave energy can be attenuated by the 3D architecture if it is added in only 20 wt*% of the paraffin matrix, as the thickness of the absorber is in the range from 2.38 to 5.00 mm. The analysis of the electromagnetic (EM) absorption mechanism reveals that the excellent EM absorption properties are related to the special 3D architecture, and therefore, the construction of graphene-based 3D heteronanostructures is effective in obtaining lightweight EM absorbers with strong absorption properties.

TT 24.6 Mon 18:00 MA 043

Continuous in-plane graphene-hexagonal boron nitride layer from a single molecular precursor — •Federica Bondino[1], Silvia Nappini[1], Igor Píš[1,2], Tevfik Onur Menteş[2], Alessandro Sala[2], Andrea Locatelli[2], Stefano Agnoli[3], Mattia Cattelan[3], and Elena Magnano[1] — [1]IOM-CNR, Laboratorio TASC, S.S. 14-km 163.5, 34149 Basovizza, Trieste, Italy — [2]Elettra - Sincrotrone Trieste S.C.p.A., S.S. 14-km 163.5, 34149 Basovizza, Trieste, Italy — [3]Department of Chemical Sciences, University of Padua, Padova 35131, Italy

We will show that it is possible to grow a continuous sp2 hybridized material composed by graphene and hexagonal-boron nitride (h-BNG)

in the same two dimensional sheet with the thermal decomposition of a single molecular precursor [1,2]. This surface-synthesis route allows an easy and controlled preparation of an high-quality h-BNG monolayer on the surface of several substrates. The temperature is the principal parameter to selectively grow the h-BNG layer in competition with hybridized B-C-N layers. The reactivity and the confinement of metal nanostructures in the interface between h-BNG and its solid substrate will be discussed in comparison with graphene. Basic processes, chemical composition, substrate interaction and changes accompanying the growth and intercalation process will be discussed based on results obtained by synchrotron radiation experimental techniques, such as high-resolution X-ray photoelectron spectroscopy and microscopy and X-ray absorption spectroscopy. 1. S. Nappini et al. Adv.Funct.Mater. 26, 1120 (2016). 2. S. Nappini et al. Carbon 120, 185 (2017).

TT 25: Frontiers of Electronic-Structure Theory: Correlated Electron Materials II (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Monday 15:00–17:15 Location: HL 001

TT 25.1 Mon 15:00 HL 001

Non-adiabatic Dynamics in Single-Electron Tunneling Devices with Time-Dependent Density Functional Theory — •Niklas Dittmann[1,2,3], Janine Splettstoesser[2], and Nicole Helbig[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden — [3]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany

The recent advance of various single-electron sources in solid-state setups has sparked interest in the investigation of electronic transport at the single-particle level. In our recent work (N. Dittmann, J. Splettstoesser, N. Helbig, arxiv:1706.04547), we put forward time-dependent density-functional theory to calculate the dynamics of interacting electrons in single-electron tunneling devices. As a physical system, we analyze a single-electron source which is built by a quantum dot tunnel-coupled to a nearby electron reservoir and driven by a time-dependent gate voltage. By using analogies with quantum-transport theory, we extract a time-nonlocal exchange-correlation potential for a Hubbard U on-site interaction on the quantum dot. The time nonlocality manifests itself in a dynamical potential step, which we explicitly link to physical relaxation time scales of the electron dynamics. Finally, we discuss prospects for simulations of larger mesoscopic systems.

TT 25.2 Mon 15:15 HL 001

Dissipative exchange-correlation functional in QED-TDDFT — •Camilla Pellegrini[1], Ilya Tokatly[2,3], and Angel Rubio[2,4] — [1]Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Nano-bio Spectroscopy Group and ETSF Scientific Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48001 Bilbao, Spain — [4]Max Planck Institute for the Structure and the Dynamics of Matter, Luruper Chausse 149, 22761 Hamburg, Germany

Time-dependent density functional theory has been recently extended to treat many-electron systems coupled to quantized electromagnetic modes. Here we discuss the implications of this approach for the theory of open quantum systems. In particular we show that in the limit of continuous spectrum of photon modes, QED-TDDFT naturally leads to time-dependent density functional theory for dissipative systems coupled to the Caldeira-Leggett bath. We consider the application to the Ohmic spin boson model and show that the developed approximation to the exchange-correlation functional describes the natural linewidth of the electronic linear density response function.

TT 25.3 Mon 15:30 HL 001

Electric and magnetic response properties of solids from the current density — •Rubén Rodríguez Ferradás[1], Pina Romaniello[2], and Arjan Berger[1] — [1]LCPQ, University of Toulouse, France — [2]LPT, University of Toulouse, France

The evaluation of the macroscopic polarization and magnetization of solids is problematic when periodic boundary conditions are used because surface effects are artificially removed. This poses a problem unless surface effects can be reformulated in terms of bulk quantities [1-5]. In this work we show the advantage of calculating electric and magnetic response properties of solids using the current density as basic variable. An efficient approach to calculate the current density is time-dependent current-density-functional theory. We will show results for optical properties of solids using a recently developed functional [6]. We will also discuss how the magnetization can be described within this framework.

[1] F. Kootstra, P.L. de Boeij, and J.G. Snijders, J. Chem. Phys. 112, 6517.

[2] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 71, 155104 (2005).

[3] P. Romaniello and P.L. de Boeij, Phys. Rev. B 71, 155108 (2005).

[4] J.A. Berger, P. Romaniello, R. van Leeuwen, and P.L. de Boeij, Phys. Rev. B 74, 245117 (2006).

[5] J.A. Berger, P.L. de Boeij, and R. van Leeuwen, Phys. Rev. B 75, 035116 (2007).

[6] J.A. Berger, Phys. Rev. Lett. 115, 137402 (2015)

TT 25.4 Mon 15:45 HL 001

Coupling Maxwell's equations to the time-dependent Kohn-Sham equations: near-field effects and electromagnetic backreaction — •Rene Jestaedt[1], Micael Oliveira[1], Angel Rubio[1,2,3], and Heiko Appel[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, USA — [3]Nano-bio Spectroscopy Group and ETSF, Universidad del País Vasco, 20018 San Sebastián, Spain

Induced currents in large molecular and condensed matter systems are non-negligible and can affect the conductivity and the optical properties of the system. In the present work, we have implemented the real-time propagation of Maxwell's equations in Riemann-Silberstein representation to use standard unitary propagation techniques in the TDDFT code octopus [1]. The Maxwell and the Kohn-Sham system are coupled via a predictor-corrector method to obtain a self-consistent time-evolution of the total system [2]. Explicitely solving the microscopic Maxwell's equations also allows us to determine the optical properties of the system directly from the Maxwell fields. We show near-field effects of a full Maxwell-matter and matter-Maxwell coupling for plasmon excitations in metallic nanoparticles [2,3] and for ring-currents in organic molecules [2].

[1] Alejandro Varas et al., J. Phys. Chem. Lett. 2015, **6**, 1891-1898 / [2] R. Jestädt et al., (to be submitted) / [3] X. Andrade et al., Physi. Chemistry Chem. Physics 2015, **17** 31371-31396

TT 25.5 Mon 16:00 HL 001

Enhanching excitation energy and charge transfer with strongly correlated light-matter interaction — •Christian Schäfer[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

Förster excitation energy and charge transfer are fundamental processes of chemical reactions and connected to interesting quantities such as correlation. Often this correlation is taken as fixed property of the system.

In the current work, we present how the coupling to cavity photons in a minimal realistic molecular system can drastically alter transfer characteristics, e.g. renders the excitation transfer to be distance independent [1,2]. The photonic interaction can imprint fermionic correlation on arbitrary distances.

The exact real-space description is suited to describe transfer and correlation in a unprejudiced ab-initio picture and allows us to extend our insights beyond common quantum-optical approximations.

[1] X. Zhong et al., Angew Chem Int Ed Engl. **56(31)**, 9034 (2017). [2] M. Slootsky et al., PRL **112**, 076401 (2014).

TT 25.6 Mon 16:15 HL 001

Effects of electronic correlations on the magnetic properties of organometallic molecules — •Sumanta Bhandary and Silke Biermann — Centre de Physique Thèorique, Ecole Polytechnique, 91128 Palaiseau, France

The realm of molecular spintronics relies on the external accessibility of molecular magnetic states. In correlated organometallic complexes, a delicate balance between the crystal field, Coulomb repulsion and dynamical hybridization between metal center and organic ligands dictates the electronic and magnetic properties and often poses challenges for an accurate theoretical modelling. We have employed density functional theory (DFT), the GW approach and Anderson's impurity model (AIM) technique to study the ground state electronic and magnetic properties of transition metal-based porphyrin and phthalocyanine molecules, both in the gas phase [1] as well as while adsorbed on surfaces. Our study reveals that the dynamical correlation effects are important in order to accurately estimate spin-transition energies, magnetic anisotropy energies as well as the ground state electronic configurations in the molecular complexes. We have explored the manipulation of surface molecule interactions to externally influence the electronic and magnetic properties of the molecular system.

[1] S. Bhandary, M. Schüler, P. Thunström, I. di Marco, B. Brena, O. Eriksson, T. Wehling, and B. Sanyal, Phys. Rev. B **93**, 155158 (2016).

TT 25.7 Mon 16:30 HL 001

Structural, electronic and optical properties of cubic and tetragonal $SrTiO_3$: a DFT study including many-body effects — •Vijaya Begum, Markus E. Gruner, and Rossitza Pentcheva — Faculty of Physics and Centre for Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg.

$SrTiO_3$ (STO) is of fundamental interest as a substrate material in oxide electronics. The bulk undergoes a phase transition from the cubic to a tetragonal structure at T=105 K accompanied by characteristic antiferrodistortive rotations of the TiO_6 octahedra. We present a systematic comparison of the performance of the gradient corrected exchange correlation functional (GGA), the strongly constrained and appropriately normed (SCAN) meta-GGA and the hybrid functional HSE06 with respect to the electronic, structural and optical properties of cubic and tetragonal STO. For the tetragonal structure, SCAN gives a significantly improved description of the structural properties, comparable to HSE06, at a computational cost similar to GGA. The experimental band gap can be reproduced within SCAN with an on-site Hubbard term ($+U$), whereas within GGA the gap is underestimated even for very high U values. We calculate the optical spectrum for both phases, including many-body effects and excitonic corrections within the GW+Bethe-Salpeter equation approach, and compare this to previous theoretical results for the cubic phase [PRB 87, 235102 (2013)] and experiment [PRB 93, 075204 (2016)]. Funding by the DFG within SFB1242, project C02 is gratefully acknowledged.

TT 25.8 Mon 16:45 HL 001

Unveiling the mysterious magnetic state of superconducting iron under pressure — •Matteo d'Astuto — Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — IMPMC, UMR CNRS 7590, Sorbonne Universités-UPMC University Paris 06, MNHN, IRD, 4 Place Jussieu, F-75005 Paris, France

Compressed iron undergoes a transition from bcc to hcp crystal structure with a loss of ferromagnetism. The magnetic state of the hcp phase has been debated for many decades and experiments give seemingly contradictory results. Mössbauer measurements find no magnetism, however x-ray emission spectroscopy finds remnant magnetism and Raman mode splitting suggests symmetry breaking due to antiferromagnetism. These paradoxical results are consistent with either a paramagnetic state with spin fluctuations faster than Mössbauer timescales or an antiferromagnetic state, afmII, which is undetectable with Mössbauer spectroscopy. We performed neutron powder diffraction measurements in the hcp phase and do not observe afmII order down to 1.8 K, while confirming the existence of a local magnetic moment in the hcp phase with x-ray emission spectroscopy and find it is intrinsic to this phase (1). This local magnetic moment disappears at 30–40 GPa, exactly the same pressure region where superconductivity disappears.

(1) B. W. Lebert, T. Gorni J.-P. Rueff, S. Klotz, M. Casula, A. Juhin, J. M. Ablett, F. Baudelet, T. Straessle, T. Hansen, A. Polian, P. Munsch, G. Le Marchand, Z. Zhang, M. d'Astuto, article in preparation.

TT 25.9 Mon 17:00 HL 001

Frist-principle and experimental characterisation of the electronic properties of CaGaSiN3 and CaAlSiN3: impact of chemical disorder — •Jan Minar[1], Ondrej Sipr[2], Robin Niklaus[3], Jonas Hausler[3], and Wolfgang Scgnick[3] — [1]New Technologies Research Center, University of West Bohemia, Pilsen, Czech Rep., — [2]FZU, Academy of Sciences, Czech Rep — [3]Department of Chemistry, University of Munich, Munich, Germany

We report a detailed investigation of the electronic, mechanical and optical properties of the recently discovered nitridogallosilicate CaGaSiN3 which has potential as a LED-phosphor host material. We focus on chemical disorder effects, originating from the Ga/Si site, and compared them to those of isostructural CaAlSiN3. We calculate the elastic moduli and the Debye temperature in terms of quasi harmonical approximation. Spectral properties like the joint density of states (JDOS) are evaluated and the absorption, reflectance and energy loss function are obtained from the dielectric function. The optical band gap of CaGaSiN3 from experiment is compared to the electronic band gap in terms of electronic DOS and band structure calculations. All properties are evaluated for different ordering models of Ga/Si while the experimentally observed substitutional disorder is accounted for by utilizing the Coherent Potential Approximation (CPA). We conclude a shrinking of the band gap for both CaGaSiN3 and CaAlSiN3 due to atomic disorder, which is unfavorable for potential phosphor applications [1]. R. Niklaus, J. Minar, J Häusler, W. Schnick, Physical Chemistry Chemical Physics 19 (13), 9292 (2017)

TT 26: Skyrmions I (joint session MA/KFM/TT)

Time: Monday 15:00–18:30 Location: EB 301

Topical Talk TT 26.1 Mon 15:00 EB 301

Structure, Energetics, and Deterministic Writing of Skyrmions in Thin Film Ferromagnets — •Felix Büttner — MIT, Cambridge, MA, USA

Room temperature skyrmions were recently observed in magnetic multilayer systems [1-4], most of them in materials with sizable Dyzaloshinskii-Moriya interaction (DMI). In this talk, I will present a unified theory that analytically describes the energy of such skyrmions, including stray fields [1]. We can now rigorously define two types of skyrmions, "stray field skyrmions" and "DMI skyrmions". DMI skyrmions can be sub-10 nm at zero field and room temperature and moved with velocities exceeding 1000 m/s at 10^{12} A/m^2.

Experimentally, I will show that skyrmions can be nucleated by spin-orbit torque current pulses without any applied fields [2]. The nucleation mechanism is robust, ultra-fast (sub-nanosecond), and extremely easy to implement. I will discuss the mechanism of the skyrmion generation and explain why DMI can replace the need for in-plane fields.

[1] Büttner et al., Nat Phys. 11, 225 (2015). [2] Woo et al., Nat Mater. 15, 501 (2016). [3] Moreau-Luchaire et al., Nat Nano. 11, 444 (2016). [4] Boulle et al., Nat Nano. 11, 449 (2016). [5] Büttner et al., arXiv:1704.08489 [6] Büttner et al., Nat Nano. 12, 1040 (2017).

TT 26.2 Mon 15:30 EB 301

Skyrmion bubble size and density control in Ta/CoFeB/MgO wedges — •Christian Denker[1], Sören Nielsen[2], Enno Lage[2], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Institut für Physik, Universität Greifswald, Germany — [2]Nanoscale Magnetic Materials - Magnetic Domains, Institute for Materials Science, Universität Kiel, Germany

After the observation of skyrmion bubbles at room temperature in Ta/CoFeB/TaO_x layers by A. Hoffmann's group, skyrmions have been found in various heavy metal/ferromagnet/oxide systems. For skyrmion generation and detection by magnetic tunnel junctions (MTJ), the Ta/CoFeB/MgO system is appealing due to high TMR ratios and its technological maturity. As a starting point typical MTJ bottom electrodes and barriers (5 nm Ta/x CoFeB/3 nm MgO) trilayers with an optional Ru capping were deposited by e-beam evaporation (MgO, Ru) and magnetron sputtering (Ta, CoFeB). We will present our results on skyrmion bubbles observed by magneto-optical Kerr effect microscopy as function of continuous variation of CoFeB thickness. The in- to out-of-plane transition for the magnetic anisotropy is found at about $x = 1.4$ nm. At slightly thinner CoFeB thicknesses skyrmions can be nucleated. Their size can be as small as 300 nm. The influence of CoFeB composition and annealing temperature on the skyrmion formation, as well as skyrmion stability will be discussed.

TT 26.3 Mon 15:45 EB 301

Small angle neutron scattering experiments of skyrmions far from equilibrium — •Alfonso Chacon[1], Marco Halder[1], Andreas Bauer[1], Wolfgang Simeth[1], André Heinemann[2], Sebastian Mühlbauer[2], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum, Garching, Germany

The prospect of the application of magnetic skyrmions in next-generation spintronic devices has recently created substantial scientific interest in this type of magnetic order. Stabilized by thermal fluctuations closed to the paramagnetic order, skyrmion lattices in cubic chiral magnets are constrained to a small window a few Kelvin wide. Recent developments have demonstrated how to expand this regime down to low temperatures by means of supercooling, electrical fields, or uniaxial pressure. Thus, it is possible to study this topological type of magnetism far from equilibrium. We report detailed small angle neutron scattering experiments on skyrmion lattices in B20 compounds at very low temperatures stabilized through fast cooling and discuss the role of disorder and magnetocrystalline anisotropies in their stabilization.

TT 26.4 Mon 16:00 EB 301

Entropy limited topological protection of skyrmions in $Fe_{1-x}Co_xSi$ — Johannes Wild[1], •Thomas Meier[1], Simon Pöllath[1], Matthias Kronseder[1], Andreas Bauer[2], Alfonso Chacon[2], Marco Halder[2], Marco Schowalter[3], Andreas Rosenauer[3], Josef Zweck[1], Jan Müller[4], Achim Rosch[4], Christian Pfleiderer[2], and Christian Back[1] — [1]Institut für experimentelle und angewandte Physik, Universität Regensburg — [2]Physik-Department, Technische Universität München — [3]Institut für Festkörperphysik, Universität Bremen — [4]Institut für Theoretische Physik, Universität zu Köln

Topologically protected magnetic textures in materials with broken inversion symmetry are considered as future high-density data storage media. The life time of these textures therefore plays a crucial role for data retention. We have used Lorentz transmission electron microscopy to infer the energetics of the topological decay of magnetic skyrmions far from equilibrium in the chiral magnet $Fe_{1-x}Co_xSi$. We investigated the decay of a lattice of sykrmions at different magnetic fields and temperatures by imaging the magnetic configuration of the system in real-time with a high speed camera. We observed that the skyrmion life time τ extracted from these movies depends exponentially on temperature following an Arrhenius law, $\tau \propto \tau_0 \exp(\Delta E/k_B T)$. The prefactor τ_0 of this Arrhenius law changes by more than 30 orders of magnitude for small changes of magnetic field reflecting a substantial reduction of the life time of skyrmions by entropic effects and thus an extreme case of enthalpy-entropy compensation.

TT 26.5 Mon 16:15 EB 301

Magnetotransport and Hall effect of MnSi thin film under pressure — •David Schroeter[1], Stefan Süllow[1], Dirk Menzel[1], Hiroyuki Hidaka[2], Hideto Okuyama[2], and Hiroshi Amitsuka[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Graduate School of Science, Hokkaido University Sapporo, Japan

In the recent years thin films of the B20 compound MnSi became subject of great interest, since the magnetic properties of bulk MnSi are modified due to the dimensional reduction and the uniaxial anisotropy with a suspected stabilized skyrmionic phase [1]. In comparison to bulk material MnSi thin film shows an enhanced ordering parameter with ongoing research about the nature of the magnetic order in thin film state [2].

The ordering temperature and critical fields of MnSi decrease with applied hydrostatic pressure, with thin film material recovering bulk values for the transition temperature at $p_{recover} \approx 2.3$ GPa and a qualitatively similar behavior to bulk MnSi with respect to the ordering temperature above $p_{recover}$ [3]. We present magnetotransport and Hall effect measurements on MnSi thin films under applied pressure of up to around 4 GPa and discuss our results concerning the magnetic phase diagram under pressure.

[1] A. B. Butenko et al., Phys. Rev. B 82, 052403 (2010).
[2] M. N. Wilson et al., Phys. Rev. B 86, 144420 (2012).
[3] J. Engelke et al., Phys. Rev. B 89, 144413 (2014).

TT 26.6 Mon 16:30 EB 301

Magnetic anisotropy in the itinerant helimagnet MnSi — •Schorsch M. Sauther[1], Andreas Bauer[1], Dirk Grundler[2], Christian Pfleiderer[1], and Marc A. Wilde[1] — [1]Phys.-Dep. E51, TU München — [2]LMGN, IMX, STI, EPF Lausanne

We report torque magnetometry in Manganese silicide (MnSi). In our experiment, we employ cantilever magnetometry in a 2D magnetic field $\vec{B} = B \cdot (\sin\varphi \quad \cos\varphi)$ to measure the torque τ resulting from the anisotropic magnetization $\vec{M}_\perp$ of a high-quality, single-crystalline bulk sample of MnSi. The angular dependence $\tau(\varphi)$ displays distinct oscillations with differently pronounced extrema. The oscillation amplitude between several extrema does not saturate for our maximum field of 4.5 T. In the field dependence $\tau(B)$ we observe an unexpected hysteresis above H_{c2}. Furthermore, the hysteretic behavior below H_{c2} changes drastically with temperature below T_c. We utilize our observations to determine the anisotropy constants and discuss our results in the context of complementary experiments[1].

[1] A. Bauer *et al.*, Phys. Rev. B **95**, 024429 (2017)

15 min break

TT 26.7 Mon 17:00 EB 301

Inelastic neutron scattering studies of magnons in the field polarized, conical and Skyrmion phase of MnSi — •Lukas Beddrich[1], Tobias Weber[3], Robert Georgii[1,2], and

Peter Böni[1] — [1]Physik-Department E21, Technische Universität München, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany — [3]Institut Laue-Langevin (ILL), 38000 Grenoble, France

Cubic chiral magnets, such as MnSi, are prototypical systems for the investigation of various spin structures. They are stabilized by the Dzyaloshinsky-Moriya interaction (DMI), which also gives rise to a universal magnon dispersion [1], [2].

Recently, the effect of non-reciprocal spin wave excitations, which generally emerge from the lack of inversion symmetry, were intensively studied in the field-polarized and helimagnetic phase of MnSi with inelastic neutron scattering [3]. Due to the excellent compatibility between the low-energy theory and the comprehensive measurements, we currently apply a related approach to describe the magnetic excitations found in the skyrmion phase.

[1] M. Janoschek et al. *Phys. Rev. B*, 81:214436, Jun 2010 doi:10.1103/PhysRevB.81.214436

[2] M. Kugler et al. *Phys. Rev. Lett.*, 115:097203, Aug 2015. doi:10.1103/PhysRevLett.115.097203

[3] T. Weber et al. *submitted for publication*

TT 26.8 Mon 17:15 EB 301

Orientation dependence of the magnetic phase diagram of the chiral magnet Cu_2OSeO_3 — •Marco Halder[1], Alfonso Chacon[1], Andreas Bauer[1], Helmuth Berger[2], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department E21, D-85748 Garching, Germany — [2]École Polytechnique Fédérale de Lausanne, Crystal Growth Facility, CH-1015 Lausanne, Switzerland

In recent years, the cubic chiral insulator Cu_2OSeO_3 attracted great scientific interest, combing the skyrmion lattice phase with strong magneto-electric coupling. We report a comprehensive study of the magnetic properties of single-crystal Cu_2OSeO_3 by means of measurements of the magnetization, ac susceptibility, and specific heat, in particular tracking the influence of crystal orientation, cooling history and demagnetizing effects on the formation of skyrmion order.

TT 26.9 Mon 17:30 EB 301

Time resolved Lorentz-TEM measurements of dynamical skyrmion lattice defects in Cu_2OSeO_3 — •Simon Pöllath[1], Johannes Wild[1], Lukas Heinen[2], Thomas Meier[1], Matthias Kronseder[1], Leonard Tutsch[1], Andreas Bauer[3], Helmuth Berger[4], Christian Pfleiderer[3], Josef Zweck[1], Achim Rosch[2], and Christian Back[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Deutschland — [2]Institut für Theoretische Physik, Universität zu Köln, Deutschland — [3]Physik-Department, Technische Universität München, Deutschland — [4]Crystal Growth Facility, École Polytechnique Fédérale de Lausanne, Schweiz

We report non-stroboscopic time resolved Lorentz-Transmission-Electron-Microscopy (LTEM) measurements of skyrmion lattice defects in the chiral magnet Cu_2OSeO_3. The multiferroic insulator hosts a hexagonal skyrmion lattice which can be observed in real space using LTEM. It is known, that the radial temperature profile caused by the illumination of the sample with the TEM electron beam sets the skyrmion lattice into rotation [1]. We utilize this effect to study the dynamics of defects and grain boundaries that naturally occur during the lattice rotation. The structural and dynamical behaviour of the defects is similar to that of 2D hexagonal particle lattices and therefore the particle character of the skyrmion in its lattice phase is stressed by our findings [2].

[1] Mochizuki, M. et al. Nat. mater. 13.3 (2014): 241-246

[2] Pöllath S, et al. PRL 118.20 (2017): 207205

TT 26.10 Mon 17:45 EB 301

Large-scale *ab initio* investigations of complex magnetic textures — •Marcel Bornemann, Sergii Grytsiuk, Paul F. Baumeister, Phivos Mavropoulos, Nikolai S. Kiselev, Samir Lounis, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We have developed a unique electronic structure code, KKR*nano* [1], specifically designed for petaFLOP computing. Our method scales linearly with the number of atoms, so that we can realize system sizes of up to half a million atoms in a unit cell. Recently, we implemented a relativistic generalization of the algorithm enabling the calculation of complex non-collinear magnetic structures in real space.
We present two applications: (i) In the helimagnet B20-MnGe different experimental groups have observed either a spin spiral in [001] direction or a 3Q-state composed of three spin spirals [2,3]. We present an *ab initio* comparison of both states. (ii) We performed a large-scale evaluation of low-lying thermal excitations, so-called "nodons", in Cr which could explain the formation of a spin density wave in this system [4].
Simulations were performed with computing resources granted by JARA-HPC, Forschungszentrum Jülich and HLRS in Stuttgart.
[1] A. Thiess *et al.*, Phys. Rev. B **85**, 235103 (2012).
[2] O.L. Makarova *et al.*, Phys. Rev. B **85**, 205205 (2012).
[3] T. Tanigaki *et al.*, Nano Lett. **15**, 5438 (2015).
[4] V. Vanhoof *et al.*, Phys. Rev. B **80**, 184420 (2009).

TT 26.11 Mon 18:00 EB 301

Giant structural response of Dzyaloshinskii-Moriya interaction in MnGe B20 compounds — •Sergii Grytsiuk, Marcel Bornemann, Markus Hoffmann, Bernd Zimmermann, Phivos Mavropoulos, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Non-centrosymmetric cubic B20 materials are currently under intensive investigation. An important feature of these materials is the competition between the antisymmetric Dzyaloshinskii-Moriya interaction (DMI) and the symmetric exchange interaction resulting in a rich variety of magnetic phases with respect to temperature, magnetic fields, material compositions and geometries. The possibility of engineering chiral structures and the effective switching between different magnetic phases requires the investigation of possible factors that influence the strength of the magnetic interactions. In this work, we show by first-principles calculations based on DFT that under pressure magnetic and structural properties of MnGe reveal a hysteretic behavior near the state where energies of high and low spin states coincide. We observe that pressure strongly enhances the DMI (by a factor 5), while the spin-stiffness gets smaller. In order to understand such giant enhancement of the micromagnetic DMI we computed atomistic DMI vectors. Surprisingly, the absolute value of the DMI vectors do not depend significantly on the lattice parameter and the enhancement of micromagnetic DMI stems mainly from the change of the DMI vectors' orientation with respect to bonds between Mn atoms.

TT 26.12 Mon 18:15 EB 301

Spin-orbit coupling effects in magnetic and response properties of B20 $A_{1-x}B_xGe$ alloys (A, B = Mn, Fe, Co, Rh) — •Sergiy Mankovsky[1], Sebastian Wimmer[1], Svitlana Polesya[1], Nicolas Martin[2], Isabelle Mirebeau[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, D-81377 Munich, Germany — [2]Lab. Léon Brillouin, CEA, CNRS, Uni. Paris-Saclay, France

The composition-dependence of the isotropic exchange (J_{ij}) and Dzyaloshinskii-Moriya interaction (DMI) ($\vec{D}_{ij}$) of $Mn_{1-x}Fe_xGe$, $Mn_{1-x}Rh_xGe$, $Mn_{1-x}Co_xGe$ and $Fe_{1-x}Co_xGe$ B20 alloys have been investigated by first-principles calculations using the relativistic multiple scattering Korringa-Kohn-Rostoker (KKR) formalism. The $D^{\alpha\alpha}$ ($\alpha = x, y, z$) elements of the DMI tensor exhibit a strong dependence on the composition, changing sign at $x \approx 0.85$ in $Mn_{1-x}Fe_xGe$ and at $x \approx 0.5$ in $Fe_{1-x}Co_xGe$, in line with previous theoretical calculations as well as with experimental results. The spin-orbit torque (SOT), anomalous and spin Hall conductivities (AHC and SHC, respectively) of $Mn_{1-x}Fe_xGe$ alloys have been investigated. A sign change at $x \approx 0.5$ is predicted for the Fermi sea contribution to the SOT, as this is closely related to the DMI. In the case of anomalous and spin Hall effects it is shown that the calculated Fermi sea contributions are rather small and the composition-dependence of these effects are determined mainly by the electronic states at the Fermi level. The spin-orbit-induced scattering mechanisms responsible for both effects are suggested to cause the minimum of the AHC and the sign change of the SHC.

TT 27: Ferroelectric Domain Walls II (joint session KFM/TT)

Organizer: Sergey Artyukhin - Istituto Italiano di Tecnologia - Genova (Italy)

Time: Monday 15:00–18:30 Location: EMH 225

Invited Talk TT 27.1 Mon 15:00 EMH 225

First-principles studies of ferroelectric and ferroelastic domain walls — •Jorge Íñiguez — Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Avenue des Hauts-Fourneaux 5, L-4362 Esch/Alzette, Luxembourg

I will present our latest theoretical predictions on how to control the properties of functional oxides, and even induce completely new behaviors, by appropriately engineering their nano-structure, domains or domain walls. I will focus on two different research directions. On one hand, I will discuss ways to engineer ferroelectric and ferroelastic domain walls so they acquire specific properties (conductive, magnetic, topological) not present in the surrounding domains. On the other hand, I will show predictions that ferroelectric domain walls can be used to control heat currents, and can even act as phonon filters. Finally, I will also describe briefly the first-principles-based (second-principles) large-scale simulation methods that we use in most of our investigations.

Works done in collaboration with many colleagues, in particular H.J. Zhao, M.A.P. Gonçalves and C. Escorihuela-Sayalero (LIST); M. Royo, J.A. Seijas-Bellido and R. Rurali (ICAMB-CSIC); and J. Junquera and P. García-Fernández (U. Cantabria). Work at LIST funded by the Luxembourg National Reserach Fund through the CORE (Grant C15/MS/10458889 NEWALLS), PEARL (Grant P12/4853155/Kreisel COFERMAT) and AFR (Grant No. 9934186) programs.

TT 27.2 Mon 15:30 EMH 225

First-principles prediction of electric skyrmions — •Mauro Gonçalves[1,2], Carlos Escorihuela-Sayalero[1], Pablo García-Fernández[2], Javier Junquera[2], and Jorge Íñiguez[1] — [1]Luxembourg Institute of Science and Technology, Belvaux, Luxembourg — [2]Universidad de Cantabria, Santander, Spain

Nowadays, nontrivial topological spin structures like skyrmions are a focus of interest, as they open the door to novel nano-technologies with huge potential impact. Some authors have discussed electric skyrmions, whereby an exotic arrangement of electric dipoles would yield skyrmion-like structures in ferroelectric materials. Indeed, the recent experimental discovery of a dipole vortices in $PbTiO_3/SrTiO_3$ superlattices [1] has added to earlier theoretical predictions of skyrmions in ferroelectric nano-composites [2], and the possibility of stabilizing electric skyrmions currently attracting a lot of attention.

Following these ideas, we have used first-principles model potentials and large-scale lattice-dynamical simulations [3] to investigate the behavior of ferroelectric nano-domains immersed in a big domain of opposite polarization. Our simulations yield the first prediction of an electric skyrmion in a single phase material. We have also found that these dipole structures can be controlled applying an epitaxial strain or external electric fields, which may open the door to interesting physics and applications.

[1] Damodaran, A. R. et al., Nature Materials **16**, 1003 EP (2017).
[2] Nahas, Y. et al., Nature Communications **6**, 8542 EP (2015).
[3] J.C. Wojdeł, et al., J. Phys.:Condens. Matter **25**, 305401 (2013).

TT 27.3 Mon 15:45 EMH 225

The impact of domains on phase transitions and the electrocaloric effect - an ab initio based study of $BaTiO_3$. — •Anna Grünebohm[1], Madhura Marathe[2], and Claude Ederer[3] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Institut de Ciència de Materials de Barcelona, Spain — [3]Materials Theory, ETH Zürich, Switzerland

The electrocaloric effect (ECE) is the adiabatic temperature change induced by a varying external electrical field [1]. Although large temperature changes arise at field-induced first order phase transitions, this response may be irreversible due to thermal hysteresis [1-3]. We present an *ab initio* based study of the impact the domain structure makes on such transitions, their thermal hysteresis, and the (reversible) caloric response. As example, we focus on the tetragonal and orthorhombic phases of $BaTiO_3$ [4].

[1] X. Moya, *et al.*, Nature Mater. **13**, 439 (2014).
[2] M. Marathe, *et al.*, Phys. Rev. B **96**, 014102 (2017).
[3] M. Marathe, *et al.*, PSS (b), **1521**, 1700308 (2017).
[4] A. Grünebohm *et al.* Euro. Phys. Lett. **115**, 47002 (2016).

15 min break

TT 27.4 Mon 16:15 EMH 225

Electronic structure and optical absorption at ferroelectric domain walls in $BiFeO_3$ from first principles — •Sabine Körbel[1,2], Stefano Sanvito[1], and Jirka Hlinka[2] — [1]School of Physics & CRANN, Trinity College, Dublin, Ireland — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

Recent publications on first principles electronic structure of ferroelectric domain walls (FE DW) in $BiFeO_3$ show some variations concerning existence and magnitude of potential steps and band bending at pristine FE DW. We investigated these properties once more, trying to improve understanding by building on previous works in a systematic way. We also tested the hypothesis that FE DW modify the light absorption properties of $BiFeO_3$.

TT 27.5 Mon 16:30 EMH 225

Formation of ferroelectric monoclinic domains in $K_{0.7}Na_{0.3}NbO_3$ thin films under different strain conditions — •Leonard von Helden[1], Martin Schmidbauer[1], Michael Hanke[2], and Jutta Schwarzkopf[1] — [1]Leibniz Institute for Crystal Growth (IKZ), Berlin — [2]Paul-Drude-Institute for Solid State Electronics (PDI), Berlin

$K_xNa_{1-x}NbO_3$ is a promising material for lead-free ferro- and piezoelectric applications due to its high piezoelectric and coupling coefficients. Moreover, monoclinic phases - which are favorable as they enable a continuous rotation of the polarization vector - can be induced by incorporating anisotropic epitaxial lattice strain in $K_xNa_{1-x}NbO_3$ thin films. Upon varying the strain conditions the symmetry and orientation of these monoclinic domains can be deliberately tailored as predicted by strain-phase calculations.[1] In order to confirm the theoretical predictions we present a systematic investigation on the ferroelectric domain formation in $K_{0.7}Na_{0.3}NbO_3$ thin films grown by MOCVD. Slightly different strain conditions were realized by the application of various (110) oriented rare earth scandate substrates. The resulting ferroelectric domain structure was investigated upon a combination of piezoresponse force microscopy and X-ray nano-diffraction. Our results reveal monoclinic M_C domains with $(001)_{pc}$ pseudocubic unit cell orientation that differ among the substrates regarding their domain wall inclination. Moreover, the additional occurrence of $(100)_{pc}$ unit cell orientation in films with a thickness above 60 nm will be discussed. [1] J. Schwarzkopf et al., Front. Mater. 4, 26 (2017).

TT 27.6 Mon 16:45 EMH 225

Phononics at ferroelectric domain walls — •Francesco Foggetti[1,2] and Sergey Artyukhin[1] — [1]Italian Insitute of Technology, Genova, Italy — [2]University of Genova, Italy

Ferroelectric domain walls are emerging as robust 2D systems with promising functionality. Recent scanning tunneling and impedance microscopy studies revealed DC and AC conductivity, 2D electron gas and modified chemistry at ferroelectric domain walls. We study phonons localized at ferroelectric domain walls, and scattering of bulk phonons off ferroelectric domain walls using continuum theory and discrete models.

15 min. break

Invited Talk TT 27.7 Mon 17:15 EMH 225

Probing STO domain walls with scanning SQUID microscopy — •Beena Kalisky — Department of Physics and Institute of Nanotechnology and Advanced Materials, Bar-Ilan University, Israel

The interface formed by growing LaAlO3 on SrTiO3 (STO), both non magnetic insulators, exhibits conductivity, superconductivity and even magnetism. It is not surprising that the symmetry of the STO substrate is a dominant player in the plethora of physical phenomena found at the interface. We first encountered the interplay between the STO ferroelastic domain walls and the interface while imaging the magnetic flux generated from the interfacial current flow. We found

that a big part of the current can be modulated over the STO domain walls and that macroscopic transport measurements are strongly affected. We then investigated the origin of the modulations. We applied local stress to the sample and imaged the change in resistivity. Surprisingly, we found that the resistivity changed mainly along the domain walls which are highly sensitive to pressure. Our study shows that the Scanning SQUID is very useful for the investigation of buried domain walls and their effect on nearby layers.

TT 27.8 Mon 17:45 EMH 225

LiNbO3 thin-film crystals: A novel class of materials for domain engineering and enhanced domain wall conductivity — •Tillmann Stralka, Alexander Hausmann, Lukas Wehmeier, and Lukas M. Eng — Institute of Applied Physics, Technische Universität Dresden, Germany

In the last years, research on ferroelectric domain wall conductivity (DWC) mostly has focused either on PLD-grown, ultra-thin ferroelectric (FE) films [1] or FE bulk-single crystals [2,3,4]. Here we extend DWC to a novel and extremely prospective class of materials, i.e. free-standing thin-film crystals made up from ultra-thin single-crystalline $LiNbO_3$ (LNO) sheets. We use 5%-Mg-doped LNO polished down to a 22-μm thickness. Beyond high-voltage- [3] and super-bandgap-illumination-induced [4] DW engineering, the sample thinness also allows to write domain patterns by low-voltage AFM lithography, resulting in fully penetrating through domains. Of central interest in these thin-film LNO crystals is the mutual interaction between neighboring DWs, hence providing a novel tool for DW shape engineering on the very local length scale. Investigations are carried out using a combination of AFM techniques (PFM, c-AFM, topography) and Cerenkov Second Harmonic Microscopy [5], as well as by monitoring the electrical transport in DWs along the crystallographic X and Y axes in LNO.
[1] J. Seidel et al., Nature Mater. **8** (2009) 229. [2] T. Sluka et al., Nature Comm. **4** (2013) 1808. [3] C. Godau et al., ACS Nano **11** (2017) 4816. [4] M. Schröder et al., Adv. Func. Mater. **22** (2012) 3926. [6] L. Wehmeier et al., Phys. Stat. Solidi **11** (2017) 1700267.

TT 27.9 Mon 18:00 EMH 225

Correlating domain wall conductivity with geometry: a real-time study via Cerenkov Second Harmonic Generation — •Christian Godau, Lukas Wehmeier, Alexander Haussmann, and Lukas Eng — Institute of Applied Physics, Technische Universität Dresden, D-01062 Dresden, Germany

Ferroelectric domain walls (DWs) have become a central topic of research these days. Especially exploring their electronic properties and domain wall conductivity (DWC) in both thin films [1,2] and single crystals (sc) [3,4,5] has become very attractive. Our recent research on sc-lithium niobate (LNO) has proven an ultra-high DWC [4] and low electronic work function [6] that both provide a solid and promising foundation for prospective electronic device application.

Here, we present a full 3D and time-resolved study by Cerenkov Second Harmonic Generation [7] when investigating the DW dynamics in sc-LNO that are subjected to electric fields. Variations of the field lead to significant changes in geometry and inclination angles of the DW, that is tracked here in real time. These changes in DW-geometry are then correlated to the current measured through the conductive DWs.

[1] J. Seidel et al., Nat. Mater. 8, 229 (2009) [2] S. Cherifi-Hertel et al., Nat. Comm. 8, 15768 (2017) [3] T. Sluka et al., Nat. Comm. 4, 1808 (2013) [4] C. Godau et al., ACS Nano 11, 4816 (2017) [5] M. Schröder et al., Mater. Res. Express 1, 035012 (2014) [6] A.-S. Pawlik et al., Nanoscale 9, 10933 (2017) [7] T. Kämpfe et al., Phys. Rev. B 89, 035314 (2014)

TT 27.10 Mon 18:15 EMH 225

Domain wall and bulk conductance in $ErMn_{1-x}Ti_xO_3$ — •Theodor Secanell Holstad[1], Donald Malcolm Evans[1], Alexander Ruff[2], Didrik René Småbråten[1], Jakob Schaab[3], Christian Tzschaschel[3], Zewu Yan[4,5], Edith Bourret[5], Sverre Magnus Selbach[1], Stephan Krohns[2], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU, Norway. — [2]Center for Electronic Correlations and Magnetism, University of Augsburg, Germany. — [3]Department of Materials, ETH, Switzerland. — [4]Department of Physics, ETH, Switzerland. — [5]Materials Sciences Division, UC Berkeley, USA.

Ferroelectric domain walls are attracting broad attention as a novel type of spatially mobile oxide interface that can be written, erased, and moved on demand. Recently, acceptor and donor doping was adapted to optimize the behavior at ferroelectric domain walls.

In this talk, I will discuss the effect of donor doping on the electronic bulk and domain wall properties in hexagonal $ErMn_{1-x}Ti_xO_3$. Density functional theory calculations show that Ti^{4+} goes to the B-site, replacing Mn^{3+}. Scanning probe microscopy measurements confirm the robustness of the ferroelectric domain template. The electronic transport at both macro- and nanoscopic length scales is characterized. The measurements demonstrate the intrinsic nature of emergent domain wall currents and point towards Poole-Frenkel conductance as the dominant transport mechanism. Aside from the insight into the electronic properties of hexagonal manganites, B-site doping adds an additional degree of freedom for tuning the domain wall functionality.

TT 28: Poster Session: Topological Topics

Time: Monday 15:00–19:00 Location: Poster B

TT 28.1 Mon 15:00 Poster B

Emergent Weyl fermion bulk excitations in TaP and NbP evidenced from solid state NMR and NQR — H. Yasuoka[1], K.M. Ranjith[1], T. Kubo[1,2], Y. Kishimoto[1,2], D. Kasinathan[1], M. Schmidt[1], B. Yan[1], H. Tou[2], C. Felser[1], A.P. Mackenzie[1], and •M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Graduate school of Science, Kobe University, Kobe, 657-8501 Japan

The monophosphides TaP and NbP belong the class of Weyl semi metals and exhibit a non centrosymmetric structure and sizable spin orbit coupling. A crossing of linearly dispersive topologically protected polarized bands at a single point in reciprocal space defines the Weyl node where the fermion mass vanishes theoretically and a giant orbital hyperfine coupling is expected [1]. ^{181}Ta quadrupole resonance(NQR) resolves three NQR lines associated with the split level transitions for the $I = 7/2$ Ta nuclear spin. The spin lattice relaxation violates the Korringa law and shows a pronounced $(1/T_1T) \propto T^2$ behaviour [2] which is assigned to the magnetic excitations of the Weyl fermions, in agreement with theoretical predictions [1]. In addition we present first ^{93}Nb NMR results from NbP single crystals. Here we investigated the anisotropic hyperfine interaction and the excitations of the $I = 9/2$ Nb nuclear spin.
[1] Z. Okvatovity et al., PRB 94 (2016)
[2] Y. Yasuoka et al., PRL 118 (2017)

TT 28.2 Mon 15:00 Poster B

Structure-Property Investigation of Superconductivity in Nb-doped Bi_2Se_3 — •Simone Munkholm Kevy[1], Laura Wollesen[1], Henriette Elisabeth Lund[2], Philip Hofmann[2], and Martin Bremholm[1] — [1]Department of Chemistry and iNano, Aarhus University, 8000 Aarhus C, Denmark — [2]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhuc C, Denmark

Topological insulators (TI) have over the past decade been studied extensively due to their interesting electronic properties that make them excellent candidates for applications in quantum computing. Bi_2Se_3 is a highly studied TI and a large number of studies have investigated the effects of doping. Of particular interest, doping of Bi_2Se_3 with Cu, Sr or Nb, leads to bulk superconductivity while the topological surface states remain intact [1-3]. In the present study, high quality crystals grown by a melt growth quench technique were investigated to reveal structure-property relations of doped Bi_2Se_3. The crystal growth conditions were explored to determine optimal growth conditions. The crystal $Nb_xBi_2Se_3$ growth by slow cooling produces compositional gradients and the as-grown crystal boules contains secondary phases that affects the elemental composition and thus the physical properties. Crystallographic studies are combined with property measurements to provide a detailed structural understanding of superconductivity in doped Bi_2Se_3.
[1] Y. S. Hor, Phys. Rev. Lett., 104, 057001, 2010.
[2] Z. Liu, J. Am. Chem. Soc., 137, 10512, 2015.

[3] Y. Qiu, arXiv:1512.03519, 2015.

TT 28.3 Mon 15:00 Poster B

Local moment spin dynamics as a probe for topological properties — •Guilherme G. Lesseux[1,2], Martin Dressel[1], Marc Scheffler[1], Jean C. Souza[2], Ricardo R. Urbano[2], Pascoal J. G. Pagliuso[2], and Carlos Rettori[2,3] — [1]1. Physikalisches Institut - Universität Stuttgart, Stuttgart, Germany — [2]"Gleb Wataghin" Institute of Physics - University of Campinas, Campinas, Brazil — [3]CCNH, Universidade Federal do ABC, Santo André, Brazil

Electron spin resonance (ESR) of diluted magnetic impurities is a powerful local technique that can directly probe the nature of the interactions between localized magnetic moments and the electronic environment as well as the local, dynamic and static, crystalline site symmetry. Therefore, ESR may be an appropriate tool to investigate metallic surface states and other related relevant features for the physics of topologically nontrivial materials. Here, we present experimental strategies to probe topological properties by means of local moment spin dynamics. Unusual ESR results in half-Heusler YPt(Pd)Bi and SmB_6 compounds are presented and discussed in terms of their topological properties.

TT 28.4 Mon 15:00 Poster B

Flat Optical Conductivity due to the Dirac nodal line in ZrSiS — •Micha Schilling[1], Artem Pronin[1], Martin Dressel[1], Bettina Lotsch[2], and Leslie Schoop[2,3] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [3]Department of Chemistry, Princeton University, Princeton, USA

In graphene, the isolated two-dimensional Dirac cones cause a universal (i.e. material-independent) interband optical conductivity: the conductivity is frequency independent and the value is set by the quantum conductance. In ZrSiS, linear dispersing bands are quasi-two-dimensional and the Dirac points form nodal lines of two types. Spin-orbit coupling (SOC) opens a small gap along one of them. It was theoretically proposed, that the interband conductivity of such a nodal-line semimetal would also exhibit a frequency-independent behavior [1]. The absolute value, however, be material dependent, related to the length of the nodal line. We investigated the optical response of ZrSiS by the means of Fourier-transform infrared spectroscopy. We measured the reflectivity over a frequency range from 6 to 3000 meV at different temperatures down to 10 K and determined the optical conductivity. Our results confirm the theoretical expectations, revealing flat optical conductivity between 30 and 300 meV. From the measurements we could estimate the length of the nodal line in the reciprocal space and the size of the SOC-induced gap [2].

[1] J. P. Carbotte, J. Phys. Condens. Matter **29**, 045301 (2017).
[2] M. B. Schilling *et al.*, Phys. Rev. Lett. **119**, 187401 (2017).

TT 28.5 Mon 15:00 Poster B

One-dimensional physics in the edge states of the high-temperature Quantum Spin Hall system bismuthene on SiC(0001) — •Raul Stühler, Felix Reis, Jörg Schäfer, and Ralph Claessen — Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

Bismuthene (a mono-atomic honeycomb lattice of Bi-atoms) chemisorbed on a SiC(0001) substrate has recently been synthesized and shown to be a promising candidate for the realization of a room-temperature Quantum Spin Hall (QSH) effect which is based on a novel QSH mechanism [1]. Experiments with angle-resolved photoelectron spectroscopy (ARPES) and scanning tunneling spectroscopy (STS) found excellent agreement with the calculated topological band structure. In particular, while the bismuthene film displays a large bulk band gap of ∼0.8eV, conducting edge states are observed at the boundaries of the honeycomb layer, e.g. at terrace steps of the substrate, as expected for a two-dimensional topological insulator (2D-TI). Here we demonstrate, by a detailed analysis of tunneling spectra, that these edge states are indeed one-dimensional (1D) and correlated in nature. The STS spectra display power law behavior with energy and temperature as well as universal scaling, consistent with the expectations for a (helical) Tomonaga-Luttinger liquid (TLL).

[1] F. Reis, G. Li, L. Dudy et al., *Science* **357**, 287 (2017).

TT 28.6 Mon 15:00 Poster B

Giant microwave magneto-conductivity in topological Insulators — •Lea Pitz-Paal, Mahasweta Bagchi, Christoph Grams, Zhiwei Wang, Yoichi Ando, and Joachim Hemberger — Universität zu Köln

Recently, locally conducting puddles were identified in the bulk-insulating topological insulator $BiSbTeSe_2$ at temperatures below 50K [1]. These puddles are the result of imperfect compensation of charged donors and acceptors in the bulk. Additionally, it was shown that these puddles in a nearly bulk-insulating topological insulator $TlBi_{0.15}Sb_{0.85}Te_2$ grow in an increasing magnetic field [2]. This was detected when observing the resulting enhancement of the DC-conductivity. The puddles are growing due to the magnetic field and therefore form a percolating current paths. In the case of $BiSbTeSe_2$ the puddles are not connected because of much better compensation. Therefore, an enhancement of the puddles size is not observable with DC-measurements in this case. Hence, to examine the puddles in $BiSbTeSe_2$, an alternative approach based on AC-measurements in magnetic field is presented here. Our measurement also show an considerably enhanced AC-conductivity with increasing magnetic field and, therefore, a growth of the puddles.

This work is supported by the DFG via SFB1238 (Cologne).

[1] N. Borgwardt *et al.*, Phys. Rev. B **93**, 245149(2016)
[2] O. Breunig *et al.*, Nat. Commun. **8**, 15545(2017)

TT 28.7 Mon 15:00 Poster B

Length scale of puddle formation in 3D topological insulators — Thomas Bömerich, Jonathan Lux, •Qingyufei Terenz Feng, and Achim Rosch — Institut für Theoretische Physik, Univeristät zu Köln, Germany

In most semiconductors and insulators the presence of a small density of charged impurities cannot be avoided, but their effect can be reduced by compensation doping, i.e. by introducing defects of opposite charge. Screening in such a system leads to the formation of electron-hole puddles, which dominate bulk transport, as first recognized by Efros and Shklovskii. Metallic surface states of topological insulators (TI) contribute extra screening channels, suppressing puddles. We investigate the typical length l_p, which determines the distance between puddles and the suppression of puddle formation close to metallic surfaces in the limit where the gap Δ is much larger than the typical Coulomb energy E_c of neighboring dopants, $\Delta \gg E_c$. In particular, this is relevant for three dimensional Bi-based topological insulators, where $\Delta/E_c \sim 100$. Scaling arguments predict $l_p \sim (\Delta/E_c)^2$. In contrast, we find numerically that l_p is much smaller and grows in an extended crossover regime approximately linearly with Δ/E_c for numerically accessible values, $\Delta/E_c \sim 35$. We show how a quantitative scaling argument can be used to extrapolate to larger Δ/E_c, where $l_p \sim (\Delta/E_c)^2/\ln(\Delta/E_c)$. Our results can be used to predict a characteristic thickness of TI thin films, below which the sample quality is strongly enhanced.

TT 28.8 Mon 15:00 Poster B

In-plane H_{c2} anisotropy of $Cu_{1.5}(PbSe)_5(Bi_2Se_3)_6$ — •Lionel Andersen, Zhiwei Wang, Thomas Lorenz, and Yoichi Ando — II. Physikalisches Institut - Universität zu Köln, Germany

The material series $(PbSe)_{5n}(Bi_2Se_3)_{3m}$ can be understood as a natural layered heterostructure. Since the end-member PbSe is topologically trivial and the other end-member Bi_2Se_3 is a well-known topological insulator, the series provides an interesting playground for the study of topological phenomena [1]. The member of this series with $n = 1$ and $m = 2$ shows strong evidence for unconventional superconductivity after Cu doping [2]. Recently the related material $Cu_xBi_2Se_3$ was proved to be a topological superconductor through the observations of a spontaneous rotational symmetry breaking [3,4]. In this contribution we present a study of the H_{c2} anisotropy observed in $Cu_{1.5}(PbSe)_5(Bi_2Se_3)_6$ obtained by resistance measurements. In addition to an out-of-plane anisotropy a clear in-plane anisotropy was found, which is difficult to be explained by a crystallographic or the associated Fermi surface anisotropy. This suggests a symmetry breaking similar to the case of $Cu_xBi_2Se_3$.

[1] K. Nakayama et al., Phys. Rev. Lett. **109**, 236804 (2012)
[2] S. Sasaki et al., Phys. Rev. B **90**, 220504 (2014)
[3] K. Matano et al., Nat. Phys. **12**, 852 (2016)
[4] S. Yonezawa et al., Nat. Phys. **13**, 123 (2017)

TT 28.9 Mon 15:00 Poster B

Electrical transport studies on the type-II Weyl semimetal candidate $W_{1-x}Mo_xTe_2$ — •Matthias Gillig[1,2], Federico Caglieris[1], Boy Roman Piening[1], Igor Morozov[1,4], Saicharan Aswartham[1], Joseph Dufouleur[1], Bernd Büchner[1,2,3], and

Christian Hess[1,2,3] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices of Emergent Materials, TU Dresden, 01069 Dresden, Germany — [4]Moscow State University, 119991 Moscow, Russia

The semimetals WTe_2 and Td-$MoTe_2$ have been the first compounds proposed as a type-II Weyl semimetals. While for these parent compounds the Weyl points are far above the Fermi level, it is presumed that mixing the two phases brings them to relevant energies.

We have performed magneto-electrical transport measurements on a series of $W_{1-x}Mo_xTe_2$ single crystals. Zero-field resistivity increases upon substituting Mo for W but keeps metallic properties. The large non-saturating magnetoresistance is reduced in between the two phases, while the Hall resistivity decreases continuously from WTe_2 to $MoTe_2$. A simple two-band analysis ascribes this behavior to suppressed charge carrier compensation and declining mobilities. Observed Shubnikov-de-Haas oscillations show no drastic changes of the electronic structure.

TT 28.10 Mon 15:00 Poster B

Quasiparticle interference pattern in superconducting quantum wells — •Mehdi Biderang[1] and Alireza Akbari[1,2] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Department of Physics, POSTECH, Pohang, Korea

Spin-orbit interaction (SOI) plays an important role in the electronic properties of solids. Particularly, when it is originating from the bulk inversion symmetry breaking combining to the asymmetry of confining potential, it moves to Dresselhaus or Rashba types of SOIs. In superconducting state, these types of SOIs may cause the parity mixing and occurrence of the accidental node in the superconducting gap. We study the symmetry of superconducting gap and its trace on the quasiparticle interference pattern for a two-dimensional superconducting quantum well grown in (110) direction, by considering the effect of the interplay of Rashba and Dresselhaus SOIs. Our theoretical results show that changing the relative strength of Dresselhaus to Rashba, from 0 to 1, leads to fix the spin quantization axis at fully mixed Dresselhaus-Rashba. Moreover, a C4 symmetry of superconducting pairing changes to C2, which is consistent with the variation of the Fermi surface topology.

TT 28.11 Mon 15:00 Poster B

Majorana bound states in monoatomic Fe-nanowires on superconducting Pb — •Carl Drechsel, Rémy Pawlak, Marcin Kisiel, Jelena Klinowaja, Tobias Meier, Shigeki Kawai, Thilo Glatzel, Daniel Loss, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland

Motivated by their potential use as topological qubits, Majorana bound states (MBS) have attracted an utmost interest. Theoretical calculations predict their occurrence in the combination of quasi-one-dimensional nanowire systems onto s-wave superconductors.

Here, we measure the spatial and electronic characteristics of topological, superconducting chains of iron atoms on Pb(110) to investigate the wave function and the localization length as fingerprint for MBSs [1]. After first observations by scanning tunneling microscopy (STM) [2,3], we demonstrate by combining STM and atomic force microscopy (AFM) at low temperature (< 5 K) that the Fe chains are mono-atomic, structured in a linear fashion, and exhibit zero-bias conductance peaks at their ends [4]. This can be interpreted as signature for a Majorana bound state [5]. From these observations, we strongly support the idea of using MBSs in Fe chains on superconducting Pb as qubits for quantum computing devices.

[1] J. Klinovaja, D. Loss, Phys. Rev. B 86, 085408 (2012)
[2] S. Nadj-Perge et al., Science 346, 602 (2014)
[3] M. Ruby et al., Phys. Rev. Lett. 115, 197 (2015)
[4] R. Pawlak et al., npj Quantum Information, 16035 (2016)
[5] V.Mourik et al., Science 336, 1003 (2012)

TT 28.12 Mon 15:00 Poster B

Stability of Majorana edge modes in an interacting Kitaev chain in presence of non-Markovian electron-phonon interaction — •Julian Schleibner, Florian Katsch, and Alexander Carmele — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik von Halbleitern, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We study a generic example of a system that fails to thermalize, namely a Kitaev chain with a bulk and topological edge-edge states [1, 2]. It is of interest to study the resilience of such Majorana modes in the presence of nearest-neighbor interaction and non-Markovian dissipation. The nearest-neighbor interaction couples the Majorana edge modes to the bulk leading to decay of the edge correlation due to dissipation into the phonon reservoir. The systems' time evolution is described and evaluated by means of Heisenberg equation of motion for small system sizes, taking into account the full hierarchy. The contributions originating from the phonon bath are calculated in second order Born factorization. The results are compared to previous studies, where the dissipation into a Markovian reservoir was described within a master equation framework, implying violation of the parity symmetry. In this case the edge correlation shows an exponential decay in homogeneous chains and a stretched exponential decay in disordered chains [3].

[1] Pal *et al.*, Phys. Rev. B **82**, 174411 (2010).
[2] Kitaev, Phys. Usp. **44**, 131 (2001).
[3] Carmele *et al.*, Phys. Rev. B **92**, 195107 (2015).

TT 28.13 Mon 15:00 Poster B

Measuring the spin structure of Majorana bound states using optical quantum dots — •Lena Bittermann[1] and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, TU Braunschweig — [2]Laboratory for Emerging Nanometrology Braunschweig

Since signatures of Majorana bound states have been found, a lot of research in this field was initiated. Despite of this, their spin structure [1] is still not well understood.

In a one dimensional semiconducting wire on top of a superconductor with an applied Zeeman field, Majorana bound states can arise at the ends of the wire to which quantum dots can be coupled [2]. Here we propose such a setup where two optical quantum dots are also connected to hole reservoirs so that photons can be created via recombination. We first perform a Schrieffer-Wolff transformation to receive the effective low energy model of the electronic system with weak coupling between the dots and the Majorana bound states. Furthermore, we use a master equation formalism to obtain the steady state solution. By analyzing the resulting photon emission spectrum, we investigate the corresponding processes of recombination to draw conclusions on the spin polarization of the Majorana bound states.

[1] D. Sticlet, C. Bena and P. Simon, PRL 108, 096802 (2012)
[2] M. T. Deng et al., Science 354, 1557 (2016)

TT 28.14 Mon 15:00 Poster B

Tunable quasiparticle poisoning in Josephson Junctions — •Daniel Frombach[1] and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, TU Braunschweig — [2]Laboratory for Emerging Nanometrology Braunschweig

The fractional Josephson effect is one of the unique features of Majorana bound states (MBS) forming in Josephson junctions [1]. However, its experimental realization still remains challenging partially due to quasiparticle poisoning potentially spoiling the 4π periodic effect. Despite first signatures of the 4π periodicity having been reported [2][3], the effect of such quasiparticle poisoning is still not well understood.

Here we propose a setup based on silicene, in which an experimental handle in the form of a perpendicular electric field exists, with which it can be possible to introduce an artificial poisoning experienced by the MBS. We analyze the poisoning effect on the current voltage characteristic of the junction and discuss the critical current as a possible indicator for the topology of the junction.

[1] L. Fu and C.L. Kane, Phys. Rev. B 79, 161408 (2009)
[2] L. P. Rokhinson et al., Nat. Phys. 8, 795 (2012)
[3] J. Wiedenmann et al., Nat. Commun. 7, 10303 (2016)

TT 28.15 Mon 15:00 Poster B

Multifractality of wavefunctions at the spin quantum Hall transition — •Daniel Hernangómez-Pérez[1], Soumya Bera[2], Ilya Gruzberg[3], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [3]Ohio State University, Department of Physics, 191 W. Woodruff Avenue, Columbus Ohio, 43210, USA

At the spin quantum Hall transition (class C) the Hall conductance for spin is quantized while charge is not conserved. Corrections to scaling are found to be small near the transition that connects two neighboring plateau states. Therefore, it lends itself as a natural testbed for analytical predictions. We here present a numerical study of the wavefunction statistics. Our results: (i) In a recent theoretical investigation [1], Bondensan et al. argue in favor of exact parabolicity of multifrac-

tal spectra near integer quantum Hall transitions. Thus motivated we investigate the class C spectrum and find that it is far from parabolic. (ii) Analytical arguments [2,3] predict a symmetry of the multifractal spectrum that we can confirm with a very high accuracy.
[1] R. Bondesan, D. Wieczorek, M. R. Zirnbauer, Nucl. Phys. B 918, 52 (2017).
[2] A. D. Mirlin, Y. V. Fyodorov, A. Mildenberger, F. Evers, Phys. Rev. Lett. 97, 046803 (2006).
[3] I. Gruzberg, A. D. Mirlin, M. Zirnbauer, Phys. Rev. B 87, 125114 (2013).

TT 28.16 Mon 15:00 Poster B

Fractional quantum Hall phenomenology in mosaic-like conductors — Ferdinand Kisslinger[1], •Dennis Rienmüller[1], Erik Kampert[2], and Heiko B. Weber[1] — [1]FAU Erlangen-Nürnberg, Lehrstuhl für angewandte Physik — [2]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf

In the early days of graphene research, fractional values of e^2/h in the two-terminal conductance were interpreted as heralding FQHE in graphene [1],[2]. Since then, a variety of detailed investigations of FQHE states in monolayer [3]-[5] were reported.
In this work, another approach was made by utilizing a simple route to generate magnetotransport data that share essential signatures with fractional quantum Hall effect. Ingredients to the generating model are, on the one hand, conducting tiles with integer quantum Hall effect as well as metallic linkers, and, on the other hand, Kirchhoff's laws. When connecting few identical tiles in a mosaic, fractional steps occur in the conductance values. Richer spectra representing several fractions occur when the tiles are parametrically varied. Parts of the simulation data are supported with purposefully designed graphene mosaics in high magnetic fields. The model can, however, not explain substructure within the last Landau level. The findings emphasize that the occurrence of FQH phenomena does not necessarily indicate interaction-driven physics.
[1] X. Du et al., Nature 462, 192(2009).
[2] K. I. Bolotin et al., Nature 462, 196(2009).
[3] C. R. Dean et al., Nat. Phys. 7, 693(2011).
[4] F. Ghahari et al., Phys. Rev. Lett. 106(2011).
[5] B. E. Feldman et al., Phys. Rev. Lett. 111(2013)

TT 28.17 Mon 15:00 Poster B

Low temperaturate properties of B20 compounds — •Timur Yasko, Georg Benka, Andreas Bauer, Christian Oberleitner, Alexander Engelhardt, and Christian Pfleiderer — Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany

Transition-metal mono-silicides crystallizing in the non-centrosymmetric space group $P2_13$ have been studied for decades due to a wide range of complex magnetic and electronic properties. Recently, the diamagnetic metal CoSi was proposed as a potential candidate material for hosting Weyl-type excitations [1]. We report on the growth of large high-quality single crystals by means of the optical floating-zone technique. Following a thorough metallurgical characterization, we present a comprehensive study of the intriguing low-temperature magnetic and transport properties of CoSi.
[1] Peizhe Tang et al., arXiv:1706.03817, 2017

TT 28.18 Mon 15:00 Poster B

Topological phase characterization of SSHH model — Daniel Duarte, Marta Prada, and •Daniela Pfannkuche — Universität Hamburg, I. Institut für Theoretische Physik, Jungiusstrasse 9, 20355 Hamburg

We study a one-dimensional interacting fermionic chain by means of density matrix renormalization group. The different spin correlation functions are studied and a phase diagram is obtained as a function of dimerization and on site interaction parameters. We find a striking phase showing finite spin edge correlations. Next we characterise the topology of the phase in terms its Zak phase and the existence of edge states. We discuss the connection between the appearance of edge-spin correlations and the Zak phase, and provide an extended phase diagram, complementing existing ones [1,2] These results could be experimentally realised in a cold atom experiment with a one-dimensional optical trap.
[1] B.-T. Ye, L.-Z. Mu, H. Fan, Phys. Rev. B 94, 165167 (2016).
[2] Da Wang, S. Xu, Yu Wang, C. Wu, Phys. Rev B 91, 115118 (2015).

TT 29: Poster Session: Cryogenic Particle Detectors and Cyotechnique

Time: Monday 15:00–19:00 Location: Poster B

TT 29.1 Mon 15:00 Poster B

Einfluss von Geometrie und Herstellungstechnologie auf das Zeitverhalten von SNSPD — Julia Brandel[1], •Oliver Brandel[1], Mario Ziegler[1], Sebastian Goerke[1], Ilya Charaev[2], Emanuel Knehr[2], Detlef Born[1], Michael Siegel[2] und Heidemarie Schmidt[1] — [1]Leibniz-Institut für Photonische Technologien e.V. (IPHT), Jena, Deutschland — [2]Karlsruher Institut für Technologie (KIT), Karlsruhe, Deutschland

Einzelphotonenzähler basierend auf ultradünnen supraleitenden Schichten (SNSPD) besitzen ein breites Anwendungsfeld von der Spektroskopie bis hin zur Quantenkryptografie, da sie in Bezug auf Dunkelzählrate und zeitlicher Genauigkeit herausragende Eigenschaften besitzen.

Die dafür eingesetzten Niobnitridschichten (NbN) wurden bislang mittels Reakivem Magnetron Sputtern hergestellt. Am IPHT wurde eine alternative Herstellungstechnologie entwickelt, mit der es möglich ist, diese Schichten durch Atomlagenabscheidung (ALD) herzustellen. Durch ALD wird neben einer idealen Schichtdickenkontrolle während des Herstellungsprozesses auch die Abscheidung auf dreidimensionalen Strukturen ermöglicht.

In unserem Beitrag werden sowohl die allgemeinen Schichteigenschaften der unterschiedlichen Herstellungstechnologien als auch der Einfluss der geometrischen Strukturierung des SNSPD untersucht.

TT 29.2 Mon 15:00 Poster B

MetroBeta: Beta Spectrometry with Metallic Magnetic Calorimeters in the Framework of the European Program of Ionizing Radiation Metrology — •Michael Paulsen[1,3], Jörn Beyer[1], Lina Bockhorn[2], Christian Enss[3], Daniel Györi[3], Sebastian Kempf[3], Karsten Kossert[2], Martin Loidl[4], Riham Mariam[4], Ole Nähle[2], Matias Rodrigues[4], and Marco Schmidt[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [3]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [4]CEA, LIST, Laboratoire National Henri Becquerel, Saclay, France

MetroBeta is a European project that aims to improve the theoretical calculation and measurement of beta spectrum shapes. The project is part of a common European program of ionizing radiation metrology. The precise knowledge of beta spectrum shapes is required for measuring the activity of pure beta emitters, thus realizing the Becquerel unit for these nuclides. Metallic magnetic calorimeters (MMCs) with the beta emitter sample embedded in the absorber have proven to be among the best beta spectrometers. Four beta spectra will be measured: Sm-151 (Q = 76.3 keV), C-14 (Q = 156.5 keV), Tc-99 (Q = 293.8 keV), Cl-36 (Q = 709.5 keV). A crucial part of the research and development is concerned with source and absorber preparation techniques, which includes producing high quality nuclide samples that need to be integrated into the MMC absorbers.

TT 29.3 Mon 15:00 Poster B

Flux ramp modulation for Microwave SQUID Multiplexing — •Daniel Richter, Mathias Wegner, Andreas Fleischmann, Sebastian Kempf, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Microwave SQUID multiplexing (μMUXing) based on non-hysteretic rf-SQUIDs appears to be the most suitable multiplexing technique to read out metallic magnetic calorimeter (MMC) arrays. The intrinsically fast signal rise time of MMCs, for example, can be maintained by providing sufficient bandwidth per channel. However, since rf-SQUIDs are intrinsically non-linear devices due to their periodic flux-to-voltage characteristic, the almost ideal linear detector response of MMCs is

degraded unless suitable counter-measures are applied. Standard feedback techniques such as flux-locked loop can't be adapted for a microwave SQUID multiplexer since individual feedback lines would have to be routed to each pixel. In contrast, modulation techniques such as flux ramp modulation provide a conceptually easy solution for linearizing the output signal of the multiplexer.

In this contribution, we will first introduce the basic concept of flux ramp modulation. We will then discuss proof-of-principle as well as comprehensive characterization measurements for which we used customized dc-SQUIDs as well as a microwave SQUID multiplexer. Finally, we will outline present challenges as well as other applications where flux ramp modulation might significantly simplify the SQUID based readout.

TT 29.4 Mon 15:00 Poster B

Superconducting GHz Resonators for Microwave SQUID Multiplexing of MMCs — •Felix Ahrens, Mathias Wegner, Andreas Fleischmann, Sebastian Kempf, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University, Germany

Microwave SQUID multiplexing is the most promising way to read out large metallic magnetic calorimeter (MMC) detector arrays. A key element of cryogenic multiplexing is superconducting GHz resonators, which provide the required frequency encoding. To maintain the very fast signal rise time of MMCs we design our resonators to have a bandwidth of $\sim$1 MHz. This value directly sets the required frequency spacing between two neighbouring channels to $\sim$10 MHz taking into account our present fabrication accuracy and the required crosstalk level below 10^{-4}. Using capacitively coupled CPW transmission line resonators, the resonance frequency f_r and the loaded quality factor Q_l of a resonator can be set by adjusting the resonator length and the geometry of the coupling capacitor. We simulate the electromagnetic properties of different coupler geometries to find a proper resonator design matching our readout requirements. Since both f_r and Q_l depend strongly on the accuracy of the physical resonator dimensions, we optimise the microfabrication process in order to minimise fabrication inaccuracies. In addition, to minimise the influence of stray light, the kinetic inductance and tunnelling systems causing low-frequency phase noise, we investigate different superconducting materials. In this contribution, we present different aspects related to the optimisation of our superconducting resonators.

TT 29.5 Mon 15:00 Poster B

Characterisation of a MMC-based integrated photon and phonon detector for $0\nu\beta\beta$ search — •Patricia Kuntz[1], Daniel Unger[1], Clemens Hassel[1], Felix Ahrens[1], Christian Enss[1], Andreas Fleischmann[1], Loredana Gastaldo[1], Yong-Hamb Kim[2], Wonsik Yoon[2], Martin Loidl[3], Xavier-Francois Navick[3], and Matias Rodrigues[3] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]IBS Center for Underground Physics, Daejeon, Rep. of Korea — [3]CEA, Saclay, France

In the search for $0\nu\beta\beta$, scintillating crystals in cryogenic experiments allow for an efficient background reduction due to active particle discrimination. This is achieved by the simultaneous measurement of heat and light generated upon the interaction of a particle in a scintillating crystal. We developed, in the framework of the AMoRE and LUMINEU experiments, for the search of $0\nu\beta\beta$ in ^{100}Mo, large area integrated photon and phonon detectors based on metallic magnetic calorimeters (MMCs) able to simultaneously measure the two signals. We will present the design of the P2 detector, which consists of a photon detector, with an expected energy resolution of $\Delta E_\mathrm{FWHM} <$ 10 eV and a demonstrated signal rise time of $\tau < 50$ μs and three phonon detectors with expected $\Delta E_\mathrm{FWHM} < 100$ eV and $\tau < 200$ μs. Furthermore, we will discuss experimental results obtained from the characterization of a P2 detector, still without any scintillating crystal, using an external x-ray calibration source. For the first time, we could investigate the time response of the four detectors on the P2 wafer, the energy resolution as well as the crosstalk among the detectors.

TT 29.6 Mon 15:00 Poster B

Towards X-ray spectroscopy with sub-eV energy resolution: Metallic magnetic calorimeters with direct sensor readout. — •Matthäus Krantz, Sebastian Kempf, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Metallic magnetic calorimeters (MMCs) are energy dispersive particle detectors that are typically operated well below 100 mK. They make use of a paramagnetic temperature sensor to convert the energy deposited by an X-ray photon within an absorber into a change of sensor magnetization which can be precisely measured using a SQUID. For state-of-the-art detectors, the temperature sensor is transformer-coupled to the input coil of a current-sensing SQUID. However, parasitic inductances in the flux transformer, as well as transformer losses, lead to a reduction of the signal size, therefore impairing the energy resolution. For this reason we have started to develop detectors with direct sensor readout for which the temperature sensor is placed on top of the SQUID loop to maximize signal coupling. In our present design the SQUID is a first-order parallel gradiometer with meander-shaped SQUID inductance. Due to the greatly enhanced flux coupling as well as optimized SQUID parameters we expect this detector to surpass our current MMC world record energy resolution of 1.6 eV (FWHM) for 6 keV X-rays and push the present limit well below 1 eV. We discuss the optimization process, design and microfabrication processes as well as very recent results for these devices.

TT 29.7 Mon 15:00 Poster B

Gamma spectroscopy to measure the ^{229}Th isomer energy using a 2-dimensional array of metallic magnetic microcalorimeters — •J. Geist[1], J. Bussmann[1], D. Hengstler[1], M. Krantz[1], R. Pons[1], P. Schneider[1], C. Schötz[1], S. Kempf[1], L. Gastaldo[1], A. Fleischmann[1], C. Enss[1], G.A. Kazakov[2], S.P. Stellmer[2], and T. Schumm[2] — [1]Heidelberg University — [2]Vienna University of Technology

The isotope ^{229}Th has a nuclear isomer state with the lowest presently known excitation energy, which possibly allows to connect the fields of nuclear and atomic physic with a potential application in a nuclear clock. In order to verify and improve the accuracy of the currently most accepted energy value, (7.8 ± 0.5) eV, we want to resolve the 29.18 keV doublet in the γ-spectrum following the α-decay of ^{233}U, corresponding to the decay into the ground and isomer state, to measure the isomer transition energy without additional theoretical input parameters.

We developed the detector array maXs-30 consisting of 8x8 metallic magnetic calorimeters with an expected energy resolution below 6 eV, providing a large detection area of 16 mm^2 to face the low rate of the 29.18 keV transitions.

In first measurements we observed the 29.18 keV transitions as a single peak with an instrumental resolution of 33 eV.A strong background contribution due to β-radiation from accumulated decay products in the ^{233}U-source was discovered. We present results of the latest measurements with an adjusted maXs-30 detector, new generation SQUIDs and an updated setup in the cryostat.

TT 29.8 Mon 15:00 Poster B

Polar-maXs: Micro-calorimeter based x-ray polarimeters — •C. Schötz[1], D. Hengstler[1], S. Kempf[1], L. Gastaldo[1], A. Fleischmann[1], C. Enss[1], G. Weber[2,3], R. Märtin[2,3], O.M. Herdrich[4], and Th. Stöhlker[2,3,4] — [1]KIP, Heidelberg University — [2]Helmholtz Institute Jena — [3]GSI Darmstadt — [4]Jena University

We are developing the x-ray detector system polar-maXs, which will combine for the first time the high energy resolution, large dynamic range and excellent linearity of magnetic micro-calorimeters with the idea of a Compton- or Rayleigh-polarimeter.

The x-ray polarimeter comprises two layers. The first layer consists of a scatterer behind a corresponding collimator. Depending on the energy range of interest and whether Compton or Rayleigh scattering is to be used, this scatterer are fabricated from low-Z or high-Z material. The active scatter area is 32mm in diameter. The second layer is the detector itself which is based on microfabricated metallic magnetic calorimeters (MMC). The scattered x-rays are detected by an array of 64 x-ray absorbers and read-out by 64 paramagnetic temperature sensors. The latter are arranged to form a rectangular frame which is protected from direct x-ray hits by the collimator. Each absorber covers an area of 1.250mm x 1.250mm and is made of 30 micrometer thick gold, to guarantee high stopping power for x-rays with energies up to 30 keV and an energy resolution of better than 20eV (FWHM) in the complete energy range. We discuss the results of Monte-Carlo simulations for a variety of scatter materials as well as first measurements at 20mK in a dilution refrigerator.

TT 29.9 Mon 15:00 Poster B

MOCCA: A 4k-pixel molecule camera for the position and energy resolving detection of neutral molecule fragments at the Cryogenic Storage Ring CSR — •Dennis Schulz[1], Steffen Allgeier[1], Christian Enss[1], Andreas Fleischmann[1],

Lisa Gamer[1], Loredana Gastaldo[1], Sebastian Kempf[1], Oldřich Novotný[2], and Andreas Wolf[2] — [1]Kirchhoff-Institute for Physics, Heidelberg — [2]Max Planck Institute for Nuclear Physics, Heidelberg

The Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg can be used to prepare and store molecular ions in their rotational and vibrational ground states, enabling state-resolved studies on electron-ion interactions. The use of Metallic Magnetic Calorimeters for particle detection allows for identifying all neutral reaction products, using the deposited energy of incident particles into MMC absorbers as a measure of the particle mass. To resolve the complete reaction kinematics, a position sensitive coincident detection of multiple reaction products is necessary.

For those measurements we designed MOCCA, a 4k-pixel molecule camera based on MMCs with a detection area of 45 mm×45 mm, which is segmented into 64×64 absorbers and read out using only 32 SQUIDs. We discuss the detector design, multi-hit capability, cross-talk and the integration of its ^{3}He/^{4}He dilution refrigerator into the setup of the CSR. We show first measurements and the expected energy resolution.

TT 29.10 Mon 15:00 Poster B

Cross Correlated Noise Thermometer for Milli-Kelvin Temperatures — •Christian Ständer, Andreas Reifenberger, Felix Mücke, Marius Hempel, Daniel Richter, Sebastian Kempf, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University.

Within our search for easy-to-use reliable thermometers for milli-Kelvin and micro-Kelvin temperatures we developed a noise thermometer, where the Johnson noise of a massive cylinder of high purity (5N) silver is monitored simultaneously by two current sensing dc-SQUIDs. Operating both SQUIDS in voltage biased mode in 2-stage SQUID configurations allows to reduce the power dissipation as well as the noise of the SQUIDS to a minimum. By cross-correlating the two SQUID signals the noise contribution of the read-out-electronics is suppressed to a marginal level even at micro-Kelvin temperatures. To further reduce the correlated amplifier noise we fabricated SQUIDs with a new design featuring minimal coupling of input and feedback coil. We compare two thermometers of this type to a previously developed noise thermometer in the temperature range from 3K down to 4mK. Statistical uncertainties below 0.5% are achieved within 10s of measurement time. Within this uncertainty no self-heating was observable at base temperature.

TT 29.11 Mon 15:00 Poster B

Quickly Tunable Rerigerator for Superconducting Quantum Circuits — •Vasilii Sevriuk[1], Kuan Tan[1], Shumpei Masuda[1], Jan Goetz[1], Matti Partanen[1], Dibyendu Hazra[1], Eric Hyyppä[1], Joonas Govenius[1], Russell Lake[2], Visa Vesterinen[3], Leif Grönberg[3], Juha Hassel[3], Slavomir Simbierowicz[3], Marton Gunyho[1], Aarne Keränen[1], Jani Tuorila[1], Tapio Ala-Nissila[4], Matti Silveri[1], Hermann Grabert[5], and Mikko Möttönen[1] — [1]QCD Labs, COMP Centre of Excellence, Department of Applied Physics, Aalto University, PO Box 13500, FI-00076 Aalto, Finland — [2]National Institute of Standards and Technology, Boulder, CO, United States. — [3]VTT Technical Research Centre of Finland Ltd, VTT, Finland. — [4]Departments of Mathematical Sciences and Physics, Loughborough University, Loughborough, United Kingdom. — [5]Department of Physics, University of Freiburg, Freiburg, Germany.

In the past decade, the research on superconducting quantum circuits has provided a great number of superior microwave components such as superconducting qubits, amplifiers, and sensors. Especially in the opertation of qubits, it is of utmost importance to be able to quickly remove any unwanted qubit excitations on demand for fast and accurate initialization. We recently introduced a device referred to as a quantum-circuit rerigerator [K. Y. Tan, et al., Nat. Commun. 8, 15189 (2017)]. In our experiments, we show how we can tune the dissipation of a superconducting resonator by orders of magnitude just by applying a bias voltage on the refrigerator. The time scale for switching the dissipation on and off is in the nanosecond range.

TT 29.12 Mon 15:00 Poster B

Applications for "Dry" Cooling with damped two-stage Pulse Tube Cryocoolers at their low temperature limit — •Jack-André Schmidt[1,2], Jens Falter[1], Bernd Schmidt[1,2], Günther Thummes[1,2], and André Schirmeisen[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany, — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen, Germany

Today's scientific research often requires cooling systems that provide low background noise and high cooling performance. Pulse Tube Cryocoolers (PTC) [1] fulfill these requirements and combine them with a regenerative system for long time measurements. PTCs are a preferable choice of "dry" cryostats because of the absence of moving parts inside the cold head.

PTCs are filled with a working gas (Helium), which is compressed and expanded in cycles of about 1-2 Hz. This induces intrinsic mechanical and thermal variation in all systems with cryocoolers. As a consequence the adaptation of PTCs to sensitive equipment is a complex procedure and needs intricate techniques for thermal as well as mechanical damping. In this work we present the intrinsic variations of PTCs with strategies to minimize the influence on delicate equipment for long time measurements [2]. Different temperature and vibration damping units and cryostat designs are discussed, together with a presentation of the cooling performance of PTCs working under these conditions.

[1] G. Thummes, Cryogenics, Vol. 38, (1998) 337
[2] R. Schrödel et al., Meas. Sci. Technol. 23 (2012) 094004

TT 29.13 Mon 15:00 Poster B

A versatile demagnetization refrigerator — •Alexander Regnat, Jan Spallek, Christopher Duvinage, and Christian Pfleiderer — Physik Department, Technische Universität München

Cooling devices providing temperatures well below 1 K are a key prerequisite for modern research and development, e.g., in materials science, quantum applications and the cooling of sensors and detectors. Here we present a versatile and compact demagnetization refrigerator for the cryogen-free generation of sub-Kelvin temperatures.

TT 29.14 Mon 15:00 Poster B

Lab::Measurement – measurement control with Perl — •Simon Reinhardt[1], Charles E. Lane[2], Christian Butschkow[1], Alexei Iankilevitch[1], Alois Dirnaichner[1], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany — [2]Department of Physics, Drexel University, Philadelphia, USA

`Lab::Measurement` is a collection of Perl 5 modules providing control of test and measurement devices. It allows for quickly setting up varying and evolving complex measurement tasks with diverse hardware. Instruments can be connected by means such as GPIB (IEEE 488.2), USB-TMC, or VXI-11 / raw network sockets via Ethernet. Internally, third-party backends as e.g. Linux-GPIB, National Instruments' NI-VISA library or Zurich Instruments' LabOne API are used, as well as lightweight drivers for USB and TCP/IP-based protocols. The wide range of supported connection backends enables cross-platform portability. Dedicated instrument driver classes relieve the user from taking care of internal or vendor-specific details. A high-level layer provides fast and flexible creation of nested measurement loops, where e.g. several input variables are varied and output data is logged into a customizable folder structure. `Lab::Measurement` has already been successfully used in several low temperature transport spectroscopy setups. It is free software and available at `http://www.labmeasurement.de/`

TT 29.15 Mon 15:00 Poster B

Phase-sensitive dynamic susceptibility measurement in a pulsed magnetic field — •Lars Postulka, Bernd Wolf, and Michael Lang — Physikalisches Institut, Goethe Universität, SFB/TR49, Frankfurt, DE

Dynamic susceptibility, commonly referred to AC susceptibility, is a powerful tool to characterize magnetic phase transition or spin relaxation processes in the presence of a magnetic field. The standard technique for accessing this quantity is based on measurements of the voltage in a coil which is induced by magnetization changes of a sample due to a small outer oscillating field. Importantly, this setup allows for a phase-sensitive detection of the susceptibility, thereby providing direct access to the dynamics of the spin system. This method is well established for the use in constant magnetic fields. However, in modern solid state physics, interesting physical phenomena emerge in high fields, conveniently accessible by the use of pulsed-field technology. Whereas various techniques to infer the in-phase part of the susceptibility are regularly used, methods to determine the out-of-phase part have not yet been reported. Here we present the first realization of an AC susceptometer for measurements in pulsed field. In particular, we focus on technical aspects including all electronic devices and a possible coil design. We prove the feasibility by measurements of the

susceptibility on a spin chain compound.

TT 29.16 Mon 15:00 Poster B

A low-temperature vector-field ultrahigh vacuum scanning tunneling microscope facility for the study of quantum materials — •Qingyu He, Xinglu Que, Lihui Zhou, Andreas Rost, and Hidenori Takagi — Max-Planck Institute ,Heisenberg Strasse 1, Vaihingen, Stuttgart, Germany

A low-temperature vector-field ultrahigh vacuum scanning tunneling microscope facility for the study of quantum materials

Scanning tunneling microscopes (STM) play a very important role in the study of quantum materials by correlating electronic properties with structures at the atomic scale. In my poster, I will present our home built ultrahigh vacuum STM facility with a base temperature of 1.2 K. A 3 T vector field as well as 9 T perpendicular to the sample surface can be applied. It features a compact design and has a long holding time. Updating with a 3He refrigerator is ongoing, which will enable us to reach a higher energy resolution.

TT 30: Poster Session: Disordered Quantum Systems

Time: Monday 15:00–19:00 Location: Poster B

TT 30.1 Mon 15:00 Poster B

On the relation between chicken eyes and superconducting vortex lattices — •Jose Benito-Llorens[1,2], Anton Fente[1,2], Edwin Herrera[1,2], Hermann Suderow[1,2], and Isabel Guillamón[1,2] — [1]Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Unidad Asociada UAM, CSIC, Departamento de Física de la Materia Condensada — [2]Instituto de Ciencia de Materiales de Madrid Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Spain

The arrangements of cells in a chicken eye are not randomly disordered, but are instead hyperuniform. Hyperuniformity is also observed in superconducting vortex lattices, even when vortex pinning centers are arranged randomly.

Here we analyze images of disordered superconducting vortex lattices taken with a scanning tunneling microscope. We analyze the potential that creates the disorder influencing the vortex lattice and present two limiting cases, random pinning and uncorrelated long range disorder created by a 1D potential at an angle with the vortex lattice. The latter is a hyperuniform potential in a somewhat trivial way, because it is a discommensuration between two ordered lattices.

We find that in both cases, the structure factor of the vortex lattice decreases to zero for large wavelengths with power laws. We discuss imaging experiments showing vortex motion and their relevance for the proposed phenomena.

Work supported by Spanish MINECO, ERC, Starting Grant and CIG Marie Curie program.

TT 30.2 Mon 15:00 Poster B

Dielectric measurements of the dynamics of atomic tunneling systems in thin-film AlO_x — •Saskia M. Meissner, Arnold Seiler, and Georg Weiss — Physikalisches Institut, Karlsruher Institut für Technologie

From the study of glasses atomic tunneling systems (TS) are well known to dominate the low temperature properties of disordered materials. They also appear in thin-film dielectrics of superconducting circuits, where AlO_x is a common material for the fabrication of Josephson junctions.

We present a broadband study of the dynamics of TS contained in thin-film disordered AlO_x ranging from kHz to GHz frequencies. The TS' density of states is probed at kHz frequencies by capacitance measurements as well as in the GHz range by tracking the resonance frequencies of superconducting microstrip resonators with embedded plate capacitors. This geometry creates a homogeneous electric field which is concentrated in the dielectric AlO_x reducing the influence of the native oxide on the surface of the Al structures.

The large bandwidth of excitation frequencies allows to verify the standard tunneling model but contrary to the predictions we measured an increasing density of TS with increasing temperature. Moreover, our observations reveal that the relaxation rates of TS are not only caused by their interaction with phonons and other TS as expected in dielectrics but also by quasiparticles penetrating the AlO_x from the superconducting Al plates.

TT 30.3 Mon 15:00 Poster B

Interaction of electrons with atomic tunneling systems in a Zr-basedsuperconducting metallic glass — •Arnold Seiler, Saskia M. Meissner, and Georg Weiss — Physikalisches Institut, Karlsruher Institut für Technologie

The low temperature properties of amorphous materials are known to be dominated by tunneling systems (TS) formed by atoms or groups of atoms that can tunnel between different configurations. Despite the success of the standard tunneling model in describing the properties of disordered dielectrics, its predictions for metallic glasses still appear incomplete.

In this work we investigate a Zr-based metallic glass by means of ultrasonic waves where the interaction of TS with quasiparticles or conduction electrons can be switched on and off by suppressing the superconductivity by a magnetic field. The onset of the relaxation process gives a clear indication of the energy relaxation rate of TS and allows to separate the underlying interactions and their coupling strength. Taking into account the temperature dependence of the finite linewidth and relaxation rate of TS in numerical calculations allows to reproduce the appearance of a crossing point of the sound velocity between normal and superconducting state.

Contrary to the expectation of a frequency-independent, logarithmic increase of the sound velocity with temperature, we found a frequency dependence of the temperature variation in the normal conducting state when changing the frequency of ultrasonic excitation from 1 GHz to 2 GHz.

TT 30.4 Mon 15:00 Poster B

Thin-film piezoelectric ZnO transducers for studies of tunneling systems in disordered materials with ultrasonic waves — •Axel Gullasch, Saskia M. Meissner, Arnold Seiler, and Georg Weiss — Physikalisches Institut, Karlsruher Institut für Technologie

The ultrasonic pulse propagation technique is a standard method for the study of fundamental properties of solids. Electron-phonon coupling in metals or semiconductors, spin-phonon interactions in magnetic systems as well as phonon coupling to collective excitations and sound propagation effects near phase transitions are a number of applications.

Ultrasonic methods are also an important tool to study atomic tunneling systems (TS) which often dominate the low temperature properties of disordered materials. In superconducting metallic glasses mechanical deformations are the method of choice to study TS and their interaction with conduction electrons.

For all these methods thin film 0.3-1 μm piezoelectric transducers are fabricated to be able to produce acoustic sound waves in the range of 0.5-2 GHz. ZnO is deposited by physical vapor deposition utilizing RF-magnetron sputtering. The quality of our ZnO-films is analyzed with an ultrasonic pulse-echo method using a probe station for lateral scanning of the piezoelectric transducers.

TT 30.5 Mon 15:00 Poster B

Low Frequency Acoustic and Dielectric Measurements of a Polymer Glass Containing Nuclear Quadrupole Moments — •Patrick Schygulla, Andreas Reiser, Annina Luck, Benedikt Frey, Nicole Assmann, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

Recent studies of glasses with nuclear electric quadrupole moments such as N-KZFS11 and HY-1 have revealed deviations in the dielectric function from the predictions of the standard tunneling model (STM), in particular an additional relaxational contribution.

We used a double paddle oscillator for acoustic and a capacitance bridge for dielectric measurements in order to investigate the elastic and dielectric susceptibility respectively at temperatures ranging from 7 to 700 mK and at frequencies between 60 Hz and 16 kHz. The examined polymer glass, FR-122P, has an atomic bromine content of 11 % with a well defined hyperfine level splitting of $\nu_Q \approx 250$ MHz. While

at higher temperatures one-phonon processes can explain the data, below the temperature of the maximum the resonant contribution to the change of sound velocity is hardly visible and in the loss data a constant contribution was found in contrast to the expected T^3-dependence. The measured results are compared to numerical calculations of different extensions to the STM accounting for the presence of quadrupole moments. Also, first results are discussed from a newly designed experimental setup allowing for selectively saturating the quadrupolar transition of the nuclei during the measurement.

TT 30.6 Mon 15:00 Poster B

Influence of Nuclear Quadrupole Moments on Dielectric Polarization Echoes — •Andreas Schaller, Marcel Haas, Robert Haase, Anna Pollithy, Sergey Tsurkan, Matthias Sinnwell, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

Many low temperature properties of amorphous solids are well described by the phenomenological standard tunneling model. However, measurements of the dielectric constant, sound velocity, and dielectric polarization echoes of glasses containing atoms carrying nuclear quadrupole moments revealed unexpected characteristics, such as magnetic field dependencies, which are not observed in glasses without nuclear quadrupole moments.

We present new results of dielectric two-pulse polarization echo measurements carried out on different multicomponent glasses and polymers containing large nuclear quadrupole moments. For all these samples the two-pulse-echo decay occurs on a comparably short timescale and we observe a dependency of the echo amplitude on the electric field strength of the excitation pulses which is weaker than for glasses without large nuclear quadrupole moments. In order to probe the echo decay at sub-μs times we developed microstructured superconducting planar resonators for which the quality factor can be determined by design. We show the results of first test measurements.

TT 30.7 Mon 15:00 Poster B

Dielectric Properties of a Brominated Molecular Glass at Low Frequencies and Low Temperatures — •Nicole Assmann, Annina Luck, Benedikt Frey, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

The low temperature behavior of amorphous solids is determined by atomic tunneling systems and can be described by the phenomenological standard tunneling model (STM). In the last two decades, several deviations from STM-like behavior have been observed which triggered a number of refinements of this model taking microscopic details of the tunneling entity and motion as well as the presence of nuclear moments into account. In order to study particularly the effect of large nuclear quadrupole splittings on the structure and dynamics of atomic tunneling systems we investigated brominated Bisphenol A diglycidether (BrDGEBA). This simply structured molecule contains about 5 % bromine which carries a very large quadrupole moment. In addition to its vitreous behaviour and well known quadrupole splitting of 250 MHz, it provides the possibility of adjusting the bromine concentration of the sample by mixing it with its unbrominated version. As a first attempt we measured the dielectric properties of an undiluted sample between 60 Hz and 16 kHz at temperatures down to 10 mK and ascertained large deviations from the STM at low frequencies combined with low temperatures.

TT 31: Dynamics in Many-Body Systems: Interference, Equilibration and Localization II (joint session DY/TT)

Time: Monday 15:30–17:45 Location: EB 107

TT 31.1 Mon 15:30 EB 107

Finite-size effects in canonical and grand-canonical quantum Monte Carlo simulations for fermions — Zhenjiu Wang, Fakher F. Assaad, and •Francesco Parisen Toldin — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We introduce a quantum Monte Carlo method at finite temperature for interacting fermionic models in the canonical ensemble, where the conservation of the particle number is enforced. Although general thermodynamic arguments ensure the equivalence of the canonical and the grand-canonical ensembles in the thermodynamic limit, their approach to the infinite-volume limit is distinctively different. Observables computed in the canonical ensemble generically display a finite-size correction proportional to the inverse volume, whereas in the grand-canonical ensemble the approach is exponential in the ratio of the linear size over the correlation length. We verify these predictions by quantum Monte Carlo simulations of the Hubbard model in one and two dimensions in the grand-canonical and the canonical ensemble. We prove an exact formula for the finite-size part of the free energy density, energy density and other observables in the canonical ensemble and relate this correction to a susceptibility computed in the corresponding grand-canonical ensemble. This result is confirmed by an exact computation of the one-dimensional classical Ising model in the canonical ensemble, which for classical models corresponds to the so-called fixed-magnetization ensemble. Our method is useful for simulating finite systems which are not coupled to a particle bath, such as in nuclear or cold atom physics.

TT 31.2 Mon 15:45 EB 107

Coupling of hydrodynamic fluctuations to diffusive modes in a one-dimensional current-carrying wire — •Philipp Weiss, Marcel Gievers, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Closed systems with conservation laws approach thermal equilibrium only algebraically slowly after a sudden perturbation. The reason is that the built-up of equilibrium fluctuations is tied to the diffusive transport of the conserved quantities which results in hydrodynamic long-time tails. A similar behavior is expected for a current-carrying wire, coupled to leads which serve as source and sink of electrons. Here, fluctuation corrections near the connections decay slowly in space along the wire. Though tailored to transport problems, the Boltzmann equation predicts exponentially fast relaxation indicating that the Boltzmann description omits crucial processes. This can be cured *ad hoc* by adding collision noise which gives rise to a stochastic Boltzmann-Langevin equation. However, the full equation is hard to solve and approximation schemes are needed when investigating a specific system.

We propose a "noisy relaxation time approximation" which satisfies the conservation laws and provides a properly correlated noise term. We examine this novel tool using the example of the one-dimensional current-carrying wire: Can we observe the expected long-distance tails? How does our approximation compare to the real dynamics? And to which extent can we control it?

TT 31.3 Mon 16:00 EB 107

Photo-carrier relaxation of correlated band insulators — •Nagamalleswara Rao Dasari[1] and Martin Eckstein[2] — [1]Friedrich-Alexander Universitat Erlangen-Nurnberg, Erlangen, Germany. — [2]Friedrich-Alexander Universitat Erlangen-Nurnberg, Erlangen, Germany.

Ionic band insulators are characterized by charge gap, which is given by staggered Ionic potential (Δ). Electronic correlations (U) in these insulators screens the charge gap and makes it smaller than the spin gap. Such correlated band insulators are realized by using simplest model Hamiltonian, i.e., Ionic Hubbard model. In this work, we have studied Ionic Hubbard model in the weak coupling limit by using non-equilibrium dynamical mean-field theory and iterated perturbation theory as an impurity solver. We find that photo-excited correlated band insulators thermalize rapidly when local coulomb interaction is greater than or equal to staggered Ionic potential (U>=Δ). However, in the opposite case where U<Δ, photo-excited system relaxes to a non-thermal steady state, and we did not see the thermalization of this state in our simulation time.

TT 31.4 Mon 16:15 EB 107

Resonant thermalization of periodically driven strongly correlated electrons — •Francesco Peronaci, Marco Schiró, and

Olivier Parcollet — Institut de Physique Théorique (IPhT), Gif-sur-Yvette, France

We study the dynamics of the Fermi-Hubbard model driven by a time-periodic modulation of the interaction within nonequilibrium Dynamical Mean-Field Theory. For moderate interaction, we find clear evidence of thermalization to a genuine infinite-temperature state with no residual oscillations. Quite differently, in the strongly correlated regime, we find a quasi-stationary extremely long-lived state with oscillations synchronized with the drive (Floquet prethermalization). Remarkably, the nature of this state dramatically changes upon tuning the drive frequency. In particular, we show the existence of a critical frequency at which the system rapidly thermalizes despite the large interaction. We characterize this resonant thermalization and provide an analytical understanding in terms of a break down of the periodic Schrieffer-Wolff transformation.

TT 31.5 Mon 16:30 EB 107

Dynamical Typicality for initial states with a preset measurement statistics of several commuting observables — •Ben Niklas Balz and Peter Reimann — Fakultät für Physik, Universität Bielefeld, Germany

We consider all pure or mixed states of a quantum many-body system which exhibit the same, arbitrary but fixed measurement outcome statistics for several commuting observables. Taking those states as initial conditions, which are then propagated by the pertinent Schrödinger or von Neumann equation up to some later time point, and invoking a few additional, fairly weak and realistic assumptions, we show that most of them still entail very similar expectation values for any given observable. This finding thus corroborates the widespread observation that few macroscopic features are sufficient to ensure the reproducibility of experimental measurements despite many unknown and uncontrollable microscopic details of the system.

TT 31.6 Mon 16:45 EB 107

Formation of Few-Electron-Complexes — •Hubert Klar — Univ. Freiburg

Systems of 2,3 or 4 electrons in the field of a nucleus are shown to posses unstable equilibrium configurations. The many-body potential energy surface has in such configurations saddle points. AS model we study a saddle point with only one fragmentation direction, and show that the diffraction of an electron wave from the corresponding potential ridge manifests itself as a novel fictitious force being temporarily attractive between electrons. Moreover that force deforms the static potential surface and predicts an energy gap. Our theory extends and translates Wannier classical ionization theory into quantum mechanics. In contrast to Cooper pairs our electronic binding mechanisme stems entirely from correlation rather than fom lattice vibrations.

TT 31.7 Mon 17:00 EB 107

Dynamic Analysis of a Scissors Structure — •Yuta Hama[1], Ichiro Ario[1], Kotaro Adachi[1], and Yuki Chikahiro[2] — [1]Hiroshima University, Higashi-hiroshima, Japan — [2]Shinsyu University, Nagano, Japan

The paper presents a new type of deployable and/or folding bridge, which can be quickly constructed in case of damages after a natural disaster. The concept of the bridge is based on the application of scissor-type mechanism, which provides its rapid deployment. The presented research reviews fundamental numerical and experimental results for the full-sized scissors structure. Experimental testing included strain and acceleration measurements in free and forced loading conditions. From these results, it was possible to estimate basic dynamic characteristics of the bridge. Besides, in order to provide a basis for development of new construction methods under gravity. This dynamic research allows for a better and safer design of the movable and foldable full-scale scissors type of bridge.

TT 31.8 Mon 17:15 EB 107

Dynamics in the ergodic phase of the many-body localization transition for a periodically driven system — •Talía L. M. Lezama[1], Soumya Bera[2], and Jens H. Bardarson[3] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm, SE-106 91 Sweden

Closed disordered interacting quantum systems can experience a many-body localization phase transition when tuning the disorder strength around its critical value. Recent studies have shown that the ergodic phase is not a common metallic phase but that it rather exhibits non-trivial mechanisms (mainly Griffiths effects) foregoing the many-body localized phase. Those mechanisms have been described in terms of dynamical quantities such as autocorrelation functions, return probability, entanglement entropy and imbalance, to mention some. Here, we study the dynamics of a Floquet model of many-body localization, focussing on the dynamical regimes on the ergodic side of the transition.

TT 31.9 Mon 17:30 EB 107

Characterizing time-irreversibility in disordered fermionic systems by the effect of local perturbations — •Giuseppe De Tomasi[1], Frank Pollmann[2], Markus Heyl[1], Shreya Vardhan[3], and Eric Heller[4] — [1]MPIPKS, Dresden, Germany — [2]TMU, Munich, Germany — [3]MIT, Cambridge, USA — [4]Harvard, Cambridge, USA

We study the effects of local perturbations on the dynamics of disordered fermionic systems in order to characterize time-irreversibility. We focus on three different systems, the non-interacting Anderson and Aubry-André-Harper (AAH-) models, and the interacting spinless disordered t-V chain. First, we consider the effect on the full many-body wave-functions by measuring the Loschmidt echo (LE). We show that in the extended/ergodic phase the LE decays exponentially fast with time, while in the localized phase the decay is algebraic. We demonstrate that the exponent of the decay of the LE in the localized phase diverges proportionally to the single-particle localization length as we approach the metal-insulator transition in the AAH model. Second, we probe different phases of disordered systems by studying the time expectation value of local observables evolved with two Hamiltonians that differ by a spatially local perturbation. Remarkably, we find that many-body localized systems could lose memory of the initial state in the long-time limit, in contrast to the non-interacting localized phase where some memory is always preserved.

TT 32: Focus Session: Chiral Topological Superconductors and Majorana Fermions

Chiral topological superconductors provide a paradigm of unconventional superconductivity. Such systems break time-reversal symmetry and exhibit rather exotic properties: they feature dispersive Majorana modes around their sample edge, and quantum vortices might host Majorana zero modes which display non-Abelian braiding statistics. This symposium aims to provide an overview of the current experimental and theoretical status as well as future directions of both chiral bulk superconductors and Shiba lattice systems presented by some of the leading experts in the field.

Organization: Katharina Franke, FU Berlin; Stephan Rachel, University of Melbourne

Time: Tuesday 9:30–12:45 Location: H 0104

Invited Talk TT 32.1 Tue 9:30 H 0104

Spin-Triplet Superconductivity in the Ruthenate — •Yoshiteru Maeno — Department of Physics, Kyoto University, Kyoto, Japan

The superconducting symmetry of Sr_2RuO_4 has been widely recognized as spin-triplet, chiral p-wave, based on a number of experimental observations as well as theoretical examinations. Although there are unresolved issues to explain, such as the strong suppression of the up-

per critical field and the first-order transition for the in-plane magnetic fields, there does not seem to be an alternative spin-singlet scenario at present capable of explaining all the key experiments [1].

In this talk, some important facts to consider towards refining the proper spin-triplet scenario are presented, such as the multicomponent order parameter characteristics of the intrinsic "1.5-K phase". This talk also addresses the issue of topological superconductivity of Sr_2RuO_4. Depending on the direction of the Cooper-pair d-vector, spinfull Dirac electron edge modes or spinless Majorana edge modes are expected.

This talk is mainly based on the collaborations and discussions with S. Kashiwaya, M. Sato, C. Hicks, A.P. Mackenzie, S. Yonezawa, Y. Yasui, K. Lahabi, and J. Aarts.

[1] A.P. Mackenzie et al., npj Quantum Materials (2017) 2:40.

Invited Talk TT 32.2 Tue 10:00 H 0104

Paths Towards Chiral d-wave Superconductivity — •Ronny Thomale — Universität Würzburg, Am Hubland, 97074 Würzburg

Starting by the discovery of integer quantum Hall effect in 1980, chiral topological states of matter have been in the focus of contemporary experimental and theoretical research. Astonishingly, despite significant effort and promising progress e.g. regarding the analysis of strontium ruthenate, unambiguous evidence for a chiral superconducting state of matter has remained an open problem until today. In this talk, we wish to sketch latest efforts to accomplish such an objective, and argue that hexagonal unconventional superconductors appear as one most interesting direction to realise chiral superconductivity which, from a mean field perspective, amounts to realising a Chern insulator of Bogoliubov quasiparticles.

Invited Talk TT 32.3 Tue 10:30 H 0104

Towards the Design of Majorana Bound States in Artificially Constructed Magnetic Atom Chains on Elemental Superconductors — •Roland Wiesendanger — Dept. of Physics, University of Hamburg, Hamburg, Germany

We demonstrate the fully-controlled bottom-up fabrication of artificial 1D atomic chains from individual magnetic Fe adatoms on high spin-orbit coupled superconducting Re(0001) substrates by STM-based atom-manipulation techniques at T=350 mK. Spin-polarized STM measurements indicate the presence of non-collinear spin textures, i.e. spin spiral ground states, stabilized by interfacial Dzyaloshinskii-Moriya interactions. Tunneling spectra measured spatially resolved on the Fe-atom chain on Re(0001) reveal the evolution of the local density of states inside the superconducting gap as well as the development of zero-energy bound states at the ends of the chain, which are distinguishable from trivial end states by systematically increasing the number of atoms within the Fe-atom chain. The experimental results will be compared with model-type calculations supporting the interpretation of the spectroscopic signatures at the ends of the chains as Majorana bound states. Such Majorana states can encode topological qubits and ultimately provide a new direction in topological quantum computation.

15 min. break.

Invited Talk TT 32.4 Tue 11:15 H 0104

Design of Majorana Modes: From Magnetic Skyrmions to Dimensional Tuning — •Dirk Morr — University of Illinois at Chicago, Chicago, USA

The experimental observation of Majorana bound states in topological superconductors represents a major breakthrough in realizing their applications in topological quantum computing and has stimulated the search for new possibilities to create and manipulate Majorana states at the nanoscale.

In this talk, I discuss the design of Majorana edge states in magnetic-superconducting hybrid structures and the ability to manipulate them through changes in the shape of the system or the creation of the magnetic skyrmions. I show that the tunneling conductance into Majorana edge states is quantized and proportional to the Chern number, C, while the chirality of the supercurrent carried by the Majorana modes reflects the sign of C, providing important insight into the nature of topological phases. Moreover I demonstrate the existence and unconventional spatial structure of superconducting triplet correlations which can be both time reversal (TR) breaking and TR preserving within the same system. Finally, I show that it is possible to continuously tune hybrid systems between 2D and 1D topological phases, and thus to change the character of the associated Majorana modes.

Invited Talk TT 32.5 Tue 11:45 H 0104

Experimental Hints of Topological Superconductivity in Hybrid Ferromagnet-Superconductor Systems — Gerbold Ménard[1], Sébastien Guissart[2], Christophe Brun[1], Raphaël Leriche[1], Mircea Trif[2], François Debontridder[1], Dominique Demaille[1], Dimitri Roditchev[3], Pascal Simon[2], and •Tristan Cren[1] — [1]Institut des Nanosciences de Paris, CNRS & Sorbonne University, Paris, France — [2]Laboratoire de Physique des Solides, CNRS & Paris-Saclay University, Orsay, France — [3]Laboratoire de physique et d'étude des matériaux, ESPCI, Paris, France

Just like insulators can present topological phases characterized by Dirac edge states, superconductors can exhibit topological phases characterized by Majorana edge states. One-dimensional topological superconductors are predicted to host zero energy Majorana fermions at their extremities. Zero bias anomalies localized at the edge of proximity induced superconducting wires were recently interpreted as fingerprints of the emergence of topological superconductivity [1,2]. By contrast, 2D superconductors have a one-dimensional boundary which would naturally lead to propagating Majorana edge states characterized by a Dirac-like dispersion. These dispersive Majorana edge states were recently observed in a Pb monolayer coupled to a nanomagnet [3]. The topological order was confirmed by the observation of Majorana bound states in vortex cores in this system.

[1] V. Mourik et al., Science 336, 1003 (2012)
[2] S. Nadj-Perge et al., Science 346, 602 (2014)
[3] G. C. Ménard, et al., Nature Comm. (2017)

TT 32.6 Tue 12:15 H 0104

Magnetic impurities on superconducting surfaces — •Nicolas Lorente — Centro de Física de Materiales and Materials Physics Center, CSIC-EHU Donostia International Physics Center, San Sebastián, Spain

A magnetic impurity on a superconducting surface can create a bound state. The state is localized to the magnetic impurity but it extends well into the superconductor and along the surface. Its energy is within the superconductor's gap. This state is a complex state caused by the weakening of Cooper pairs due to the magnetic exchange field produced by the impurity. If another magnetic impurity is approached, the Shiba states can start interacting. If their spins are aligned, they can form bonding and antibonding states. As the number of impurities increases forming a chain of impurities, the Shiba states also increase forming Shiba bands. Under certain conditions, some of these bands can cross the Fermi energy, closing the superconducting gap. This can give rise to changes in the topological electronic structure of the system. As a consequence, if the chain is not infinite, bound states at the edges of the chain are actually Majorana fermions. I will show model calculations analyzing the case of Cr chains on a β-Bi_2Pd superconductor.

TT 32.7 Tue 12:30 H 0104

Search for topological superconductivity in the proximitized, quantum-spin-Hall edge state of bismuth bilayers — •Berthold Jaeck[1], Yonglong Xie[1], Sangjun Jeon[1], Aris Alexandradinata[2], B. Andrei Bernevig[1], and Ali Yazdani[1] — [1]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [2]Department of Physics, Yale University, New Haven, CT 06520, USA

Two-dimensional topological insulators host helical, one-dimensional (1D) modes that are protected by time-reversal symmetry. Proximity induced superconductivity on such edge modes is predicted to be topological in nature and provide a platform for realization of Majorana zero modes. Previously, scanning tunneling microscopy (STM) studies have found evidence for topological edge modes in bismuth (Bi) bilayers on the surface of bulk Bi(111) (1). By epitaxially growing thin films on the surface of Nb, we have successfully induced superconductivity into (111) oriented Bi films. Using high-resolution STM spectroscopy and quasi-particle interference mapping, we characterize the nature of both the normal and the superconducting properties of Bi bilayer edge modes. We find the 1D edge mode to develop a hard superconducting gap that appears to be spectroscopically distinct from the 2D surface gap of the bilayer islands. We will describe these and other experiments designed to elucidate the nature of superconductivity and search for signatures of topological superconductivity in these 1D topological edge states.

[1] I. Drozdov et al., Nature Phys. 10 (2014) 664.

TT 33: Nanotubes and Nanoribbons

Time: Tuesday 9:30–11:30 Location: H 0110

TT 33.1 Tue 9:30 H 0110

Excitons in MoS_2 nanoribbons: width and localization effects. — •Pino D'Amico[1], Deborah Prezzi[1], Andrea Ferretti[1], and Elisa Molinari[2,1] — [1]CNR-NANO-S3, Via Campi 213/a I-41125 Modena, Italy — [2]Physics, Computer Science and Mathematics Departement, University of Modena and Reggio Emilia, Via Campi 213/a I-41125 Modena, Italy

The formation of 1D wires of carriers at the edges of MoS_2 nanoribbons (NRs) represents a case study for spontaneous polarization effects. The spatial confinement and the charge accumulation at the edges make MoS_2-NRs a perfect candidate to investigate interaction effects at the nanoscale, also in view of possible applications in solar-energy devices [1,2]. While the electronic and optical properties of MoS_2 bulk monolayers have been the focus of an intense research, the investigation of MoS_2-NRs is at the early stages. We will present a first principle investigation of the electronic structure and optical absorption of MoS_2-NRs as a function of the NR width, as obtained within the framework of many-body perturbation theory, according to the G0W0 plus Bethe-Salpeter-Equation scheme. We will show that both width-dependent and width-independent mechanisms emerges in the formation of excitonic excitations, and we will explain the relationship between those two mechanisms and the edge-localization of the carriers. Since the investigated MoS_2-NRs are metallic, the present work deals with the fundamental issue of the presence of excitons in metals[3].

[1] M. Gibertini et al., Nat. Commun. 5, 5157(14).
[2] M.Gibertini and N. Marzari, Nano Lett. 15, 6229(15).
[3] F. Wang et al., PRL 99, 227401(07).

TT 33.2 Tue 9:45 H 0110

Doubled quasi-bound states in metallic zigzag carbon nanotubes: an *ab initio* perspective — •Kristjan Eimre[1], Gilles Buchs[2], Dario Bercioux[3,4], Carlo Pignedoli[1], and Daniele Passerone[1] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland — [2]Centre Suisse d'Electronique et de Microtechnique (CSEM) SA, Switzerland — [3]Donostia International Physics Center (DIPC), Spain — [4]IKERBASQUE, Basque Foundation of Science, Spain

The introduction of defects into single-walled carbon nanotubes (SWNTs) can induce electron confinement, enabling the implementation of new SWNT-based quantum devices, such as room temperature single-electron transistors [1].

By means of density funtional theory we compute the electronic structure of metallic zigzag SWNTs, 50 nm long, with defects. Scanning tunneling spectroscopy (STS) simulations are performed to obtain the local density directly comparable to STS experiments.

We show that a particular configuration of the defects produces a doubling of the quasi-bound states in the zigzag nanotube. Our predictions are supported by an experimental case where a partially suspended zigzag tube shows split quasi-bound states between defects induced by Ar^+ ions [2].

[1] Postma, H. W. C et al. *Science* 293, 76 (2001)
[2] Buchs, G. et al. *Phys. Rev. Lett.* 102, 245505 (2009)

TT 33.3 Tue 10:00 H 0110

Carbon nanotube transfer into complex devices with commercial quartz tuning forks — •Patrick Steger, Alexander Albang, Stefan Blien, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040, Regensburg, Germany

For experiments in the GHz regime we intend to couple suspended, clean carbon nanotubes (CNTs) to a superconducting coplanar waveguide (CPW) resonator. However, device fabrication is still challenging. Wet chemical processing as well as plasma etching can cause contamination and defects in the nanotubes while the conditions during CVD needed for nanotube growth can destroy superconducting on-chip circuitry.

To increase our fabrication yield we have developed a fork transfer method that allows us to separate the CVD process for CNT growth from the rest of the device fabrication. CNTs are grown between the tips of a commercial quartz tuning fork. In a subsequent step the tubes are transferred to the device containing dc electrodes as well as superconducting RF circuitry. Our transfer setup allows in situ precharacterization of the CNT during the transfer process. When a suitable CNT is found, the transfer process is completed by cutting the tube with current pulses at both ends.

We show first results of CNTs successfully transferred to a niobium CPW resonator device. Transport measurements at millikelvin temperatures show characteristics of a low number of high quality nanotubes and confirm the feasibility of transparent contacts.

TT 33.4 Tue 10:15 H 0110

Influence of defect-induced deformations on electron transport in carbon nanotubes — •Fabian Teichert[1,3,5], Christian Wagner[1,2], Alexander Croy[4], and Jörg Schuster[3,5] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Center for Microtechnologies (ZfM), Technische Universität Chemnitz, Chemnitz, Germany — [3]Dresden Center for Computational Materials Science (DCMS), Dresden, Germany — [4]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, Dresden, Germany — [5]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

We theoretically investigate the influence of defect-induced long-range deformations in carbon nanotubes on their electronic transport properties using a density-functional-based tight-binding (DFTB) model [1]. The geometry optimization leads to a strong reconstruction of the atoms close to the defect and an additional long-range deformation. The impact of both structural features on the conductance is systematically investigated for various tubes with vacancies.

We find that the long-range deformation additionally affects the transmission spectrum and the conductance compared to the short-range reconstruction. The conductance of larger CNTs is overall less affected implying that the influence of the long-range deformation decreases with increasing tube diameter. Our results indicate that the long-range deformation must be included in order to reliably describe the electronic structure of defective, small-diameter CNTs.

[1] F. Teichert et al., arXiv:1705.01753 [cond-mat.mes-hall]

TT 33.5 Tue 10:30 H 0110

Renormalization group study of competing low-temperature phases in single-wall carbon nanotubes — Wen-Min Huang[1], •Junichi Okamoto[2,3], and Ludwig Mathey[2,3] — [1]Department of Physics, National Chung-Hsing University, Taichung 40227, Taiwan — [2]Zentrum für Optische Quantentechnologien and Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

Carbon nanotubes (CNs) are intriguing one-dimensional systems where various electronic states emerge from their microscopic details. Examples are superconducting states in CNs embedded in a zeolite matrix [1], Mott insulating states in ultraclean CNs [2], and Wigner crystals in semiconducting CNs [3]. Here, we theoretically investigate the low-temperature phase diagrams of single-wall CNs by a renormalization group method. Important ingredients are: (i) electron-phonon interactions that may induce superconductivity or Peierls distortion and (ii) electronic correlations that may cause Mott insulating states. We discuss some preliminary consequences of the competition among these phases.

[1] Z. K. Tang et al., Science 292, 2462 (2001)
[2] V. V. Deshpande et al., Science 323, 106 (2009)
[3] V. V. Deshpande and M. Bockrath, Nat. Phys. 4, 314 (2008)

TT 33.6 Tue 10:45 H 0110

Dark states in a carbon nanotube quantum dot - theory — Michael Niklas[1], Michael Schafberger[2], •Andrea Donarini[1], Nicola Paradiso[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

The dark states are the key to interpret the transport characteristics of a class of single electron transistors based on carbon nanotubes (CNT) quantum dots. The emergence of the dark states relies on the (quasi) valley degeneracy of the CNT and on the particular coupling to the metallic leads. The difference between the tunneling phases to the

two electrodes is the most relevant parameter of the theory. Besides characterizing the dark states, this phase difference determines also the precession dynamics of the pseudospin associated to the orbital degeneracy. This theory predicts current suppression with a specific gate and bias dependence which accurately matches the experimental results.

TT 33.7 Tue 11:00 H 0110

Dark states in a carbon nanotube quantum dot - experiment — Michael Niklas[1], Michael Schafberger[2], Andrea Donarini[1], •Nicola Paradiso[2], Christoph Strunk[2], and Milena Grifoni[1] — [1]Institute of Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Illumination of three level atoms (λ-systems) by detuned lasers can pump electrons into a coherent superposition of hyperfine-split levels which can no longer absorb light. Because fluorescent light emission is then suppressed, the coherent superposition is known as a *dark state*. We report an all-electric analogue of this destructive interference effect in a carbon nanotube quantum dot. A dark state is in this case a coherent superposition of states with opposite angular momentum which is fully decoupled from either the drain or the source leads. The emergence of dark states impacts the current-voltage characteristics, where missing current steps are observed depending on the sign of the applied source-drain bias. Our results demonstrate for the first time coherent-population trapping by all-electric means in an artificial atom.

TT 33.8 Tue 11:15 H 0110

Coupling a terahertz cavity to a carbon nanotube quantum dot — •F. Valmorra[1,2], K. Yoshida[3], L. Contamin[1], T. Cubaynes[1], M. Dartiailh[1], M. Desjardins[1], S. Massabeau[1], K. Hirakawa[3], J. Mangeney[1], A. Cottet[1], and T. Kontos[1] — [1]Laboratoire Pierre Aigrain, CNRS UMR 8551, ENS, 24 rue Lhomond, 75005 Paris, France — [2]Early-Postdoc Fellow of the Swiss National Science Foundation — [3]Institute of Industrial Science, University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan

One of the most interesting aspects of science is the fundamental, coherent interaction of light and matter, down to the quantum level of countable photons and single electronic transitions. Such kind of investigations gave birth to the field of cavity-Quantum ElectroDynamics and later to circuit-QED. Mesoscopic QED uses quantum dots as the matter part, aiming at the realisation of spin-qubits and at the investigation of fundamental physical phenomena. While these investigations have focussed on the microwave range, it comes natural to extend them to the THz, where the energies of the quantum dots realised in a carbon nanotube lie. We thus couple the QD to a THz-split-ring resonator: the transport characterisation of the device shows a region of suppressed conductance, close to zero bias, as large as the photon energy. This gap is reminiscent of the Franck-Condon blockade effect transposed to photons. Such system paves the way towards more complex condensed matter studies and the demonstration of strong coupling pushing forward optoelectronics and quantum optics in the THz frequency range.

TT 34: Superconductivity: Tunneling and Josephson Junctions

Time: Tuesday 9:30–13:00 Location: H 2053

Invited Talk TT 34.1 Tue 9:30 H 2053

Non-Equilibrium Spin- and Charge Transport Phenomena in Superconductor-Ferromagnet Hybrid Structures — •Torsten Pietsch — Department of Physics, University of Konstanz, Germany

Over the past few years, hybrid superconducting nanostructures attracted tremendous interest in condensed matter physics due to their great potential in dissipation-less spintronic devices with unprecedented switching rates. The practical realization of such devices, however, requires a complete understanding of the transfer and the dynamics of spin- and charge currents between superconducting (S) and ferromagnetic (F) circuit elements, as well as the coupling between spin- and charge degrees of freedom in these systems. Here we explore both local and non-local transport properties of lateral, superconducting spin-valves and ferromagnetic Josephson junctions. In diffusive S-FS'-S proximity junctions, the spin-polarized spacer leads to a non-sinusoidal current-phase relationship, which is investigated via the occurrence of Shapiro steps in the IV characteristics under microwave irradiation depending on the magnetization state of the F spacer. An interesting question remains, whether superconducting triplet pair correlations can be induced in extended S-F-S junctions incorporating a long ferromagnetic spacer with a dynamic magnetization via magnon scattering. The latter would provide means to generate spin-polarized supercurrents in S/F heterojunctions for superconducting spintronic applications.

TT 34.2 Tue 10:00 H 2053

Influence of Microwaves on Magnetic Switching in Nb-Al/AlO$_x$-(Nb)-PdFe-Nb Josephson Junctions — •Roberta Caruso[1,2], Davide Massarotti[1,2], Aymen Ben Hamida[3], Vitaly Bol'ginov[4], Alessandro Miano[1], Igor Vernik[5], Valery Ryazanov[4,6], Oleg Mukhanov[5], Francesco Tafuri[1,2], and Giovanni Piero Pepe[1,2] — [1]Dipartimento di Fisica, Università degli Studi di Napoli Federico II, I-80125 Napoli, Italy — [2]CNR-SPIN Institute - Superconductors, Innovative Materials and Devices, UOS Napoli, I-80100 Napoli, Italy — [3]National University of Science and Technology MISiS, Moscow, Russia — [4]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka 142432, Russia — [5]Hypres, Inc., 175 Clearbrook Road, Elmsford, New York 10523, USA — [6]Faculty of Physics, National Research University Higher School of Economics, Moscow, Russia

Superconducting circuits have found application in various fields, due to their high speed and high energy efficiency. However, the practical, large scale application of these circuits is limited by the lack of compatible energy-efficient, high-speed and high capacity random access memories. In 2012 Nb-Al/AlO$_x$-(Nb)-PdFe-Nb have been proved to be random access magnetic memories compatible with RSFQ logic. However, the performances of such devices can be limited by the external addressing circuitry. Here we discuss the effect on magnetic switching of RF fields, in particular the enhancement of the separation between the 0 level and the 1 level when an external microwave field is applied, and its consequences on the performances of these devices.

TT 34.3 Tue 10:15 H 2053

Fluxoid-periodicity crossover from $\frac{h}{2e}$ to $\frac{h}{e}$ in Al nano-loops — •Rebekka Garreis[1], Julian Braun[1], Christopher Espy[1], Omri Sharon[2], Florian Strigl[1], Yosef Yeshurun[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics and Institute of Nano Technology and Advanced Materials, Bar-Ilan University, 5290002 Ramat-Gan, Israel

In a multiply connected superconductor, the fluxoid is quantized in units of $\Phi_0 = \frac{h}{2e}$, where the 2e is a hallmark of electron pairing in the superconductor. Theoretical studies [1] have predicted that in superconducting nano-loops with length-scale $a < \xi_0$ the dominant periodicity of the flux is $2\Phi_0$ rather than Φ_0. Aluminum is a natural choice of material for experimental verification of this prediction because of its relatively large bulk coherence length ($\xi_0 = 1.6\,\mu$m). First measurements on aluminum networks with loop sizes of roughly 320 nm and 420 nm at temperatures between 300 and 1400 mK reveal usual Little-Parks flux periodicity of Φ_0 at low temperatures and indicate a crossover to $2\Phi_0$ periodicity at temperatures above 1300 mK. So far, the relatively low critical field of aluminum, in particular close to the transition temperature, and the large period of small loops, allowed the measurement of one Φ_0 period only. To be able to achieve a full experimental verification, measurements on networks with a loop size of 500 nm at temperatures between 1100 and 1550 mK are performed.

TT 34.4 Tue 10:30 H 2053

Renormalization of Charging Energy in superconducting Single Electron Transistors — •Susanne Sprenger, Thomas Lorenz, and Elke Scheer — Universität Konstanz

A small island connected by two tunnel junctions and a gate electrode

forms a single electron transistor (SET) that shows Coulomb blockade (CB) effects. In the case of weak-coupling, Orthodox Theory (OT) can be used to quantitatively describe the behavior of these devices even when considering superconducting transport [1,2].

Transport in the strong-coupling regime, however, is not yet fully understood and difficult to address with traditional SETs. We present a measurement scheme where all coupling regimes can be addressed. The sample is composed of an AlO_x tunnel barrier and a mechanically controllable break junction, that can be tuned throughout all coupling regimes. When tuning the sample from the orthodox regime to higher couplings the transport properties are changing, which is most prominent in the superconducting state. We observe a renormalization of the charging energy for intermediate couplings as well as the disappearance of the CB for very high couplings, similar to the findings of [3].

[1] R. J. Fitzgerald, Phys. Rev. B 57, R11073(R) (1997)
[2] K. K. Likharev, Proc. IEEE 87, 606 (1999)
[3] S. Jezouin, Nature 536, 58-62 (2016)

TT 34.5 Tue 10:45 H 2053

Evidence of Shapiro steps in hysteretic nanobridge weak link Josephson junctions — •Connor Shelly, Patrick See, Jane Ireland, and Jonathan Williams — National Physical Laboratory, Hampton Rd, Teddington, TW11 0LW, United Kingdom

We present experimental work demonstrating the response of superconducting nanobridge Josephson junctions to microwave irradiation. Our nanobridge devices exhibit hysteretic current-voltage characteristics (IVC) below 7 K. In this regime the devices enter a resistive state when the applied current is increased to a value greater than the junction critical current I_c. When the applied current is then reduced, the nanobridge remains in the resistive state until the re-trapping current I_r is reached, where $I_r < I_c$. Unlike traditional tunnel junctions it is widely considered that the origin of this hysteresis is thermal with the device remaining in a non-superconducting state such that$T > T_c$ on the re-trapping branch of the IVC [1-3]. However we present evidence of Shapiro steps in the hysteretic branch of the IVC.

[1] W. J. Skocpol, M. R. Beasley, M. Tinkham, J. Appl. Phys. 45, 4054, (1974)
[2] D. Hazra, L. M. A. Pascal, H. Courtois, A. K. Gupta, Phys. Rev. B 82, 184530 (2010).
[3] A. Blois, S. Rozhko, L. Hao, J. C. Gallop, E. J. Romans, Supercond. Sci. Technol. 30, 014003 (2017).

TT 34.6 Tue 11:00 H 2053

Tunneling spectroscopy of superconducting $In_xSn_{1-x}Te$ nano-plates — •Fan Yang, Mengmeng Bai, Zhiwei Wang, and Yoichi Ando — Institute of Physics II, University of Cologne, Zuelpicher Str. 77, 50937 Cologne, Germany

With indium doping, superconductivity can be induced in SnTe, a well-known topological crystalline insulator. Due to the possible co-existence of superconductivity and non-trivial band topology, $In_xSn_{1-x}Te$ provides a promising platform for searching for topological superconductivity.

In this talk, we present our study on the point-contact spectroscopy of superconducting $In_xSn_{1-x}Te$ nanostructures. $In_xSn_{1-x}Te$ nano-plates were grown on Si/SiO_2 substrates via vapor-transport method. After the growth, Au contacts with naturally formed tunnel barrier were fabricated on selected nano-plates. The conductance spectra of Au contacts were measured in a dilution refrigerator, and non-trivial sub-gap features were observed in several Au contacts at the tunnel limit. The preliminary results are presented and discussed.

15 min. break.

TT 34.7 Tue 11:30 H 2053

Transport properties of an electron-hole bilayer/superconductor hybrid junction — •D. Bercioux[1,2], T.M. Klapwijk[3], and F.S. Bergeret[1,4] — [1]Donostia International Physics Center (DIPC), Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]Kavli Institute of Nanoscience Delft University of Technology — [4]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, 20018 Donostia-San Sebastián, Spain

We investigate the transport properties of an electron-hole bilayer (EBL) contacted with normal and superconducting leads. We assume that the EBL hosts an exciton condensate (EC) described by a BCS-like model with a gap in the quasiparticle density of states. Contrary to the existing proposal based on Coulomb drag measurements [1,2], we show that the existence of the EC via transport measurements in the sub-gap regime. Here, transport properties are determined by the competition of the standard Andreev reflection at the interface between the superconductor/EC with crossed reflection at the semi-metal/EC. The latter converts electrons from one layer to the other [2]. We show that the existence of a finite gap manifests in a minimum of the conductance at low voltage bias [3].

[1] Croxall et al., Phys. Rev. Lett. 101, 246801 (2008).
[2] Rontani & Sham, Phys. Rev. Lett. 94, 186404 (2005).
[3] DB, Klapwijk, & Bergeret Phys. Rev. Lett. 119, 067001 (2017).

TT 34.8 Tue 11:45 H 2053

Spin-flip enhanced thermoelectricity in superconductor-ferromagnet bilayers — •Ali Rezaei, Akash Kamra, Peter Machon, and Wolfgang Belzig — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We study the effects of Zeeman-splitting and spin-flip scattering in a superconductor (S) on the thermoelectric properties of a tunneling contact to a metallic ferromagnet (F) using the Green's function method. A giant thermopower has been theoretically predicted and experimentally observed in such structures. This huge thermoelectric effect is attributed to the spin-dependent particle-hole asymmetry in the tunneling density of states in the S/F heterostructure. Here, we evaluate the S density of states and thermopower for a range of temperatures, Zeeman-splitting, and spin-flip scattering. In contrast to the naive expectation, we find that the spin-flip scattering strongly enhances the thermoelectric performance of the system in the low-field and low-temperature regime. This is attributed to a complex interplay between the charge and spin conductances caused by the softening of the spin-dependent superconducting gaps. The maximal value of the thermopower exceeds k_B/e by a factor of ~ 5 and has a nonmonotonic dependence on Zeeman-splitting and spin-flip rate. We also demonstrate that the incoherent broadening leads to a drastic reduction of the thermoelectric performance.

[1] A. Rezaei, A. Kamra, P. Machon, W. Belzig, arXiv:1711.11538v1

TT 34.9 Tue 12:00 H 2053

Yu-Shiba-Rusinov states in magnetic Josephson junctions — •Andreas Costa, Denis Kochan, and Jaroslav Fabian — University of Regensburg, 93040 Regensburg, Germany

Superconductivity and ferromagnetism are two nominally antagonistic states of matter, which lead to extraordinary physical phenomena when combined in one system. Perhaps most striking is the emergence of 0-π transitions in magnetic Josephson junctions. We study the bound state spectrum in S/I/S Josephson junctions in which the interlayer (I) hosts point-like scalar and magnetic impurities. In addition to Andreev-like subgap states, stemming from the coherent coupling of the superconductors (S), magnetic impurities give rise to superimposed Yu-Shiba-Rusinov (YSR)-like states. We show that these states have genuine features, which can be tuned by changing the junction characteristics and allow to clearly identify the states in STM experiments. Particularly interesting are zero-energy YSR-like states in the center of the superconducting gap, which form for a wide range of accessible junction configurations. By calculating the Josephson current flow across the system from the spectrum, we unravel a unique connection between these zero-energy YSR-like states and the appearance of 0-π transitions in the current flow. Our findings shed new light on the physics of 0-π transitions in Josephson junctions.

This work was supported by DFG SFB Nos. 689 and 1277, by the European Union's Horizon 2020 research and innovation programme under Grant agreement No. 696656, and by the International Doctorate Program Topological Insulators of the Elite Network of Bavaria.

TT 34.10 Tue 12:15 H 2053

Charge Transfer across a Scanning Tunneling Microscope Junction in Presence of a Macroscopic Impedance — •Simon Dambach[1], Christian R. Ast[2], Björn Kubala[1], Jacob Senkpiel[2], Markus Etzkorn[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems, Ulm University, Ulm, Germany — [2]MPI for Solid State Research, Stuttgart, Germany

When it comes to probing electronic structure on an atomic scale, scanning tunneling microscopy has evolved into one of the most powerful and versatile experimental techniques over the last decades. Recent progress in pushing the energy resolution to the low energy scales that are necessary for resolving extremely sharp spectral features (e.g., su-

perconducting gaps, Yu-Shiba-Rusinov states, or Kondo peaks) has led to the development of an ultra-precise scanning tunneling microscope operating at 15 mK [1]. At these low temperatures, the device is operated at the quantum limit, i.e., the granularity of the current becomes non-negligible. The ultimate resolution is limited here by the electromagnetic interaction of the tunneling charge quantum with the surrounding and the capacitative noise of the junction.

In this talk, we provide a theoretical study of the electrical current across a scanning tunneling microscope junction in presence of an environmental macroscopic impedance. On the basis of $P(E)$ theory, which describes the probability for a loss or gain in energy during a tunneling process, we obtain corrections to the $I(V)$ characteristics which reproduce data of current measurements with high accuracy.
[1] C. R. Ast et al., Nat. Commun. **7**, 13009 (2016)

TT 34.11 Tue 12:30 H 2053

Single Channel Josephson Effect in a High Transmission Tunnel Junction — •Christian R. Ast[1], Jacob Senkpiel[1], Simon Dambach[2], Björn Kubala[2], Ciprian Padurariu[2], Berthold Jäck[1], Markus Etzkorn[1], Juan Carlos Cuevas[3], Joachim Ankerhold[2], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Institut für Komplexe Quantensysteme, Universität Ulm — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

Andreev bound states lie at the heart of many phenomena involving scattering with superconductors, such as Yu-Shiba-Rusinov states, Majorana bound states, or the Josephson effect. In most cases it is sufficient to approximate the Josephson effect by an ensemble of many, nearly opaque transport channels. However, in scanning tunneling microscopy (STM), where only very few transport channels are realized and arbitrary transmissions can be achieved, this approximation may break down and the full energy-phase relation of the Andreev bound states has to be considered. Using the manipulation techniques available to STM, we exploit a single atom contact at high transmission to demonstrate the consequences of single channel transport for the Josephson effect. We demonstrate single channel transport through the analysis of multiple Andreev reflections at various transmission setpoints and discuss the transition from the tunneling approximation to the full Andreev bound state description in the dynamical Coulomb blockade regime.

TT 34.12 Tue 12:45 H 2053

Phase-dependent heat transport in multi-terminal Josephson junctions — •Sun-Yong Hwang and Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Phase-coherent heat transport has received a lot of attention recently as it offers the possibility to control heat flows at the nanoscale with the same precision as charge currents [1]. Thus, phase-coherent caloritronics provides not only fundamental insights into heat transport at the nanoscale but can also lay the foundations for future thermal logic and energy management in small electric circuits.

Here, we investigate the phase-dependent linear thermal conductance in multi-terminal Josephson junctions. The thermal conductance in our system can be controlled via the magnetic flux through the junction and the phase bias configuration among the superconductors. Remarkably, the phase- and flux-controlled heat can show a strongly unidirectional transport property which can be utilized for a heat circulator or a highly efficient cooler.
[1] A. Fornieri, F. Giazotto, Nat. Nanotechn. 12, 944 (2017).

TT 35: Superconductivity: Fe-based Superconductors - 122 and Theory

Time: Tuesday 9:30–13:00 Location: A 053

TT 35.1 Tue 9:30 A 053

Soft phonons reveal finite nematic correlation length in $Ba(Fe_{0.94}Co_{0.06})_2As_2$ — •Frank Weber[1], Michael Merz[1], Thomas Wolf[1], Rafael Fernandes[2], Jörg Schmalian[1], and Dmitry Reznik[3] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota, 55455, USA — [3]Department of Physics, University of Colorado at Boulder, Boulder, Colorado, 80309, USA

Nematicity is ubiquitous in electronic phases of high-T_c superconductors, particularly in the Fe-based systems. While several experiments have probed nematic fluctuations, they have either been restricted to uniform, i.e. $\mathbf{q} = 0$ fluctuations, or measure momentum-averaged effects. Here, we investigate the behavior of finite-momentum nematic fluctuations near $\mathbf{q} \approx 0$ by utilizing the anomalous softening of transverse acoustic phonon modes in optimally doped $Ba(Fe_{0.94}Co_{0.06})_2As_2$. We determine the nematic correlation length and find that it sharply changes its T-dependence at T_c, revealing a strong connection between nematicity and superconductivity.

TT 35.2 Tue 9:45 A 053

Superconductivity induced changes of the phonon lifetime in $Ba(Fe_{0.94}Co_{0.06})_2As_2$ — •Maximilian Kauth[1], Frank Weber[1], John-Paul Castellan[1], Thomas Wolf[1], Thomas Keller[2], and Dimitry Reznik[3] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Max-Planck-Institute for Sodid State Research, Stuttgart, Germany — [3]Department of Physics, University of Colorado atBoulder, Boulder, Colorado, 80309, USA

We have investigated the life time of the transversal acoustic (TA) phonon mode in the Fe-based high-temperature superconductor $Ba(Fe_{0.94}Co_{0.06})_2As_2$ along the [100] direction. We used the thermal neutron triple axis spectrometer (TAS) 1T at LLB at CEA Saclay and the neutron resonant spin echo (NRSE) technique at the TRISP spectrometer at the MLZ in Garching [1]. This phonon mode is the soft mode of the structural phase transition present in lower doped samples. Recent measurements showed evidence that it is sensitive to nematic fluctuations in this compound [2]. We observe a clear maximum of the TA phonon linewidth at the superconducting transition temperature $T_C \approx 24$ K with both measurement techniques (regular TAS and NRSE). This is the first experimental evidence of changes of the phonon lifetime in Fe-based superconductors.
[1] MPI for Solid State Research et al., Journal of large-scale research facilities, 1, A37 (2015).
[2] F. Weber et al., arXiv:1610.00099 (2016).

TT 35.3 Tue 10:00 A 053

Uniaxial strain control of spin-polarization in multicomponent nematic order of $BaFe_2As_2$ — T. Kissikov[1], •R. Sarkar[2], S. L. Bud'ko[3], P. C. Canfield[3], R. M. Fernandes[4], and N. J. Curro[2] — [1]Department of Physics, UC Davis, CA 95616, USA — [2]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [3]Ames Laboratory Department of Physics and Astronomy,ISU Ames, Iowa 50011, USA — [4]School of Physics and Astronomy, UMN Minneapolis, Minnesota 55455, USA

The iron-based high temperature superconductors exhibit a rich phase diagram reflecting a complex interplay between spin, lattice, and orbital degrees of freedom. The nematic state observed in many of these compounds illustrates this complexity, by entangling a real-space anisotropy in the spin fluctuation spectrum with ferro-orbital order and an orthorhombic lattice distortion. A more subtle and much less explored fact of the interplay between these degrees of freedom arises from the sizable spin-orbit coupling present in these systems, which translates anisotropies in real space into anisotropies in spin space. Here, we present a new technique enabling nuclear magnetic resonance under precise tunable strain control, which reveals that upon application of a tetragonal symmetry-breaking strain field, the magnetic fluctuation spectrum in the paramagnetic phase of $BaFe_2As_2$ also acquires an anisotropic response in spin-space.

TT 35.4 Tue 10:15 A 053

Superconductivity with broken time reversal symmetry in $Ba_{1-x}K_xFe_2As_2$ single crystals — •Vadim Grinenko[1,2], Philipp Materne[1], Rajib Sarkar[1], Sirko Kamusella[1], Kunihiro Kihou[3], Chul-Ho Lee[3], Shavkat Akhmadaliev[4], Dmitriy Efremov[2], Stefan-Ludwig Drechsler[2], Hubertus Luetkens[5], and Hans-Henning Klauss[1] — [1]Institute for Solid State and Material Physics, TU Dresden, 01069 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [3]National Institute of Advanced

Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8560 Japan — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [5]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland

Over the last years a lot of theoretical and experimental efforts have been made to find states with broken time reversal symmetry (BTRS) in multi-band superconductors below the superconducting transition temperature (T_c). In particular, it was theoretically proposed that in the $Ba_{1-x}K_xFe_2As_2$ system either an $s+is$ or an $s+id$ BTRS state may exist at high doping levels in a narrow region of the phase diagram. Here we report the observation of an enhanced zero field muon spin relaxation rate at $T^* \lesssim T_c$ for a high quality crystalline samples in the doping range $0.8 \gtrsim x \gtrsim 0.7$. We found that T^* is strongly doping dependent. Our results are consistent with the multi-band $s+is$ superconducting state in $Ba_{1-x}K_xFe_2As_2$ in this doping range.

TT 35.5 Tue 10:30 A 053

Mass enhancements and band shifts in hole overdoped Fe-based pnictide superconductors: KFe_2As_2 and $CsFe_2As_2$ — •S.-L. Drechsler[1], H. Rosner[2], V. Grinenko[3], S. Aswartham[1], I. Morozov[4], L. Ming[4], A. Boltalin[4], K. Kihou[5], C. H. Lee[5], T. K. Kim[6], D. Evtushinsky[7], J.M. Tomczak[8], S. Johnston[9], and S. Borisenko[1] — [1]IFW-Dresden, Germany — [2]MPI-CPfS Dresden, Germany — [3]TU Dresden, Germany — [4]Moscow University, Russia — [5]AIST, Tsuk. Japan — [6]Diamond Light Source, U.K. — [7]Ec. de Fed., Lausanne, Switzerland — [8]Vienna-University of Technology, Austria — [9]Tennesee University, Knoxville, USA

The interplay of high- and low energy (LE) mass renormalizations with band shifts as seen in the positions of van Hove singularities (VHS) in the normal state of the strongly correlated and most hole-overdoped AFe_2As_2 (A122), A = K,Rb,Cs Fe pnictides is discussed phenomenologically from ARPES data and band structure (GGA) with full spin-orbit coupling and microscopically applying the GW-self-energy. The increase of the Sommerfeld coefficient γ from K122 to Cs122 is ascribed to an enhanced coupling to LE bosons in the vicinity of a quantum critical point to an yet unknown incommensurate phase different from the tetragonal Mott phase. We find no sizable increase of correlation for Cs122 in contrast to scenarios proposed in the literature. The ARPES positions of VHS as compared with GGA and GW results point to slightly weaker correlations in accord with the low-T susceptibility data and the reduced Wilson ratio $\chi(0)/\gamma$. Other quasi-2D systems with generic VHS and their el-el interactions are briefly discussed.

TT 35.6 Tue 10:45 A 053

Synthesis and Characterization of $YbFe_2As_2$ Single Crystals — •Nilotpal Ghosh[1], Santhosh Raj[2], and R Navamathavan[2] — [1]Science and Engineering Research Board, Department of Science and Technology, Vasant Kunj, New Delhi, India — [2]School of Advanced Sciences ,VIT University, Chennai, Tamilnadu, India

We report synthesization of a new compound $YbFe_2As_2$ crystals using melt growth technique. The crystals have been characterized by Scanning Electron Microscopy (SEM) and Energy Dispersive X-ray Analysis (EDX). Rietveld refinement of crushed single crystals has shown that the $YbFe_2As_2$ has monoclinic unit cell structure. Transport measurement has shown metallic behavior with a down turn in resistivity around 17K for $YbFe_2As_2$ which is similar to superconducting transition. The detailed magnetic studies by SQUID on these crystals have revealed the co-existence of strong antiferromagnetic and weak ferromagnetic characteristics. Influence of anti-ferromagnetic spin fluctuation in the normal state transport property has been found. Effect of oxygen adsorption on $YbFe_2As_2$ have been studied in detail.
[1] S. S. Raj, N. Ghosh, R. Navamathavan, J. Supercond. Novel Magnetism 30 (2017) 287;
[2] S. S. Raj, N. Ghosh, R. Navamathavan, Mater. Res. Express 4 (2017) 086101;

TT 35.7 Tue 11:00 A 053

Interplay of magnetism and superconductivity in the triclinic $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$ system — •Felix Brückner[1], Vadim Grinenko[1], Rajib Sarkar[1], Maksym Surmach[1], Hubertus Luetkens[2], Dmytro Inosov[1], and Hans-Henning Klauss[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, Villigen, Switzerland

Among iron-based superconductors, $Ca_{10}Pt_3As_8(Fe_{1-x}Pt_xAs)_{10}$ is the first system with a triclinic crystal structure. The usually tetragonal symmetry of the characteristic FeAs layers is slightly distorted by insertion of a skutterudite-like interlayer.

We report comprehensive studies of magnetic probe experiments including ^{75}As and ^{195}Pt nuclear magnetic resonance (NMR), muon spin rotation and inelastic neutron scattering (INS). Broadening of NMR spectra below $T^* \sim 45$ K provides evidence for static magnetic correlations far above the superconducting $T_c = 13$ K. At T^*, a sudden drop of the spin-lattice relaxation rate, that is insensitive to external magnetic field up to 30 T, is observed. INS spectra exhibit a resonant mode at higher energies just below T^*. This was previously interpreted as a manifestation of preformed cooper pairs, which can be ruled out by ^{195}Pt Knight-shift experiments. Furthermore an additional magnetic transition at 3 K and strong but slow magnetic fluctuations peaking at ~ 120 K are detected by NMR. In addition to the magnetic probe investigations, we compare our results with transport measurements and specific heat studies.

15 min. break.

TT 35.8 Tue 11:30 A 053

Consequences of Orbital Selectivity for Magnetism and Superconductivity in Fe-based Superconductors — •Andreas Kreisel[1], Brian Andersen[2], and Peter Hirschfeld[3] — [1]Universität Leipzig, Germany — [2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark — [3]University of Florida, Gainesville, FL, United States

Recently, it has been observed that electronic correlations in iron pnictides and chalcogenides affect electrons in different d-orbitals quite differently. The resulting reduced coherence of the quasiparticle states has consequences for the normal state properties and affects the superconducting state. The renormalization of the d_{xy} orbital is known to be largest, thus its quasiparticle weight smallest. In the Fe based systems, this leads to a reduction of Néel type (π,π) magnetic fluctuations and makes stripe fluctuations relatively stronger. Within a modified spin fluctuation pairing theory, this makes the sign-changing s-wave state more competitive. In this work, we investigate these effects of orbital selectivity with a focus on the FeSe system, which allows us to study the effect of nematicity due to the breaking of tetragonal symmetry without magnetic order at low temperatures. Consequences include different renormalization of the d_{yz} and d_{xz} orbital states, leading to an anisotropic superconducting order parameter and enhancements of the $(\pi,0)$ magnetic fluctuations, an effect seen in neutron scattering experiments. The strongest effects of the reduced coherence are observed in the KFe_2As_2, system where we discuss implications for the superconducting order parameter.

TT 35.9 Tue 11:45 A 053

Orbital loop currents in iron-based superconductors — •Markus Klug[1], Jian Kang[2], Rafael M. Fernandes[2], and Jörg Schmalian[1,3] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany — [2]School of Physics and Astronomy, University of Minnesota, Minneapolis, Minnesota 55455, USA — [3]Institute of Solid State Physics, Karlsruhe Institute of Technology, D-76344 Eggenstein-Leopoldshafen, Germany

We show that the stripe spin-density wave state commonly observed in the phase diagrams of the iron-based superconductors necessarily triggers loop currents characterized by charge transfer between different Fe 3d orbitals. This effect is rooted on the glide-plane symmetry of these materials and on the existence of an atomic spin-orbit coupling that couples states at the X and Y points of the 1-Fe Brillouin zone. We show that the two main manifestations of the orbital loop currents are the emergence of magnetic moments in the pnictide/chalcogen site and an orbital-selective band splitting in the magnetically ordered state, both of which could be detected experimentally. Our results highlight the unique intertwining between orbital and spin degrees of freedom in the iron-based superconductors, and reveal the emergence of an unusual correlated phase that may impact the normal state and superconducting properties of these materials.

TT 35.10 Tue 12:00 A 053

Mixed magnetic order in iron pnictides — •Chris Koschenz and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, Germany

Multiband and multiorbital physics are crucial for understanding superconductivity and magnetism in iron pnictides. We present recent

results for multiorbital Hubbard models representative of iron pnictide compounds using restricted and unrestricted generalized Hartree-Fock methods. The generalized Hartree-Fock method introduced by [1] allows to study phases with mixed magnetic order. In this talk, we revisite the magnetic phases in the vicinity of superconductivity for compounds for which a reentrance of tetragonal magnetic order was found [2,3]. We employ a realistic multiorbital model for $Ba_{1-x}Na_xFe_2As_2$ and $Ba_{1-x}K_xFe_2As_2$ and elucidate the role played by orbital effects. Furthermore, we study the coexistence and competition of tetragonal or mixed magnetic order with superconductivity as well as the possibility of phase separation (mixed phases).

[1] E. Langmann and M. Wallin, J. Stat. Phys. **127** (2007) 825
[2] S. Avci *et al.*, Nature Comm. **5** (2014) 3845
[3] M. Gastiasoro, B. Anderson, Phys. Rev. B **92** (2015) 140506(R)

TT 35.11 Tue 12:15 A 053

Collective modes and short-time dynamics of time-reversal symmetry broken superconductors — •Marvin A. Müller[1], Pengtao Shen[2], Maxim Dzero[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, German — [2]Department of Physics, Kent State University, Kent, OH 44242 USA

Motivated by the recent observation of the time-reversal symmetry broken state in K-doped $BaFe_2As_2$ systems, we theoretically study the collective modes and the short time dynamics of this state using density-matrix theory on an effective four-band model with two hole and two electron pockets. Hole doping moves the electron bands away from the Fermi surface and leads to frustration between superconducting channels. This results either into $s+is$ or $s+id$ superconductivity, which are both time-reversal symmetry breaking (TRSB) states. Consequently, the Higgs and Leggett modes are coupled and the superconducting ground state accommodates a variety of collective modes. In extremely overdoped systems with incipient electron bands, we find the Higgs mode at $\omega = 2\Delta_h$ with an absent Leggett mode similar to a two band model. At dopings before the TRSB occurs and within the TRSB state, we uncover a new coupled collective mode both in the amplitude and in the relative phase of the superconducting gaps. This mode becomes gapless at the boundaries of the TRSB state.

TT 35.12 Tue 12:30 A 053

Superconductivity in presence of spin-orbit coupling in strongly electron-doped iron-based superconductors — •Jakob Böker[1], Felix Ahn[1], Peter Hirschfeld[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics, University of Florida, Gainesville, FL 32611, USA

Motivated by recent experimental reports on sizeable spin-orbit coupling (SOC) in the iron pnictides, we study the SOC induced mixing of the spin singlet and the spin triplet pairing for the leading s- and d-wave superconducting instabilities. We focus on highly electron doped systems where only electron $d_{yz}/d_{xz}/d_{xy}$ pockets are present at the M-point of the two-iron unit cell. Using a orbitally projected effective low energy model for the iron pnictides with pairing driven by atomic onsite interactions, we present the gap structure close to Fermi level and discuss consequences of the induced triplet pairing to experiment.

TT 35.13 Tue 12:45 A 053

Enhanced Nernst effect by nematic fluctuations in an iron based superconductor — •Steffen Sykora[1], Christoph Wuttke[1], Federico Caglieris[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

Nematic fluctuations are expected to enhance superconductivity in iron based superconductors which undergo a transition to nematic order. Motivated by recent Nernst effect measurements we investigate theoretically transport properties within a minimal electronic model consisting of two orbitals, with interactions that enhance nematic fluctuations. We apply a many-particle renormalization method to calculate current-current correlation functions and show that the correlation between currents in perpendicular directions are particularly enhanced by interactions between different orbitals. This property gives rise to a direct coupling of the Nernst effect to nematic fluctuations. We discuss our results in the context of recent Nernst effect experiments in $BaFe_2As_2$.

TT 36: Correlated Electrons: 1D Theory

Time: Tuesday 9:30–12:15 Location: HFT-FT 101

TT 36.1 Tue 9:30 HFT-FT 101

Dynamical measurement of the interaction strength in helical Luttinger Liquids — •Tobias Müller[1], Ronny Thomale[1], Björn Trauzettel[1], Erwann Bocquillon[2], and Oleksiy Kashuba[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg — [2]Laboratoire Pierre Aigrain, Ecole Normale Supérieure-PSL Research University, CNRS, Université Pierre et Marie Curie-Sorbonne Universités, Université Paris Diderot-Sorbonne Paris Cité, 75231 Paris Cedex 05

Based on an equations of motion description of helical Luttinger Liquids we propose a setup to measure the interactions inside a one-dimensional wire directly. Using a capacitively coupled gate rather than purely ohmic contacts we can extract the Luttinger parameter both directly and in the low frequency expansion of a frequency-resolved conductivity measurement. We also discuss the influence of the precise form of the change in interactions at ohmic contacts within the setup.

TT 36.2 Tue 9:45 HFT-FT 101

Superconducting proximity effect in a helical Luttinger liquid coupled to single-electron sources — •Flavio Ronetti[1,2], Matteo Carrega[3], Jérôme Rech[2], Thibaut Jonckheere[2], Thierry Martin[2], and Maura Sassetti[1] — [1]Università di Genova and CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy. — [2]Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France. — [3]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Piazza San Silvestro 12, I-56127 Pisa, Italy.

The superconducting proximity effect in a helical Luttinger liquid induces correlations between left-movers and right-movers channels and, in the presence of the Rashba spin-orbit coupling, also between particles in the same channel [1]. We focus on the injection of single-electrons through a periodic train of Lorentzian pulses [2] along a helical Luttinger liquid coupled to a superconductor. We analyze the current-noise in this setup when a single channel or both channels are coupled to a single-electron source [3]. The presence of electron-electron interactions and Rashba coupling is considered and we suggest some possible experimental signatures of their strength.

[1] P. Virtanen, P. Recher, Phys. Rev B 85, 035310 (2012)
[2] J. Dubois et al., Nature (London) 502, 659 (2013).
[3] F. Ronetti et al., in preparation (2017).

TT 36.3 Tue 10:00 HFT-FT 101

Coherence and decoherence in beamsplitters for interacting edge state electrons — Andreas Schulz, •Imke Schneider, Sebastian Eggert, and James Anglin — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern

Recent studies have shown that simple intersections between one-dimensional channels can act as coherent beam splitters for non-interacting electrons. Here we examine how coherent splitting at such quantum wire crossings is affected by inter-particle interactions. We use the one-loop renormalization group to derive the effective impurity which represents the intersection within Luttinger liquid theory at low energy. For the special case of Luttinger K = 1/2, we compute exact time-dependent expectation values of charge density as well as density-density correlation functions. We find that when multiple charge density wave packets encounter the impurity from different directions, reflection and splitting of the packets depends on their relative phases, raising the prospect of Luttinger interferometry.

TT 36.4 Tue 10:15 HFT-FT 101

Tuning the Drude Weight of Dirac-Weyl Fermions in One-Dimensional Ring Traps — Manon Bischoff[1], Johannes Jünemann[1,2], Marco Polini[3], and •Matteo Rizzi[1] — [1]Institut

für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany — [3]Istituto Italiano di Tecnologia, Graphene Labs, Genova, Italy

We study the response to an applied flux of an interacting system of Dirac-Weyl fermions confined in a one-dimensional (1D) ring. Combining analytical calculations with density-matrix renormalization group results, we show that tuning of interactions leads to a unique many-body system that displays either a suppression or an enhancement of the Drude weight – the zero-frequency peak in the ac conductivity – with respect to the non-interacting value. An asymmetry in the interaction strength between same- and different-pseudospin Dirac-Weyl fermions leads to Drude weight enhancement. Viceversa, symmetric interactions lead to Drude weight suppression. Our predictions can be tested in mixtures of ultracold fermions in 1D ring traps.
[1] Bischoff *et al.*, arXiv:1706.02679

TT 36.5 Tue 10:30 HFT-FT 101

The resonant state at filling factor 1/2 in chiral fermionic ladders — •Andreas Haller[1], Matteo Rizzi[1], and Michele Burrello[2] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

Helical liquids have been experimentally detected in both nanowires and ultracold atomic chains as the result of strong spin-orbit interactions. In both cases the inner degrees of freedom can be considered as an additional space dimension, providing an interpretation of these systems as synthetic ladders, with artificial magnetic fluxes determined by the spin-orbit terms. In this work, we analyze such a quasi-one-dimensional ladder geometry and characterize the helical state which appears at filling factor 1/2. This state is generated by a gap arising in the spin sector of the corresponding Luttinger liquid and can be interpreted as the one-dimensional (1D) limit of a fractional quantum Hall state of bosonic pairs of fermions. We study its main features, focusing on entanglement properties and correlation functions and support our analytic results with matrix product state simulations.

TT 36.6 Tue 10:45 HFT-FT 101

Observation of a hierarchy of modes in an interacting 1D system — •Christopher J B Ford[1], Yiqing Jin[1], Maria Moreno[1], Wooi Kiat Tan[1], Anne Anthore[2], Jon P Griffiths[1], Ian Farrer[1], Geraint A C Jones[1], David A Ritchie[1], Oleksandr Tsyplyatyev[3], and Andrew Scholfield[4] — [1]University of Cambridge, UK — [2]Paris Diderot University, France — [3]University of Frankfurt, Germany — [4]University of Birmingham, UK

At low excitation energies, a system of interacting one-dimensional (1D) electrons can be described theoretically as a Tomonaga-Luttinger liquid. However, it is only in the last few years that theoreticians have developed models of the behaviour at energies comparable to the Fermi energy, predicting 'replicas' of the dispersion relation offset by multiples of the Fermi wave-vector. We measure momentum-resolved tunnelling of electrons between 1D wires formed within a GaAs heterostructure and a 2D electron gas used as a spectrometer and have previously found well-resolved spin-charge separation at low energy with appreciable interaction strength. Now we have detected structure resembling replicas, which dies away quite rapidly at high momentum, in line with the most recent theory.[1] We have fabricated arrays of wires with lengths between 1 and 20μm, after developing a reliable technique to make thousands of 'air-bridges' on each device. The replicas seem strongest in the short wires,[2] again as predicted by the theory.
[1] Tsyplyatyev *et al.*, Phys. Rev. Lett., **114**, 196401 (2015)
[2] Moreno *et al.*, Nat. Commun. **7**, 12784 (2016)

15 min. break.

TT 36.7 Tue 11:15 HFT-FT 101

Systematic reduction of Thermodynamic Bethe Ansatz equations by means of Bäcklund hierarchies — •Eyzo Stouten and Andreas Klümper — Bergische Universität Wuppertal, 42097 Wuppertal, Germany

For integrable systems there is an established way to calculate thermodynamics through the Thermodynamic Bethe Ansatz. The conventional method necessarily involves the characterization of the full spectrum of the Hamiltonian via combinatorial means. An alternative approach is to study the leading eigenvalue of a column to column or quantum transfer matrix (QTM), which is related to an infinite family of QTM by factorization of the bilinear fusion relations (of Hirota type). By studying the analyticity of the constituents of the QTM one can rewrite the fusion relations into non-linear integral equations (NLIE) that characterize the leading eigenvalue. This transformation only depends on some knowledge of the partial spectrum of the QTM.

To extract the thermodynamic properties at finite temperatures the infinite hierarchy of NLIE is truncated to a finite set at the cost of introducing a finite set of auxiliary equations. In previous works these auxiliary equations could only be derived in a heuristic manner for low rank systems. The goal of this research is to derive them in a systematic way by factorization of a set of bilinear Bäcklund equations and extending to arbitrary rank. The use of Bäcklund relations is inspired by a series of papers [1] where they where introduced because of their relation to the Hirota equations and the related fusion relations.
[1] Zabrodin et al., Nucl. Phys. B 790 (2008) 345

TT 36.8 Tue 11:30 HFT-FT 101

DC-Conductance of one-dimensional correlated systems derived by DMRG — •Jan-Moritz Bischoff and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Deutschland

We present an efficient method [1] for computing the zero-temperature linear conductance of correlated one-dimensional systems using the density-matrix renormalization group (DMRG). Like in [2], the model expresses the conductance as limits of dynamical correlation functions in finite systems within Linear Response Theory. These correlation functions can be calculated by dynamical DMRG. We tested the method first on non-interacting models for comparison with exact results and in order to determine an appropriate scaling of frequency, system size and spectral broadening. In addition, we extended the procedure to interacting systems using the one-dimensional spinless fermion model. The results were in good agreement with field-theoretical predictions (combined with the Bethe Ansatz solution) for the renormalization of conductance in a pure Luttinger liquid, as well as for the effects of an impurity in a Luttinger liquid [3]. We were also able to simulate the experimental more relevant setup of a wire that is coupled to leads and will present our first results.
[1] J.-M. Bischoff, E. Jeckelmann, PRB 96, 195111 (2017)
[2] D. Bohr, P. Schmitteckert, P.W. Wölfle, Europhys. Lett., 73, 246 (2006)
[3] C.L. Kane, M.P.A. Fisher, PRB 46, 15233 (1992)

TT 36.9 Tue 11:45 HFT-FT 101

Effective narrow ladder model for a spinless fermion wire on a semiconducting substrate — •Anas Abdelwahab and Eric Jeckelmann — Institut für Theoretische Physik, Leibniz Universität Hannover, Hannover, Germany

A spinless fermion wire coupled to a 3D-tight-binding substrate is approximated by a few-leg narrow ladder model (NLM) using the exact mapping introduced in Refs.[1] and [2]. Three phases are distinguished, namely, a one-component Luttinger liquid, a charge-density-wave (CDW) and a doped band insulator. We investigated the convergence of the single-particle excitation gap with increasing number of legs in the NLM. We confirm that the NLM is a good approximation to the 3D wire-substrate model in the one-component Luttinger liquid and the CDW phases. The NLM describes only qualitatively the doped band-insulator phase. The quantum phase transitions between the three phases are investigated as function of the wire-substrate coupling. The critical nearest-neighbor interactions increase with increasing the wire-substrate coupling.

Support from the DFG through the Research Units FOR 1700 is gratefully acknowledged.
[1] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B 96, 035445 (2017).
[2] A. Abdelwahab, E. Jeckelmann, and M. Hohenadler, Phys. Rev. B 96, 035446 (2017).

TT 36.10 Tue 12:00 HFT-FT 101

Spectral flow for an integrable staggered superspin chain — •Konstantin Hobuss and Holger Frahm — Institut für Theoretische Physik, Leibniz Universität Hannover

The flow of the low energy eigenstates of a $U_q[sl(2|1)]$ superspin chain with alternating fundamental (3) and dual ($\bar{3}$) representations is studied as function of a twist angle determining the boundary conditions. The finite size spectrum is characterized in terms of scaling dimensions and quasi momenta representing the two families of commuting transfer matrices for the model which are even and odd under the interchange $3 \leftrightarrow \bar{3}$, respectively. Based on the extrapolation of our finite size data we find that under a variation of the boundary conditions

from antiperiodic to periodic for the fermionic degrees of freedom levels from the continuous part of the spectrum flow into discrete levels and vice versa. The implications of our results on the underlying conformal field theory which describes the continuum limit are discussed.

TT 37: Skyrmions II (joint session MA/TT/KFM)

Time: Tuesday 9:30–13:15 Location: EB 301

TT 37.1 Tue 9:30 EB 301

Low temperature magnetic field mapping on Néel-skyrmions in GaV4Se8 — •Franziska Seifert[1], Felix L. Kern[1], István Kézsmárki[2], Daniel Wolf[1], Bernd Büchner[1], and Axel Lubk[1] — [1]Leibniz Institute for Solid State and Materials research Dresden, Germany — [2]University of Augsburg, Germany

Skyrmions are promising candidates for magnetic memory devices, because of their small size, thermal stability and high mobility. Here we report on Skyrmion mapping in GaV4Se8 carried out on our dedicated cryo TEM fitted with a continuous-flow liquid He cryostat, facilitating electron holography and Lorentz TEM down to 7K. Bulk GaV4Se8 is predicted to show Neel type skyrmions below 18K under applied magnetic field between 0.10T and 0.45T mT. Using Lorentz TEM, we characterized the cycloidal and skyrmionic phase of thin GaV4Se8 lamellas in dependence of temperature and applied magnetic field. By mapping the magnetic phase diagram of the thin film we identify magnetic textures that are not considered in the bulk phase diagram. We discuss the origins of these in terms of crystal symmetries and strain prevailing in the thin film slab geometry.

TT 37.2 Tue 9:45 EB 301

Probing skyrmion lattice phase by NMR in GaV_4S_8 — •Markus Prinz-Zwick, Norbert Büttgen, Vladimir Tsurkan, Martina Schädler, and István Kézsmárki — Center of electronic correlation and magnetism, University of Augsburg

With the discovery of Néel-Type skyrmions forming in a skyrmion lattice (SkL) in the lacunar spinel GaV_4S_8, the characterization and analysis of such polar axially symmetric skyrmion host materials gained general interest. From a microscopic point of view we want to elucidate the local distribution of internal magnetic fields associated with the SkL and probe spin excitations using Nuclear Magnetic Resonance(NMR) spectroscopy. Since the stability of the SkL phase is limited to the sub-Tesla range, this is a highly challenging issue. Here, we report NMR results within the SkL-phase in the lacunar spinel GaV_4S_8, and the first so called zero-field NMR measurements, where the internal field of the V_4 cubanes was exploited to perform ^{51}V measurements for applied magnetic fields $0 < \mu_0 H < 100\,\mathrm{mT}$.

TT 37.3 Tue 10:00 EB 301

Optically induced demagnetization and coherent spin excitations in GaV4S8 — •Fumiya Sekiguchi[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], István Kézsmárki[2], and Paul H. M. van Loosdrecht[1] — [1]Institute of Physics 2, University of Cologne, 50937 Cologne, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Skyrmions are quasiparticle-like topological spin textures stabilized in non-centrosymmetric crystals with Dzyaloshinskii-Moriya interactions. For potential applications and a better understanding of their nature, it is important to understand their creation and annihilation dynamics, as well as their collective excitation spectrum. Here we employ time resolved magneto-optical Kerr experiments to study the magnetization dynamics in the lacunar spinel GaV4S8 which hosts novel cycloid and Néel-type skyrmion magnetic ground states. The experiments show the emergence of a slow demagnetization process in the magnetically ordered states. In addition, we observe coherent collective spin excitations in both the cycloid and skyrmion phases.

TT 37.4 Tue 10:15 EB 301

Temperature dependence of the cubic anisotropy in the room-temperature skyrmion host $Co_9Zn_9Mn_2$ — •Bertalan György Szigeti[1], Dieter Ehlers[2], Kosuke Karube[3], István Kézsmárki[2], Hans-Albrecht Krug von Nidda[2], Markus Preissinger[2], Vladimir Tsurkan[2], Yusuke Tokunaga[3], Yasujiro Taguchi[3], and Yoshinori Tokura[3] — [1]Department of Physics, Budapest University of Technology and Economics,1111 Budapest, Hungary — [2]Experimental Physik V, EKM, Universität Augsburg, 86135 Augsburg — [3]RIKEN Centre for Emergent Matter Science (CEMS), Wako 351-0198, Japan

The β-Mn-type Co-Zn-Mn alloys are cubic chiral room temperature skyrmion hosts already studied by Lorentz transmission electron microscopy, magnetization and small-angle neutron scattering[1]. Spin wave spectroscopy of the Dzyaloshinskii-Moriya interaction has been measured for $Co_8Zn_8Mn_4$ and $Co_9Zn_9Mn_2$[2]. $Co_9Zn_9Mn_2$ can host metastable skyrmions in zero magnetic field below its $T_C \approx$ 400 K Curie-temperature[3]. In this work we present ESR measurements in the field polarized state of $Co_9Zn_9Mn_2$ to investigate the temperature dependence of the cubic magnetocrystalline anisotropy and its influence on the properties of the meta-stable skyrmion lattice state. We found strong correlation between the change in the anisotropy and the trigonal to square lattice transformation of the skyrmion state.

[1] Tokunaga, Y., et al., Nat. Commun. 6, 7638 (2015), [2] Takagi, R., et al., Phys. Rev. B 95, 220406 (2017), [3] Karube, K., et al., arXiv:1709.08047 (2017).

TT 37.5 Tue 10:30 EB 301

Effects of Magnetocrystalline Anisotropy on the Triangular to Square Lattice Transformation of Skyrmions — •Markus Preissinger[1], Dieter Ehlers[1], Kosuke Karube[2], István Kézsmárki[1], Hans-Albrecht Krug von Nidda[1], Bertalan Szigeti[3], Yusuke Tokunaga[2], Yasujiro Taguchi[2], Yoshinori Tokura[2], and Vladimier Tsurkan[1] — [1]Experimentalphysik V, EKM, Universität Augsburg, 86135 Augsburg — [2]RIKEN Centre for Emergent Matter Science (CEMS), Wako 351-0198, Japan — [3]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary

The β-manganese-type alloy $Co_8Zn_8Mn_4$ exhibits a helical state below the Curie-temperature $T_c \approx 300\,\mathrm{K}$ [1]. Below the phase transition, between 300 K and 284 K, an equilibrium skyrmion lattice state occurs in weak magnetic fields in the range of 400 Oe. This state can be quenched down to lower temperatures by rapid field cooling. Below 150 K the metastable triangular skyrmion lattice transforms into a square lattice [2]. The magnetocrystalline anisotropy in the ferromagnetic phase was determined by ferromagnetic resonance measurements. We discuss its impact on the phase transition between the two types of skyrmion lattices. On cooling, the increasing cubic anisotropy constant K_1 seems to drive the phase transition of the skyrmion lattice between 150 K and 40 K. The temperature dependence of the corresponding critical fields turns out to be correlated to the anisotropy constant K_1.

[1] T. Hori et al., J. Magn. Magn. Mater. **310**, 1820–1822 (2007).
[2] K. Karube et al., Nature Materials **15**, 1237–1243 (2016).

TT 37.6 Tue 10:45 EB 301

Incommensurate magnetic systems studied with the multi-purpose three-axis spectrometer (TAS) MIRA at FRM II — •Robert Georgii[1], Tobias Weber[1,2], Georg Brandl[1], and Peter Böni[3] — [1]Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Institut Laue Langevin (ILL), Grenoble, France — [3]Physik Department E21, TU München, Garching, Germany

Incommensurate magnetic structures like Helimagnons and Skyrmions are currently intensively studied. Due to their large size and rigid structure they often show very low-lying excitations, where most of the interesting physics is taking place below some meV. The cold-neutron three-axis spectrometer MIRA is an instrument optimized for such low-energy excitations. Its excellent intrinsic resolution makes it ideal for studying incommensurate magnetic systems. Here we will present several examples for the dynamics of such structures which have been measured with MIRA.

TT 37.7 Tue 11:00 EB 301

Induction mapping of the 3D Spin Texture of Skyrmions in Thin Helimagnets — •Sebastian Schneider[1,2], Daniel Wolf[1], Matthew J. Stolt[3], Song Jin[3], Darius Pohl[1], Bernd

Rellinghaus[1], Marcus Schmidt[4], Bernd Büchner[1], Sebastian T. B. Goennenwein[2], Kornelius Nielsch[1,2], and Axel Lubk[1] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]University of Wisconsin-Madison, Madison, USA — [4]MPI CPfS, Dresden, Germany

Envisaged applications of skyrmions in magnetic memory and logic devices crucially depend on the stability and mobility of these topologically non-trivial magnetic textures in thin films. We present for the first time experimental evidence for a characteristic 3D modulation of the skyrmionic spin texture towards the sample surface. Inherent to this structure is the gradual change of the Bloch nature of the skyrmion in the depth of the film to surface chiral twists. By combining focal series inline electron holography (EH), and off-axis EH to quantitatively reconstruct the projected magnetic field pertaining to both the helical and the skyrmion lattice phase in single crystal nanoplates of the isotropic chiral magnet $Fe_{0.95}Co_{0.05}Ge$ nanoplate with electron tomography and magnetostatic simulations of the fields, we extract quantitative information on the 3D spin texture of skyrmions. Our results highlight the relevance of surfaces for the formation of skyrmions in thin film geometries and pave the way towards a surface-induced tailoring of the skyrmion structure.

15 minutes break

Topical Talk TT 37.8 Tue 11:30 EB 301

Composite topological excitations in ferromagnet-superconductor heterostructures — •Kjetil Hals — Department of Engineering Sciences, University of Agder, 4879 Grimstad, Norway

Heterostructures of conventional superconductors and ferromagnets are currently attracting considerable interest because of their potential use for realizing topological superconductivity. The combination of spin-orbit coupling in the superconductor and the lack of inversion symmetry of these heterostructures leads to a magnetoelectric coupling between the magnetic and superconducting order parameters [1, 2]. In this talk, I demonstrate that the magnetoelectric coupling causes magnetic skyrmions and superconducting vortices to bind, forming skyrmion-vortex pairs (SVPs) which represent topological excitations of the hybrid system [1]. I determine the conditions under which a bound SVP is formed, and characterize the range and depth of the effective binding potential through analytical estimates and numerical simulations. Furthermore, I develop a semiclassical description of the coupled skyrmion-vortex dynamics and discuss how SVPs can be controlled by applied spin currents.

[1] K.M.D. Hals, M. Schecter, M. S. Rudner, Phys. Rev. Lett. 117, 017001 (2016). [2] K. M. D. Hals, Phys. Rev. B 95, 134504 (2017).

TT 37.9 Tue 12:00 EB 301

Magnetoelectric effect and orbital magnetization in skyrmion crystals: new ways for detection and characterization of skyrmions — •Börge Göbel[1], Alexander Mook[2], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Skyrmions are small magnetic quasiparticles, which are uniquely characterized by their topological charge and their helicity. We present theoretically how both properties can be determined without relying on real-space imaging [1].

The topological Hall effect of electrons allows to distinguish skyrmions from antiskyrmions by sign of the topological Hall conductivity [2,3] and the orbital magnetization [1]. Here, we predict a magnetoelectric effect in skyrmion crystals [1], which is the generation of a magnetization (polarization) by application of an electric (magnetic) field. Its dependence on the skyrmion helicity fits that of the classical toroidal moment of the spin texture and allows to differentiate skyrmion helicities: it is largest for Bloch skyrmions and zero for Néel skyrmions. We predict distinct features in the magnetoelectric polarizability that can be used to detect and characterize skyrmions in experiments.

[1] B. Göbel et al., submitted.
[2] B. Göbel et al., Phys. Rev. B **95**, 094413 (2017).
[3] B. Göbel et al., New J. Phys. **19**, 063042 (2017).

TT 37.10 Tue 12:15 EB 301

Antiferromagnetic skyrmion crystals: generation and topological spin Hall effect — •Börge Göbel[1], Alexander Mook[2], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Skyrmions are topologically nontrivial, magnetic quasi-particles, that are characterized by a topological charge. A regular array of skyrmions—a skyrmion crystal (SkX)—features the topological Hall effect (THE) of electrons [1,2], that, in turn, gives rise to the Hall effect of the skyrmions themselves.

We present a generally applicable method to create stable antiferromagnetic skyrmion crystals (AFM-SkXs) by growing a two-sublattice SkX onto a collinear antiferromagnet. As an example we show that both types of skyrmion crystals—conventional and antiferromagnetic—exist in honeycomb lattices. While AFM-SkXs do not show a THE, they exhibit a topological spin Hall effect [3]. The zero skyrmion Hall effect carries over to isolated AFM skyrmions as well. They can move in straight lines, at higher velocities and need lower driving currents compared to conventional skyrmions [4,5].

[1] B. Göbel et al., Phys. Rev. B **95**, 094413 (2017).
[2] B. Göbel et al., New J. Phys. **19**, 063042 (2017).
[3] B. Göbel et al., Phys. Rev. B **96**, 060406(R) (2017).
[4] J. Barker et al., Phys. Rev. Lett. **116**, 147203 (2016).
[5] X. Zhang et al., Sci. Rep. **6**, 24795 (2016).

TT 37.11 Tue 12:30 EB 301

Topological Hall effect in Heusler compound $Mn_{1.4}PtSn$ — •Praveen Vir, Nitesh Kumar, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Skyrmions are topologically stable vortex-like spin structure which are considered as potential candidate for future high density memory devices. They have been detected in many chiral and polar compounds such as MnSi, FeGe, Co-Mn-Zn, GaV_4S_8 etc. Recently, with the help of Lorentz transmission electron microscopy, one new vortex like spin structure, so called antiskyrmions have been discovered in Mn-based tetragonal Heusler compound $Mn_{1.4}PtSn$ and $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Antiskyrmion has been predicted to be anti-particle of Néel or Bloch type skyrmions becuase they annihilate with conventional skyrmions [2]. They are also topologically stable and consist of topological winding number or skyrmion number +1 [3]. Due to this topologically stable spin nature, it can give rise to non-vanishing Berry phase in real space. In other words, there could be nonzero topological Hall effect. Here, we report large topological Hall effect in single crystal of antiskyrmion hosting compounds $Mn_{1.4}PtSn$.

TT 37.12 Tue 12:45 EB 301

Prospecting anti-skyrmions in ultra-thin Co films deposited on W(110) — •Flaviano José dos Santos, Bernd Zimmermann, Stefan Blügel, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Recently, the possibility of anti-skyrmion formation in magnetic films on substrates with low symmetry due to anisotropic Dzyaloshinskii-Moriya interactions (DMI) has been demonstated [1]. Experimentally, such anisotropic DMI has been found for Co-films on W(110) [2]. Motivated by these findings, we investigated from first-principles the tensor of magnetic interactions of films containing up to three layers of Co reconstructed on W(110) surface as a continuation of our previous study [3]. We use the full-potential relativistic Korringa-Kohn-Rostoker Green function method combined with a technique employing infinitesimal rotations to access the different components of the tensor. The anisotropy, magnitude and sign of the interactions are analysed in detail with a focus on the DMI. Using atomistic spin dynamics simulations, we prospect and demonstrate the existence of skyrmions and anti-skyrmions, which depend strongly on the thickness of Co films. Finally, we unveil the spin-wave excitations characterising the topologically distinct skyrmionic objects.

Work supported by the Brazilian agency CAPES (Project No. 13703/13-7) and the European Research Council (ERC-consolidator Grant No. 681405-DYNASORE). [1] Nat. Commun. 8, 308 (2017); [2] Phys. Rev. B 95, 214422 (2017); [3] Phys. Rev. B 95, 134408 (2017).

TT 37.13 Tue 13:00 EB 301

Material systems for skyrmions in Co-based ferro-/antiferromagnetically (FM/AFM) coupled multilayers — •Hongying Jia, Bernd Zimmermann, Gustav Bihlmayer, and Stefan Blügel — Peter Grünberg Institut and Institute for Ad-

vanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Magnetic skyrmions, in particular AFM skyrmions, are considered as ideal candidates for high storage density information carriers due to the suppressed skyrmion Hall effect and a smaller size by canceling the dipolar fields. So far searching for materials that can host AFM skyrmions is still a challenging task. Magnetic multilayers (MMLs) with composite structures provide a great opportunity to design materials that can host spin-spirals, skyrmions or magnetic domains with optimal properties. Here we will present the qualitative trends of magnetic exchange interactions throughout a wide range of {Z|Co|Pt} MMLs (Z=3d: Cu, Zn; 4d: Tc∼Cd; 5d: Au). The AFM coupling in between the Co layers was observed in {Z|Co|Pt} MMLs (Z=Zn, Ru, Rh, Cd). The effects of 3d-4d-5d hybridization between Co and the nonmagnetic metals, in particular the effects around the Fermi level, on the magnetic interactions will be discussed. The correlation between the electric interface dipole moments and the sign and magnitude of the Dzyaloshinskii-Moriya interaction will be also discussed.

We acknowledge financial support from the MAGicSky Horizon 2020 European Research FET Open project (#665095) and computing time at JURECA from Jülich Supercomputing Center and JARA-HPC.

TT 38: Magnetocaloric Effects (joint session MA/TT)

Time: Tuesday 9:30–12:45 Location: EB 407

TT 38.1 Tue 9:30 EB 407

A DFT and Monte Carlo approach to simulating the magnetocaloric effect in magnetovolume-coupled materials — •Nuno Fortunato[1,2], João Amaral[2], Gercsi Zsolt[3], João Gonçalves[2], Vitor Amaral[2], Hongbin Zhang[1], Oliver Gutfleisch[1], Vitalij Pecharsky[4], Karl Sandeman[5], and Lesley Cohen[5] — [1]TU Darmstadt, Germany — [2]CICECO, Universidade de Aveiro, Portugal — [3]Physics, Trinity College Dublin, Ireland — [4]Ames Laboratory, United States — [5]Department of Physics, Imperial College London, United Kingdom

Magnetic refrigeration is an emergent technology promising for eco-friendly and more energy efficient refrigeration applications, using the magnetocaloric effect (MCE). Magnetovolume effects contribute significantly to the MCE, however the estimation of MCE with magnetovolume effects remains a challenge. In this work, we simulate the MCE using a microscopic model solved by Monte Carlo methods that evaluate the thermodynamic density of states. The magnetic interaction (J_{ij}) between local moments is considered a function of volume (v), together with external field (H) and lattice volume terms: $H = -\frac{1}{2}\Sigma J_{ij}(v) S_i.S_j + \frac{1}{2}Kv^2 - HM$, where K is compressibility.

Simulation results are compared with the experimental data of Gd, the typical benchmark material for room-temperature magnetic cooling applications. We show that such a simple model quantitatively reproduces experimental data for the MCE and the magnetostriction. This work paves the way to a 'ground-up', fast computational approach to optimize and search for magnetic refrigerant materials.

TT 38.2 Tue 9:45 EB 407

Spin dynamics of magnetocaloric compounds under magnetic field investigated with inelastic neutron scattering measurements — •Nikolaos Biniskos[1,2], Karin Schmalzl[1], Stephane Raymond[2], and Thomas Brückel[3] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science at ILL, 71 avenue des Martyrs, 38000 Grenoble, France — [2]Univ. Grenoble Alpes, CEA, INAC, MEM, 38000 Grenoble, France — [3]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT, 52425 Jülich, Germany

The magnetocaloric effect (MCE) is a temperature or entropy change of a material subject to a variation of magnetic field and is the basic principle of magnetic refrigeration. This technique is considered as promising for a more environmentally friendly and efficient use of energy. However, the microscopic mechanisms at play are to be revealed and the key ingredients are to be identified in order to design new materials. In order to understand the fundamental driving force of the MCE, a microscopic study of magnetism with inelastic neutron scattering (INS) measurements is necessary. To this aim, the spin dynamics of MnFe4Si3 and Mn5Si3, that exhibit the direct and inverse MCE, respectively, have been investigated with INS measurements under different magnetic fields and temperatures. It is evidenced that the inverse MCE of Mn5Si3, the cooling by adiabatic magnetization, is associated with field induced spin-fluctuations, contrary to the usual suppression of fluctuations by a magnetic field that is observed in the direct MCE of MnFe4Si3 [1]. [1]N. Biniskos et al., Phys. Rev. B 96 104407 (2017).

TT 38.3 Tue 10:00 EB 407

Element-specific view on La(FeSi)$_{13}$ — •Katharina Ollefs[1], Markus E. Gruner[1], Fabrice Wilhelm[2], Andrei Rogalev[2], Ilya Radulov[3], Alexandra Terwey[1], Benedikt Eggert[1], Maria Krautz[4], Konstantin Skokov[3], Werner Keune[1], Oliver Gutfleisch[3], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg- Essen, Germany — [2]European Synchrotron Radiation Facility, Grenoble, France — [3]Functional Materials, Technical University Darmstadt, Darmstadt, Germany — [4]Institute for Complex Materials, IFW Dresden, Dresden, Germany

Due to its large magneto-caloric effect, the itinerant electron metamagnet La(FeSi)$_{13}$ is of great interest for its potential use in solid state refrigeration. In order to better understand the magnetic interactions in this material and how they change at the transition, we have performed x-ray absorption measurements. X-ray magnetic circular dichroism measurements in the low temperature phase at the Fe K-edge and La $L_{2,3}$-edges reveal not only a magnetic moment on Fe but also a sizable magnetic moment in the 5d states of La. Magneto-optical sum-rule analysis and DFT calculations indicate an anti-parallel alignement of the Fe and La spin moment and a small orbital moment on La also anti-parallel to spin moment. Disentangling the different magnetic moment contributions in La(FeSi)$_{13}$ may reveal additional sources for hysteresis and might shed light on the thermodynamic role of the particular magnetic degrees of freedom.

Funding by the DFG (SPP1599) is acknowledged.

TT 38.4 Tue 10:15 EB 407

Dynamic effects of the magneto-elastic phase transition in a Fe$_2$P-type magnetocaloric alloy — •Maximilian Fries[1], Pfeuffer Lukas[1], Tino Gottschall[1,2], Franziska Scheibel[1,3], Konstantin Skokov[1], Youri Skourski[2], Mehmet Acet[3], Michael Farle[3], Jochen Wosnitza[3], and Oliver Gutfleisch[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, 64287 Darmstadt — [2]Hochfeldlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden — [3]Fakultät für Physik und CENIDE, Universität Duisburg-Essen, 47057 Duisburg

Magnetic refrigeration could be an efficient alternative refrigeration technology if operated at high cycling frequencies [1]. In order to investigate if the magnetocaloric materials are applicable in a high-frequency cooling device we measured the adiabatic temperature change ΔT_{ad} of a Fe$_2$P-type alloy [2] under different field-change rates ranging from 0.93 Ts^{-1} in a permanent-magnet-based Halbach setup to 2700 Ts^{-1} in pulsed fields. We observed that a field-rate independent second-order like phase transition always overlaps with the first-order phase transition leading to a non-saturating behavior of ΔT_{ad} even in fields up to 20 T. By measurements under different field pulse rates we show that the first-order phase transition cannot follow the fast field changes, resulting in a distinct field-dependent hysteresis of ΔT_{ad}.

[1] O. Gutfleisch et al., Philosophical Transactions of the Royal Society A 374 (2016) 20150308. [2] M. Fries et al., Acta Materialia 132 (2017) 222

TT 38.5 Tue 10:30 EB 407

Decoupling of the magnetostructural transition in magntocaloric La-Fe-Si alloys — •Yanyan Shao[1,2], Konstantin Skokov[2], Francois Guillou[3], Dmitriy Yu Karpenkov[2], Mingxiao Zhang[1], Oliver Gutfleisch[2], and Jian Liu[1] — [1]Ningbo Institute of Material Technology and Engineering, CAS, 315201 Ningbo, China — [2]Material Science, TU Darmstadt, 64287 Darmstadt, Germany — [3]European Synchrotron Radiation Facility, 38000 Grenoble, France

The giant magnetocaloric effect occurs when a magnetic material un-

dergoes a first-order magnetic transition, which usually involves the coupling of magnetic and lattice contributions [1]. In order to investigate in detail the evolution of the magnetostructural phase transition, both magnetocaloric (dT(H)) and magnetovolume (dV(H)) effects in La1.7Fe11.6Si1.4 alloy were measured simultaneously. We observed that under isothermal conditions, only heat transfer occurs first, whereas the structural transition takes place in higher fields, where the heat transfer is already in progress or almost completed. The shift between the magnetic and structural transitions is 0.27 T, which clearly indicates a decoupling effect. The decoupling effect was also confirmed by X-ray absorption (lattice contribution) and by magnetic circular dichroism (change in magnetic system). We will discuss different reasons for the decoupling effect. [1]V. K. Pecharsky et al., Physical Review Letters. 91 (2003) 197204.

TT 38.6 Tue 10:45 EB 407

Correlation of microstructural and magnetic properties of Mn-Fe-P-Si magnetocaloric compounds — •Lukas Pfeuffer[1], Maximilian Fries[1], Enrico Bruder[1], Tino Gottschall[2], Semih Ener[1], Léopold Diop[1], Thorsten Gröb[1], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Fachbereich Materialwissenschaft, TU Darmstadt, 64287, Darmstadt, Germany — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany

Mn-Fe-P-Si alloys of Fe2P-type are very promising candidates for magnetocaloric applications. Extensive studies dealing with the optimization of the chemical composition have been published in recent years. However, the microstructure and its effect on the thermomagnetic properties are rarely discussed in literature. For this reason, we processed Mn-Fe-P-Si samples using a powder-metallurgical approach and characterized their microstructure and magnetocaloric behaviour. SEM, EDX, EBSD and XRD studies display small amounts of a cubic secondary phase showing a distinct phosphorous depletion and a characteristic arrangement at the triple junctions of the Fe2P grains. A shift in saturation magnetization, transition temperature and isothermal entropy change as a function of the secondary phase fraction can be observed. A significant influence of the metal/non-metal ratio on the above mentioned properties could be investigated. Additionally, all the prepared samples reveal a virgin effect shown thermomagnetically and with temperature dependent optical microscopy.

TT 38.7 Tue 11:00 EB 407

Influence of substitutions, hydrostatic pressure and magnetic field on the MnNiGe system — •Andreas Taubel, Tino Gottschall, Maximilian Fries, Tom Faske, Konstantin P. Skokov, and Oliver Gutfleisch — TU Darmstadt, Institute of Material Science, Alarich-Weiss-Str. 16, 64287 Darmstadt, Germany

An enhancement in the energy efficiency of cooling devices for household refrigeration and air conditioning can provide worldwide savings in energy and CO_2 emissions. An alternative to conventional gas compression refrigerators is solid state based magnetocaloric cooling with the potential of increased energy efficiency. The MM'X materials family provides promising magnetocaloric effects with sharp phase transitions for the MnNiGe and MnCoGe systems.

We studied the isostructural substitutions of Fe for Mn and Si for Ge, which enhance the ferromagnetic character of the low temperature phase, allow for a precise tuning of the transition temperature and reduce the amount of expensive Ge in the compounds. Since a magnetic field shifts the transition temperature by 1 K T^{-1}, the phase transition cannot be induced completely in small fields. We directly measured a maximum adiabatic temperature change of 1.3 K for the first magnetic field application of 1.93 T [1]. Therefore, the large sensitivity towards hydrostatic pressure (72 K GPa^{-1}) enables an additional stimulus to induce the phase transition more efficiently for Fe- and Si-substituted (Mn,Fe)Ni(Ge,Si) compounds.

This work was supported by DFG (Grant No. SPP1599).

[1] A. Taubel et al., J. Phys. D: Appl. Phys. 50, 464005 (2017)

15 minutes break

TT 38.8 Tue 11:30 EB 407

Exploring three-dimensional temperature gradients in magnetic tunnel junctions: Anomalous Nernst effect — Ulrike Martens[1], Torsten Huebner[2], Henning Ulrichs[3], Oliver Reimer[2], Timo Kuschel[2], Ronnie Tamming[4], Chia-Lin Chang[4], Raanan Tobey[4], Andy Thomas[5], Markus Münzenberg[1], and •Jakob Walowski[1] — [1]Universität Greifswald, Greifswald, Germany — [2]Bielefeld University, Bielefeld, Germany — [3]Universität Göttingen, Göttingen, Germany — [4]University of Groningen, Groningen, The Netherlands — [5]IFW Dresden, Institute for Metallic Materials, Dresden, Germany

We measure the anomalous Nernst effect (ANE) generated on a nanometer length scale by micrometer sized temperature gradients in magnetic tunnel junctions (MTJs). The ANE is extracted by analyzing the influence of in-plane temperature gradients on the tunnel magneto-Seebeck effect (TMS) in in-plane magnetized MTJs based on CoFeB electrodes with uniaxial magnetic anisotropy and an MgO tunnel barrier. The direction controlled temperature gradients are created by a focused laser spot. The spatial extent of the measured effects is defined by the MTJ size, while the spatial resolution is given by the laser spot size and the step size of its lateral translation. The measurement method is highly sensitive to low voltages and yields an ANE coefficient of $K_N \approx 1.6 \cdot 10^{-8} \frac{\mathrm{V}}{\mathrm{TK}}$ for CoFeB. At such sensitivity, the generated ANE effect allows to expand the MTJs' functionality from simple memory storage to nonvolatile logic devices and opens new application fields e.g. direction dependent temperature sensing.

TT 38.9 Tue 11:45 EB 407

Anomalous Nernst effect in carbon doped Mn_5Ge_3 and Mn_5Si_3 thin films — •Sasmita Srichandan, Sihao Deng, and Christoph Sürgers — Karlsruhe Institute of Technology, Physikalisches Institut, PO Box 6980, 76049 Karlsruhe, Germany

Carbon doped Mn_5Ge_3 shows enhanced magnetic properties compared to pure Mn_5Ge_3 which makes $Mn_5Ge_3C_x$ suitable for spintronics applications. The magnetotransport properties of ferromagnetic Mn_5Ge_3, $Mn_5Ge_3C_{0.8}$ and $Mn_5Si_3C_{0.8}$ systems have been previously investigated [1]. In this present work, the thermal-magnetotransport properties, in particular the anomalous Nernst effect (ANE), have been experimentally investigated in thin films of $Mn_5Ge_3C_{0.8}$, $Mn_5Si_3C_{0.8}$ and Mn_5Ge_3 on Ge (111). The ANE coefficients for all the films show the same positive sign at high temperatures until at about 100 K the sign changes to negative for $Mn_5Ge_3C_{0.8}$ and Mn_5Ge_3 films but not for $Mn_5Si_3C_{0.8}$ film. This behavior follows the same change of sign behavior previously observed in the anisotropic magnetoresistance ratio and ordinary Hall coefficient for these films. The change of sign of the ANE is the direct consequence of the Mott relation in our ferromagnetic films [2] even if the sign of the anomalous Hall coefficient remains unchanged. In addition, a possible contribution from the spin Seebeck effect to the transverse thermo-voltage has been addressed.

[1] C. Sürgers et al. Phys. Rev. B **90**, 104421(2014)
[2] T. Miyasato et al. Phys. Rev. Lett. **99**, 086602(2007)

TT 38.10 Tue 12:00 EB 407

An experimental design to measure the spin Nernst effect — •Sandra Gottwals[1], Thierry Crozes[2], and Georg Schmidt[1,3] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Nanostrukturierte Materialien, Halle — [2]Institut Néel, CNRS, Grenoble — [3]Martin-Luther-Universität Halle-Wittenberg, Interdisziplinäres Zentrum für Materialwissenschaften, Halle

Like the spin Hall effect to the ordinary Hall effect the spin Nernst effect compares to the Nernst effect. A thermal gradient in a material with sufficient spin orbit coupling generates a spin current and spin accumulation perpendicular to the gradient. We are developing a setup to measure the resulting spin accumulation and magnetic moment using micro SQUIDs. The sample design is rather complex because it needs at least two micro SQUIDs to measure the spin accumulation on two opposite sides of a Pt layer together with superconducting stripes to measure the local temperature. On top of these a Pt layer and a heater with the necessary electrical insulation need to be processed. We present the results and current status of our development. On all superconducting structures the critical current needs to be measured simultaneously.

TT 38.11 Tue 12:15 EB 407

A tool for detecting complex magnetic configurations — •Alexander Fernández Scarioni[1], David Schroeter[2], Xiukun Hu[1], Sibylle Sievers[1], Dirk Menzel[2], Stefan Süllow[2], and Hans W. Schumacher[1] — [1]Physikalish-Technische Bundesanstalt (PTB), Braunschweig, Germany — [2]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

The anomalous Nernst effect (ANE) is a simple and powerful tool to detect the average magnetization in a single nanowire. Using this simple thermoelectrical measurement one can precisely track the position

and motion of a single Domain Wall in a metallic nanowire with perpendicular magnetization anisotropy with a resolution below 20 nm [1]. This makes the ANE a candidate for detecting the magnetization in nanowires made of complex materials such as the ones that show a Dzyaloshinskii-Moriya Interaction (DMI), even also single skyrmions in nanowires. We are going to show thermoelectric ANE measurements on a nanowire with DMI were we can identify the different components of the magnetization.

[1] P. Krzysteczko et al., Phys. Rev. B. 95, 220410(R) (2017)

TT 38.12 Tue 12:30 EB 407

Magneto-Seebeck Tunneling Across a Vacuum Barrier — •Cody Friesen and Stefan Krause — Department of Physics, University of Hamburg, Jungiusstr. 11A, 20355 Hamburg, Germany

The tunneling magneto-Seebeck (TMS) effect has been intensively studied both for its potential applications in e.g. waste heat recycling in electronics, and for the insights it can provide into fundamental solid state phenomena. This effect has been measured in planar junctions [1] and, as will be described in this talk, can also be measured using spin-polarized scanning tunneling microscopy (SP-STM).

The experiments were performed at low temperatures ($T = 50\,\mathrm{K}$) and in UHV conditions, on the Fe/W(110) multilayer system [2], using a laser-heated bulk Cr tip and active bias compensation. The non-collinear spin structures present in this sample system, and the atomic-scale lateral resolution of SP-STM, allowed for the imaging of a continuous range of relative tip-sample magnetization orientations.

Here, as in planar junctions, the measurement of the temperature gradient between electrodes is a significant challenge. We have estimated the tip-sample temperature difference using a linear thermal tip expansion model. To verify this, we have also directly predicted the Seebeck coefficient S using tunneling bias spectroscopy. We found these approaches to be in good agreement, suggesting a convenient spectroscopic approach to determining S on the atomic scale, even in the absence of a temperature gradient.

[1] M. Walter *et al.*, Nat. Mater. **10**, 10 (2011).
[2] S. Meckler *et al.*, Phys. Rev. Lett. **103**, 15 (2009).

TT 39: Focus Session: Quantum Nanophotonics in Solid State Systems I (joint session HL/TT)

Photonic quantum technologies provide revolutionary concepts and innovative solutions in the fields of sensing, communication and computing in the so called "second quantum revolution". Activities in this area involve light-matter interaction, light propagation, light manipulation and light detection, mainly at the single photon level. The Focus Session aims at presenting and discussing the current status of quantum nanophotonics, open challenges as well as future directions and perspectives in this very active field of solid state research.

Organizers: Alexander Szameit(U Rostock), Ruth Oulton (U Bristol), and Stephan Reitzenstein (TU Berlin)

Time: Tuesday 9:30–15:45 Location: EW 201

Invited Talk TT 39.1 Tue 9:30 EW 201

Exploring the limits of position measurement with optomechanics — Sergey A. Fedorov, Vivishek Sudhir, Nils J. Engelsen, Ryan Schilling, Hendrik Schütz, Amir H. Ghadimi, Mohammad J. Bereyhi, Dalziel J. Wilson, and •Tobias J. Kippenberg — Institute of Physics (IPHYS), École polytechnique fédérale de Lausanne, 1015 Lausanne, Switzerland

Optomechanics provides a platform to investigate the quantum limits on position measurements and extend quantum control to macroscopic objects. We utilized a microdisk optical cavity with a nanobeam mechanical oscillator in the near-field to perform sensitive measurements of the oscillator position. At cryogenic temperatures, we attained a measurement rate approaching the thermal decoherence rate. Using the measurement record as an error signal, we feedback-cooled the oscillator to a mean phonon number of 5.3 (16% ground state probability). In the same system, we observed ponderomotive squeezing of light and distilled quantum sideband asymmetry from the thermal noise using measurement-based feedback. At room temperature, we demonstrated quantum correlations of light and used these quantum correlations to enhance force sensitivity. However, thermal decoherence remains a major obstacle in our experiments—any potential quantum state preparation must be performed within the decoherence time. Therefore, we have developed ultra-high quality factor mechanical resonators, capable of hundreds of coherent oscillations at room temperature. We are now working to integrate these oscillators with an optical cavity to enable operation in the measurement-backaction dominated regime.

Invited Talk TT 39.2 Tue 10:00 EW 201

On-chip integration of superconducting single photon detectors — •Wolfram Pernice — Universität Münster, Physikalisches Institut, Heisenbergstr. 11, 48149 Münster

Nanophotonic circuits employ waveguiding devices to route light across quasi-planar integrated optical chips in analogy to electrical wires in integrated electrical circuits. Using materials with high refractive index allows for confining light into sub-wavelength dimensions as efficient optical wires. Interaction with the environment is possible through near-field coupling to the evanescent tail of propagating optical modes, given that the measurable system is close to the waveguide surface. The interaction length can then be conveniently tailored by simply choosing a sufficiently long waveguide. This approach is particularly interesting for designing highly sensitive detectors which are able to register individual photons. Because nanophotonic circuits are well-suited for the study of single photon effects on chip, such detectors constitute a fundamental building block for emerging quantum photonic technologies. I will present recent progress on waveguide integrated single photon detectors, with a focus on superconducting nanowire single photon counters. Besides covering the basics of single photon threshold detection, advanced designs for multi-photon and coherent detection will be discussed. In combination with waveguide coupled single photon sources, such detectors are promising ingredients for fully integrated quantum circuits. The heterogeneous integration with nanophotonic circuits allows for implementing compact hybrid systems for non-classical optics in a chipscale framework.

TT 39.3 Tue 10:30 EW 201

Indistinguishable single photons from a quantum dot coupled to a ridge waveguide — •Lukasz Dusanowski[1], Soon-Hong Kwon[1,2], Christian Schneider[1], and Sven Höfling[1] — [1]Technische Physik, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Department of Physics, Korea University, Seoul 136-701, Korea

Here we report on resonance fluorescence of an InAs/GaAs quantum dot coupled to a distributed Bragg-reflection ridge waveguide. The pulsed, resonant excitation was carried out from the top of the waveguide and emitted photons collected from the side facet of the ridge after 2 mm travel distance. Based on the calculations and time-resolved-measurements coupling efficiency into waveguide was estimated to be around 20%. In this case highly linearly polarized photons have been observed with a single-photon purity of >99% and indistinguishability >95% demonstrating a realistic pathway for on-chip quantum photonics.

TT 39.4 Tue 10:45 EW 201

Deterministic integration of QDs into on-chip multimode interference couplers via in-situ electron beam lithography — •Peter Schnauber[1], Johannes Schall[1], Samir Bounouar[1],

Jin-Dong Song[2], Theresa Hoehne[3], Sven Burger[3], Tobias Heindel[1], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut fuer Festkoerperphysik, Technische Universitaet Berlin, Berlin, Germany — [2]Korea Institute of Science and Technology, Seoul, Korea — [3]Zuse Institut Berlin, Freie Universitaet Berlin, Berlin, Germany

The deterministic integration of quantum emitters into on-chip photonic elements is crucial for the implementation of scalable on-chip quantum circuits. Recent activities include multistep-lithography[1] as well as AFM tip transfer[2]. Here we report on the deterministic integration of single QDs into on-chip beam splitters using single step in-situ electron beam lithography[3]. In order to realize 50/50 coupling elements acting as central building blocks of on-chip quantum circuits we chose tapered multimode interference (MMI) splitters which feature relaxed fabrication tolerances and robust 50/50 splitting ratio. We demonstrate the functionality of the deterministic QD-waveguide structures by μPL spectroscopy and photon cross-correlation between the two MMI output ports. The latter confirms single-photon emission and on-chip splitting associated with $g^{(2)}(0) < 0.5$.

[1] Coles et al., Nature Communications 7, 11183 (2016)
[2] Zadeh et al., Nano Letters 16, 2289 (2016)
[3] Gschrey et al., Nature Communications 6, 7662 (2015)

15 min. break.

Invited Talk TT 39.5 Tue 11:15 EW 201

Integrated III-V nonlinear quantum optical devices — •Gregor Weihs — Institut für Experimentalphysik, Universität Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria

For fundamental tests of quantum physics as well as for quantum communications, non-classical states of light are an important tool. In this talk, we will present our work on nonlinear AlGaAs waveguides. Most III-V semiconductors exhibit a large second-order optical nonlinearity, but phase-matching the nonlinear interaction is notoriously difficult. As a solution Bragg-reflection waveguides (BRW) allow efficient creation of photon pairs through spontaneous parametric down-conversion. They have the potential to be integrated with a pump laser on the chip for a miniaturized room-temperature entangled photon pair source.

In our BRWs we can create high-fidelity polarization and time-bin entangled photon pairs, which cover a large frequency band in the low-loss telecommunication window, suitable for serving multiple users through wavelength division multiplexing. For all our applications it is important that we can design the desired linear and nonlinear properties, which in turn makes precise characterization necessary. For this purpose we have developed a Fourier-transform Fabry-Perot spectroscopy technique, which yields the relevant device parameters with superior accuracy. Finally, we will present our latest results on devices that integrate electrically injected lasers and the nonlinear conversion and give an outlook on the possible integration of other optical elements on-chip.

TT 39.6 Tue 11:45 EW 201

Temporally adjustable photon pairs from semiconductor waveguides — •K. Laiho[1,2], B. Pressl[2], A. Schlager[2], S. Auchter[2], H. Chen[2], T. Günthner[2], H. Suchomel[3], J. Gessler[3], M. Kamp[3], S. Höfling[3,4], C. Schneider[3], and G. Weihs[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut für Experimentalphysik, Universität Innsbruck, Technikerstr. 25, 6020 Innsbruck, Austria — [3]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]School of Physics & Astronomy, University of St Andrews, St Andrews KY16 9SS, UK

Semiconductor Bragg-reflection waveguides (BRWs) are efficient photon-pair sources and well suited for integrated optics. These monolithic structures are made of AlGaAs and profit from its strong second order optical non-linearity. Our BRWs rely on type-II parametric down-conversion (PDC) achieved via spatial mode matching.

In order to become truly practical, BRWs need to be reliably fabricated and applicable in various quantum optics tasks. Our simulations show that too coarse tolerances in fabrication easily distort the design properties. Further, we experimentally investigate the characteristics of PDC emission, verify the indistinguishability of photon pairs and prepare polarization entangled states with a temporally adjustable degree of entanglement [1]. To conclude, a careful study of the PDC process parameters is necessary for controlling and manipulating the BRW's performance in the investigated tasks.

[1] A. Schlager et al., Opt Lett. 42, 2102 (2017) and references therein.

TT 39.7 Tue 12:00 EW 201

On-chip hybrid quantum photonic circuits — Ali W. Elshaari[1], Iman Esmaeil Zadeh[2], Andreas Fognini[2], Dan Dalacu[3], Philip J. Poole[3], Michael E. Reimer[4], Val Zwiller[1,2], and •Klaus D. Jöns[1] — [1]Applied Physics Department, KTH Stockholm, Sweden — [2]Kavli Institute of Nanoscience, TU Delft, The Netherlands — [3]National Research Council of Canada, Ottawa, Canada — [4]Institute for Quantum Computing, University of Waterloo, Canada

Quantum communication applications require a scalable approach to integrate bright on-demand sources of entangled photon-pairs in complex on-chip quantum circuits. Currently, the most promising sources are based on III/V semiconductor quantum dots. However, complex photonic circuitry is mainly achieved in silicon photonics due to the tremendous technological challenges in circuit fabrication. We take the best of both worlds by developing a new hybrid on-chip nanofabrication approach [1], allowing to integrate III/V semiconductor nanowire quantum emitters into silicon-based photonics. We demonstrate for the first time on-chip generation, spectral filtering, and routing of single-photons from selected single and multiple nanowire quantum emitters all deterministically integrated in a CMOS compatible silicon nitride photonic circuit [2]. Our new approach eliminates the need for off-chip components, opening up new possibilities for large-scale quantum photonic systems with on-chip single- and entangled-photon sources.

[1] I. Esmaeil Zadeh et al., Nano Lett. 16(4), 2289-2294 (2016).
[2] A. W. Elshaari et al., Nat. Commun. 8, 379 (2017).

TT 39.8 Tue 12:15 EW 201

Reconfigurable integrated optical circuits on an stretchy polymer chip — •James A. Grieve[1], Kian Fong Ng[1], Filip Auksztol[1], Manuel J.L.F. Rodrigues[2], Neo Ho[2], José Viana-Gomes[2,3], and Alexander Ling[1,3] — [1]Centre for Quantum Technologies, National University of Singapore, Singapore — [2]Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore — [3]Department of Physics, National University of Singapore, Singapore

We describe the development of a waveguide platform in the flexible, stretchy polymer polydimethylsiloxane (PDMS). The pliable substrate enables tuning of integrated optical components by mechanical deformation of the host chip, overcoming a key limitation in many bespoke waveguide platforms. We illustrate this capability via the continuous on-chip tuning of a beamsplitter. We also apply these techniques to continuously coupled photonic random walks. Here, appropriate deformation of the chip allows reconstruction the spatial evolution of light in a coupled 1D array by observation of the end face alone. The PDMS platform is compatible with visible wavelengths and is insensitive to polarization, making it a compelling candidate for the integration of quantum optics experiments.

TT 39.9 Tue 12:30 EW 201

Confined microcavity polaritons: effect of trap geometry on potential shape — •Alexander Kuznetsov, Paul Helgers, Klaus Biermann, and Paulo Santos — Hausvogteiplatz 5-7, 10117 Berlin, Germany

Micorcavity (MC) exciton-polaritons (MPs) result from the strong light-matter coupling. MPs may be quantum-confined using micrometer-sized static potentials (traps). Arrays of such traps have been suggested for quantum-simulators. The latter require energy- and spatial overlap of wave functions of trapped single polaritons and thus precise control of the trap shape and size. In this work, we investigate the two-dimensional and three-dimensional confinement of MPs in traps produced by shallow etching and overgrowth of (Al,Ga)As MC. Using low-temperature photoluminescence, atomic-force microscopy and numerical modeling we correlate trap shape and size with the energy spectrum and spatial profile of MPs wave functions. We find that the um-sized potential is of neither purely square nor parabolic type. We show that the trap potential is anisotropic due to the different overgrowth kinetics along [-110] and [-1-10] directions. We present a model to explain non-degenerate energy levels in the emission spectra of confined MPs, which also predicts the minimum size and confinement strength of MPs traps.

TT 39.10 Tue 12:45 EW 201

Photo-luminescence of defects in GaAs double quantum

wells in the trion blockade regime — •Mingyun Yuan, Alberto Hernández-Mínguez, Colin Hubert, Klaus Biermann, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Electrostatic traps are commonly used to control excitons in double quantum well (DQW) structures, in our case a GaAs/AlGaAs DQW. When the traps are biased to the flat-band regime, only direct (i.e. in the same QW) excitons and trions can be formed. Away from the flat-band, indirect (in different QWs) excitons appear due to their favorable binding energies. At the edge of the flat-band, we observe a narrow regime in which the photo-luminescence (PL) of direct excitons, trions and indirect excitons is supressed, while unexpected narrow spectral lines from individual emission centers become visible.

We conclude that such PL spectra arise from trion blockade. The excess charge of a trion cannot break away and tunnel to the second QW, since the resulted direct exciton would have a higher energy. However, if defect states with sufficiently lower energies exist in the second QW, the excess charge can tunnel and recombine with such a defect, emitting photons during the process. By moving the sub-micron excitation spot we can map out the precise location and the density of these emission centers. Their intensity saturates with increasing excitation power, indicating their single-photon nature. This phenomenon in the trion blockade regime can assist engineering of defects in a DQW. The potential of using them as single photon sources can also be explored.

TT 39.11 Tue 13:00 EW 201

Enhanced single-photon emission from a CdSe quantum dot in a ZnSe nanowire featuring a bottom-up photonic shell — Mathieu Jeannin[1], Thibault Cremel[2], Teppo Häyrynen[3], •Niels Gregersen[3], Edith Bellet-Amalric[2], Gilles Nogues[1], and Kuntheak Kheng[2] — [1]Université Grenoble Alpes, CNRS, Institut Néel, Grenoble, France — [2]Université Grenoble Alpes, CEA, Grenoble, France — [3]DTU Fotonik, Technical University of Denmark, Kongens Lyngby, Denmark

A quantum dot in a semiconductor nanowire represents an attractive platform for an efficient single-photon source. While demonstrations so far have mainly been for III-V materials, the II-VI platform offers the possibility of room-temperature operation, where CdSe quantum dots inserted in ZnSe nanowires have demonstrated the ability to emit single photons at 300 K.

In this work, we present a bottom-up approach to fabricate a photonic nanowire-like structure around such CdSe quantum dots by depositing an oxide shell using atomic-layer deposition. Simulations suggest that the intensity collected in a 0.6 NA microscope objective can be increased by a factor 7 with respect to the bare nanowire case. Combining micro-photoluminescence, decay time measurements, and numerical simulations, we obtain a fourfold increase in the collected photoluminescence from the quantum dot. We show that this improvement is due to an increase of the quantum-dot emission rate and a redirection of the emitted light.

45 min. break.

Invited Talk TT 39.12 Tue 14:00 EW 201

Hybrid waveguide platforms for quantum optics — •Michal Bajcsy — IQC, University of Waterloo, Waterloo, ON, Canada

While often challenging to implement, combining systems and building blocks from different areas of quantum optics and nanophotonics can open avenues for realizing novel devices and for studies of previously unexplored phenomena. I will describe three hybrid nanophotonic platforms my group has been exploring in the past few years.

In the first platform, we attempt to integrate superconducting-nanowire single-photon detectors with waveguide arrays laser-written in glass. In the second platform, we propose to couple individual quantum emitters, such as trapped atoms, colour centres, or quantum dots, with dispersion engineered chiral waveguides to implement deterministic single-photon subtraction. Our third platform combines hollow-core waveguides with dielectric metasurfaces acting as mirrors to realize integrated Fabry-Perot cavities that can be designed to be polarization selective.

TT 39.13 Tue 14:30 EW 201

Heterogeneous quantum networks: Combine QDs with long lived atomic quantum memories — •Janik Wolters[1], Lucas Béguin[1], Roberto Mottola[1], Jan-Philipp Jahn[1], Andrew Horsley[1], Fei Ding[2], Armando Rastelli[3], Oliver G. Schmidt[2], Richard J. Warburton[1], and Philipp Treutlein[1] — [1]Universität Basel, Department Physik, Switzerland — [2]IFW Dresden, Germany — [3]Johannes-Kepler Universität Linz, Austria

Semiconductor quantum dots (QDs) are excellent single-photon sources, providing triggered single-photon emission at a high rate and with high spectral purity. Independently, atomic ensembles have emerged as one of the best quantum memories for single photons, providing high efficiency storage and long memory lifetimes. We aim at combining these two disparate physical systems to exploit the best of both worlds. For this, the bandwidth mismatch between QDs typically emitting GHz-broad photons and atomic lines of 10 MHz width must be solved. We demonstrate a scheme to generate temporally shaped narrow-bandwidth single photons with QDs [1], and we push forward an EIT-based quantum memory to store broadband photons in a dense ensemble of 87Rb atoms [2].

[1] L. Béguin et al., On-demand semiconductor source of 780 nm single photons with controlled temporal wave packets, arXiv:1710.02490 (2017).

[2] J. Wolters et al., Simple atomic quantum memory suitable for semiconductor quantum dot single photons, Phys. Rev. Lett. 119 060502 (2017).

TT 39.14 Tue 14:45 EW 201

Rare-earth doped nanoparticles with millisecond-long spin coherence lifetime — •Diana Serrano[1], Jenny Karlsson[1], Alexandre Fossati[1], Alban Ferrier[1,2], Alexandre Tallaire[1], and Philippe Goldner[1] — [1]Institut de Recherche de Chimie Paris (IRCP), UMR 8247 CNRS Chimie-Paristech, 11 rue Pierre et Marie Curie, 75005 Paris — [2]Sorbonne Universités, UPMC Université Paris 06, 75005, Paris, France

Nanoscale systems possessing long-lived spins and the ability to coherently couple to light are highly demanded for quantum devices implementations. Several approaches, like NV centers in diamond, semiconductor quantum dots are intensively investigated in the field, where an outstanding challenge is to preserve properties, and especially optical and spin coherence lifetimes, at the nanoscale. Here, we investigate for the first time the spin coherence properties of rare-earth doped nanoparticles. Using all-optical techniques, we observed spins echoes and measured spin coherence lifetimes up to T2=2.9 ms at 5 K. Moreover, we achieve spin T2 extension using all-optical spin dynamical decoupling and observe high fidelity between excitation and echo phases. Rare-earth doped nanoparticles are thus the only reported nano-material in which optically controlled spins with millisecond coherence lifetimes have been observed.

Acknowledgement:

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TT 39.15 Tue 15:00 EW 201

Cavity Optomagnonics — •Silvia Viola Kusminskiy[1], Florian Marquardt[1,2], Hong Tang[3], and Jasmin Graf[1,2] — [1]Max Planck for the Science of Light, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [3]Yale University, New Haven, USA

In optomagnonics, light couples coherently to collective magnetic excitations in solid state systems. This topic is of high interest for quantum information processing platforms at the nanoscale, and recent experiments have demonstrated the optomagnonic coupling for the first time. In this talk, I show how to obtain the microscopic optomagnonic Hamiltonian starting from the Faraday effect and discuss the optically-induced classical nonlinear dynamics for a homogeneous magnetic mode. A unique feature of optomagnonic systems is moreover the possibility of coupling light to spin excitations on top of magnetic textures. For the case of a microdisk geometry, I discuss the coupling between magnon modes in the presence of a magnetic vortex, and light confined to whispering gallery modes.

TT 39.16 Tue 15:15 EW 201

Quantization of three-dimensional leaky and lossy cavities using quasinormal modes — •Sebastian Franke[1], Stephen Hughes[2], Andreas Knorr[1], and Marten Richter[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, EW 7-1, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Department of Physics,Engineering Physics and Astronomy,Queen's University, Kingston, Ontario, Canada K7L 3N6

Open cavity systems, e.g. plasmonic metal nanoparticles or micropillar cavities, are of high interest in modern research on quantum optics and quantum plasmonics. However, the dissipative character of these systems prevents the use of a canonical quantization scheme with the open cavity photon modes.

We develop a rigorous quantization scheme using a Green's function approach[1] of an inhomogeneous and dispersive medium, and quasinormal modes[2] (QNMs) with complex eigenfrequencies $\tilde{\omega}_\mu$ and complex eigenfunctions $\tilde{\mathbf{f}}_\mu$ as a basis for the mode expansion of the quantization. In this way we obtain suitable annihilation and creation operators for modified QNMs to create QNM multi-photon Fock states. Applications to density matrix equations and comparison to the Jaynes-Cummings model will be shown, including extensions to the multimode case.

[1]T. Gruner, and D.-G. Welsch, *Phys. Rev. A* **53**, 1818, 1996
[2]P. T. Leung, S. Y. Liu, and K. Young, *Phys. Rev. A* **49**, 3057, 1994

TT 39.17 Tue 15:30 EW 201

Quantum correlations of strongly-coupled emitters inside a nanoantenna-enhanced plasmonic cavity — •Matthias Hensen[1], Tristan Kenneweg[2], Tal Heilpern[3], Stephen K. Gray[3], and Walter Pfeiffer[2] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Center for Nanoscale Materials, Argonne National Laboratory, 9700 Cass Avenue, Lemont, Illinois 60439, USA — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Plasmon-mediated strong coupling between spatially separated and thus selectively addressable quantum emitters is a worthwhile goal for conveying quantum optical many-body interactions to ultrafast timescales. For this purpose we employ a recently demonstrated hybridization scheme [1] that combines the longevity and waveguide character of an elliptical plasmon cavity with the strong field enhancement of nanoantennas positioned in the associated focal spots. Quantum dynamical simulations reveal an oscillatory exchange of excited state population and a notable degree of entanglement between the attached quantum emitters over a distance of 1.8 μm [2].
Presently, we study coherent control and time-resolved spectroscopy of quantum emitter-related nonclassical photon correlations in this device and show first results.

[1] Aeschlimann et al., *Light: Science & Applications* 6, e17111 (2017)
[2] Hensen et al., *ACS Photonics*, doi:10.1021/acsphotonics.7b00717

TT 40: Dual-Method Approaches to Quantum Many-Body Systems II

To make an impact on possible applications, theoretical approaches for correlated many-body systems must allow for studying more realistic models and lead to more accurate predictions as compared to what is achievable nowadays. This requires, on the one hand, the development of specialized tools which are mathematically and/or algorithmically demanding. On the other hand, an emergent promising approach to make significant progress beyond toy-model understanding of many-body physics is the combined use of two or more complementary methods. The demand for such type of approaches is growing. The two session of contributed talks will provide an overview of recent successes in such dual-(multi-)method approaches involving analytical as well as numerical tools, and will indicate prospects for future directions.

Compilation: Volker Meden, RWTH Aachen; Stefan Wessel, RWTH Aachen

Time: Tuesday 10:00–13:00 Location: H 3010

TT 40.1 Tue 10:00 H 3010

A practical guide to training neural networks of quantum many body systems — •Thomas C. Lang, Jonas B. Rigo, and Andreas M. Läuchli — Institute for Theoretical Physics, University of Innsbruck, Austria

Encoding the representation of the electronic wave function of a minuscule fragment of a crystal is a nearly impossible task. learning promises to cut through the complexity and to allow for efficient encoding of a vastly complex system in a limited number of degrees of freedom by identifying the subtle, yet relevant signatures of phases of matter. We assess the efficiency and practical limits of the representational power of basic neural networks for the many body wave functions of quantum spin systems. We identify the types of wave functions, bases and network topologies, which are favorable and investigate what features the neural networks learn and how to exploit them in scaling up the network. Finally, we comment on the predictive power and entanglement properties of neural networks trained on small portions of the full phase space.

TT 40.2 Tue 10:15 H 3010

A simple tensor network algorithm for 2d steady states — •Roman Orus — Johannes Gutenberg-Universität, Mainz, Germany

Here we present a tensor network algorithm that approximates steady-states of 2d quantum lattice dissipative systems in the thermodynamic limit. The implementation of our method is remarkably simple and efficient. We prove the validity of the approach by computing the steady states of dissipative quantum Ising and XYZ models, relevant to address controversies in dissipative systems of interacting Rydberg atoms, and benchmark our simulations with a variational algorithm based on product and correlated states. Our results support the existence of a first order transition in the dissipative Ising model, while we find no evidence for a bistable region.

TT 40.3 Tue 10:30 H 3010

Non-Abelian Symmetries in Tensor Network Algorithms — •Philipp Schmoll[1,2] and Román Orús[1] — [1]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [2]Graduate School Materials Science in Mainz, Staudingerweg 9, 55128 Mainz, Germany

In recent years Tensor Networks (TNs) have emerged as a natural language to describe quantum states of matter by capturing the amount and local structure of entanglement in the system. They provide an efficient framework to study quantum many-body properties with many remarkable applications such as the Density Matrix Renormalization Group (DMRG) for 1d systems proposed by S. White. The Projected Entangled Pair State (PEPS) ansatz has proven to be a versatile tool for 2d systems with topological order, both chiral and non-chiral. However, at the current stage simulations in 2d are strongly limited due to the complexity of the systems. In this respect, a big step needs to be taken to have a versatile implementation of non-abelian symmetries (such as SU(2) or SU(3)) in 2d PEPS algorithms, which will allow to advance significantly in the study of many relevant systems (e.g., frustrated antiferromagnets, chiral topological spin liquids, ...). In this talk I will report on recent advances in this direction at our group in Mainz.

TT 40.4 Tue 10:45 H 3010

Entanglement properties of the Hubbard chain model — •Francesco Parisen Toldin and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We study the entanglement properties for a bipartition of the one-dimensional Hubbard model. By means of a recently-developed Quantum Monte Carlo method which exploits the replica trick [1], we sample the spin correlations of the entanglement Hamiltonian, and compare our results with those for an open chain of the same size of the entanglement cut. We further introduce a dimerization of the hopping constants, which gives rise to a distinctive behavior in the correlations, depending whether the entanglement cut creates a topological or a trivial phase.

[1] F. F. Assaad, T. C. Lang, F. Parisen Toldin, Phys. Rev. B 89, 125121 (2014)

TT 40.5 Tue 11:00 H 3010

Microscopical justification of the eigenstate thermalization hypothesis (ETH) — •Nils O. Abeling and Stefan Kehrein — Institut für Theoretische Physik, Fakultät für Physik, Georg-August-Universität Göttingen

The ETH postulates how isolated quantum many-body systems thermalize. It is essential to the understanding of thermalization and implicates various thermodynamic relations [1]. While there are several numerical verifications of the ETH ([2]), only few analytical arguments have been found so far. They, in particular, are based on semiclassical approaches [3]. Another argument was given by J. Deutsch who showed how a small interaction which is modelled by a random matrix leads to thermalization [4]. Our work adopts this idea and analyzes whether and how a generic quantum system can be treated as a random matrix. To do this we employ the flow equation method that performs continuous unitary transformations to map an initial Hamiltonian to an effective Hamiltonian. The latter takes on a banded form and is compared to a random matrix. By studying the statistical properties of the numerically obtained matrices we are able to use the analytical flow equation approach to close the gap in Deutsch's reasoning. Our results depict the first step towards a microscopic justification of the eigenstate thermalization hypothesis.

[1] L. D'Alessio et al., Adv. in Phys. Vol. 65, Iss. 3 (2016)
[2] M. Rigol, V. Dunjko, and M. Olshanii, Nature 452 (2008)
[3] M. Srednicki, Phys. Rev. E 50 (1994)
[4] J.M. Deutsch, Phys. Rev. A 43 (1991)

TT 40.6 Tue 11:15 H 3010

Quantum dynamics from classical networks — •Markus Schmitt[1,2] and Markus Heyl[1] — [1]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany — [2]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany

The efficient representation of quantum many-body states with classical resources is a key challenge in quantum many-body theory. In our work [1] we analytically construct classical networks for the description of the quantum dynamics in transverse-field Ising models that can be solved efficiently using Monte Carlo techniques. With this construction we compute transient dynamics of transverse-field Ising models in one, two, and three dimensions. We include a mapping to equivalent artificial neural networks and explore the utility of the obtained network structures for numerical time-evolution using a time-dependent variational principle.

[1] M. Schmitt and M. Heyl, arXiv:1707.06656

15 min. break.

TT 40.7 Tue 11:45 H 3010

Exact long time evolution of spinless fermion systems from a highly correlated initial state — •Kristof Harms, Lorenzo Cevolani, Stefan Kehrein, and Salvatore Manmana — Institut für Theoretische Physik, Universität Göttingen

Using time-dependent density matrix renormalization group (tDMRG), we analyze the time evolution of density-density correlations in one-dimensional spinless fermion systems after a global quench of the Hamiltonian. In particular, quenches to free fermion systems are considered. In this case, the time evolution can in fact be obtained exactly up to arbitrary times when providing the four-point propagators of the initial state, which are computed via DMRG at high accuracy. Taking this approach, we are able to both study the dynamics directly after the quench, as well as the long-time behavior. We obtain a ballistic lightcone structure and study the region outside in detail. For gapless initial states, we observe temporal oscillation outside the lightcone which we relate to the initial state and the dispersion relation of the quenched Hamiltonian.

Financial support by DFG CRC1073 (project B03) is gratefully acknowledged.

TT 40.8 Tue 12:00 H 3010

Geometry of driven-dissipative phase transitions — •Mikhail Pletyukhov[1], Dmitry Krimer[2], and Maarten Wegewijs[1,3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Institute for Theoretical Physics, TU Wien, Austria — [3]Peter Grünberg Institute, Forschungszentrum Jülich, Germany

Recent progress in the study of driven dissipative phase transitions in open quantum systems has raised the question how hysteretic phenomena in many-body systems can be appropriately understood on a quantum level, going beyond the common semiclassical mean-field description. In this talk we explain how hysteresis generically arises when accounting for a typical measurement time. We directly tie this to the eigenmodes of a nonunitary Lindblad dynamics of which a metastable state is composed. The metastable state attained on this given measurement timescale depends on the whole experimental procedure (a sequence of all preceding runs). This dependence must be accounted for at every subsequent experimental run. We show that different branches in the parametric dependence of observables then emerge naturally from the linear quantum master equation. Interestingly, these metastable states can be understood in terms of their path-dependent amplitudes in the Liouvillian-eigenmode expansion. Such amplitudes are familiar from pumping problems in quantum transport that can be related to geometric "phases" of the Landsberg type.

TT 40.9 Tue 12:15 H 3010

Driven-dissipative phase transitions of open quantum systems from a Floquet-Liouville perspective — •Viktor Reimer[1], Mikhail Pletyukhov[1], and Vladimir Gritsev[2] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Institute for Theoretical Physics, University of Amsterdam, Netherlands

The study of driven-dissipative open quantum systems prompted the emergence of a plethora of interesting new physics inaccessible to their equilibrium counterparts. Combining Floquet's theorem with the general Liouvillian approach to open quantum systems provides powerful tools to investigate such systems beyond the adiabatic limit.

Here, we present a general method to calculate the quasistationary state of a driven-dissipative system coupled to a transmission line with arbitrary coherent driving strength and modulation frequency of system parameters. Our first application of the method is the two level system with time-dependent parameters and we explore the regime where the breakdown of the adiabaticity condition happens even for a slow time modulation. Secondly, we apply our method to a driven three level Λ-system exhibiting electromagnetically induced transparency (EIT) and observe how the time modulation modifies the latter phenomenon.

Our focus however lies on the third application – the single-mode Kerr nonlinearity model – where driving is considered across the bistability point of the dissipative phase transition. In this talk I discuss the behaviour of observables in the quasistationary time regime and the critical regime of parameters.

TT 40.10 Tue 12:30 H 3010

Finding purifications with minimal entanglement — •Johannes Hauschild[1], Eyal Leviatan[2], Jens H. Bardarson[3], Ehud Altman[4], Michael P. Zaletel[5], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot 7610001, Israel — [3]Department of Physics, KTH Royal Institute of Technology, Stockholm SE-10691, Sweden — [4]Department of Physics, University of California, Berkeley, CA 94720 — [5]Department of Physics, Princeton University, Princeton, NJ 08540, USA

Purification is a tool that allows to represent mixed quantum states as pure states on enlarged Hilbert spaces. A purification of a given state is not unique and its entanglement strongly depends on the particular choice made. Moreover, in one-dimensional systems, the amount of entanglement is linked to how efficiently the purified state can be represented using matrix-product states (MPS). We introduce an MPS based method that allows to find the minimally entangled representation by iteratively minimizing the second Rényi entropy [1]. First, we consider the thermofield double purification and show that its entanglement can be strongly reduced especially at low temperatures. Second, we show that a slowdown of the entanglement growth following a quench of an infinite temperature state is possible.

[1] J. Hauschild et al., arXiv:1711.01288

TT 40.11 Tue 12:45 H 3010

A time-dependent variational description latttice gauge theories. — Ignacio Cirac[1], Eugene Demler[2], Tao Shi[1,3], and •Pablo Sala[1,4] — [1]Max Planck Institute for Quantum Optics, Garching, Germany — [2]Harvard University, Cambridge, Massachusetts — [3]Institute of Theoretical Physics, Beijing, China —

[4]Technical University of Munich, Germany

Fermionic Gaussian states are completely characterized by their two-point correlation functions. These are collected in the so-called covariance matrix, which then becomes the main object in their description. We derive a time-dependent variational description of (1+1)-dimensional gauge theories using the framework of lattice gauge theories as well as fermionic Gaussian states. We compare our results to previously obtained results via matrix product states for ground-state properties and real-time dynamics. Specifically, we investigate the phase transition between the string and string-breaking phases, and the dynamical properties in the massive Schwinger model and other non-Abelian generalizations.

TT 41: Frustrated Magnets - Spin Liquids - Experiments

Time: Tuesday 10:15–13:00 Location: H 3005

TT 41.1 Tue 10:15 H 3005

Yb- delafossites as pseudo spin 1/2 triangular magnets: magnetism, specific heat, NMR and the quest for spin liquids — •M. Baenitz[1], K.M. Ranjith[1], P. Schlender[2], J. Sichelschmidt[1], R. Sarkar[3], S. Khim[1], D.A. Sokolov[1], H.H. Klauss[3], H. Yasuoka[1], A.P. Mackenzie[1], D.S. Inosov[3], and Th. Doert[2] — [1]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [2]TU Dresden, Department of Chemistry and Food Chemistry, D-01062 Dresden, Germany — [3]TU Dresden, Institute of Solid State Physics, D-01062 Dresden, Germany

$S = 1/2$ triangular quantum magnets (TQM) are rare and discussed as ideal quantum spin liquids (QSL)[1]. Recently the pseudo $S = 1/2$ TQM $YbMgGaO_4$ was identified as a QSL candidate [2]. Delafossites share the same space group and the planar triangular spin arrangement so we started working on Yb based delafossites. These systems are rare ($AYbO_2$ (A=Ag,Na)) and a low T pseudo spin S=1/2 state is in question. As for T-> 0 the magnetism of Yb compounds is determined by i)the crystalline electric field (CEF) and ii) the exchange frustration, replacing the oxygen by another chalcogen might tune the magnetism. $NaYbS_2$, $LiYbS_2$ and $NaLuS_2$ were synthesized in poly- and single- crystalline form and bulk- (magnetization, specific heat) and local- methods (Na- Li- NMR, ESR, μSR) were applied. Our studies evidence pseudo spin $S = 1/2$ magnetism and an absence of magnetic order (T > 300 mK) which identifies (AM)YbS_2 (AM=Li, Na) as a new promissing candidate for a QSL ground state.

[1] L.Savary et al., Rep. Prog. Phys. 80 (2017).
[2] J.A.M. Paddison et al., Nature Phys. 13,(2017).

TT 41.2 Tue 10:30 H 3005

Low temperature properties of the triangular antiferromagnet $KBaYb(BO_3)_2$ — •K. Kavita, S. Bachus, Y. Tokiwa, A. A. Tsirlin, and P. Gegenwart — Experimental Physics VI, University of Augsburg, Germany

Geometrically frustrated magnetic materials host new exotic states such as quantum spin liquids (QSL). A recent example is the QSL candidate $YbMgGaO_4$, with the triangular lattice of pseudospin-1/2 Yb^{3+} ions. A crucial part, to understand the physics of $YbMgGaO_4$, is to identify leading interaction terms that may extend beyond nearest neighbors. To this end, we studied $KBaYb(BO_3)_2$, where the Yb^{3+} ions are also arranged on a triangular lattice, whereas the distance between nearest neighbors is comparable to the next nearest neighbor distance in $YbMgGaO_4$. Our polycrystalline samples confirm the rhombohedral symmetry of $KBaYb(BO_3)_2$ with the space group $R\bar{3}m$. Magnetic susceptibility data down to 1.8 K revealed a Curie-Weiss temperature of about 20 mK with antiferromagnetic couplings. Furthermore, we report heat capacity down to 60 mK, which also indicates a very small exchange coupling.

TT 41.3 Tue 10:45 H 3005

Spin-1 triangular antiferromagnet $BaMoP_2O_8$ — •Jan Hembacher[1], Alexander Tsirlin[1], Danis Badrtdinov[2], and Clemens Ritter[3] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Ural Federal University, Yekaterinburg, Russia — [3]Institute Laue Langevin, B. P. 156, 38042, Grenoble, France

We present magnetic properties of a spin-1 antiferromagnet $BaMoP_2O_8$. It crystallizes in the $C2/m$ space group, resulting in a layered crystal structure with the triangular arrangement of the magnetic Mo^{+4}-ions. Frustrated interaction geometry leads to a broad maximum in the magnetic susceptibility around 50 K followed by the long-range ordering at 21 K. Neutron diffraction reveals the collinear stripe order with the reduced ordered moment of 1.48 μ_B compared to 2 μ_B expected for a spin-1 ion. The effects of spatial anisotropy, spin-orbit coupling, and metal-ligand covalency will be discussed.

TT 41.4 Tue 11:00 H 3005

A new three dimenisional quantum spin liquid — •Shravani Chillal[1], Yasir Iqbal[2], Harald O. Jeschke[3], Jose A. Rodriguez-Rivera[4,5], Robert Bewley[6], Pascal Manuel[6], Dmitry Khalyavin[6], Paul Steffens[7], Ronny Thomale[8], A. T. M. Nazmul Islam[1], Johannes Reuther[1,9], and Bella Lake[1,10] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Indian Institute of Technology Madras, Chennai , India — [3]Okayama University, Okayama, Japan — [4]NIST Center for Neutron Research, Gaithersburg, USA — [5]University of Maryland, USA — [6]ISIS Facility, STFC Rutherford Appleton Laboratory, UK — [7]Institut Laue-Langevin, Grenoble, France — [8]Julius-Maximilian's University of Würzburg, Würzburg, Germany — [9]Freie Universität Berlin, Berlin, Germany — [10]Technische Universität Berlin, Berlin, Germany

Quantum spin liquid (QSL) is a highly entangled magnetic state characterized by the lack of static magnetism, however, accompanied by highly correlated excitations known as spinons. While there are few experimental examples of QSL in two dimensionally frustrated lattices, very little is known about the possibility in three dimensional (3D) Heisenberg systems. Here we report a new type of 3D lattice that enables spin liquid behavior in a so called hyper-hyperkagome lattice which manifests in the compound $PbCuTe_2O_6$. Using a combination of experiment and theory we show that this system satisfies all the requirements for a quantum spin liquid including the absence of static magnetism and the characteristic continuum of spinon excitations.

TT 41.5 Tue 11:15 H 3005

Crystal growth and magnetic characterization of novel kagome-type materials — •Christian Klein, Mahmoud Abdel-Hafiez, and Cornelius Krellner — Goethe-University, D-60438 Frankfurt am Main, Germany

Kagome-lattices are promising materials to investigate frustrated quantum spin systems with a possible quantum spin liquid (QSL) ground state [1]. High-quality single crystals are essential to distinguish between disordered magnetic ground-states and a true QSL.

We report on synthesis and characterization of Co-derivates of the spin-1/2 antiferromagnet material Barlowite ($Cu_{4-x}Co_x(OH)_6BrF$). The kagome-layers are build up by copper ions and separated from each other through a transition-metal cation, so that a quasi-two-dimensional system is created [2]. The non-magnetic material $Zn_4(OH)_6BrF$ was synthesized to determine the magnetic contributions to the kagome-physicsThe synthesis was carried out under hydrothermal conditions. Single Crystals of Co-doped Barlowite were obtained as well as polycrystalline samples of the Zn-analogue of Barlowite. Characterization of the samples was done by magnetic measurements to determine the susceptibility and magnetic ordering. Furthermore heat capacity measurements were performed to investigate phase transitions and magnetic ordering at low temperature.

[1] P. A. Lee, Science 321, 1306 (2008).
[2] H. Jeschke et al., PRB 92, 094417, (2015).

15 min. break.

TT 41.6 Tue 11:45 H 3005

Frozen state and spin-gap behavior in a new kagome magnet $Fe_4Si_2Sn_7O_{16}$: An NMR study — •S. Dengre[1], R. Sarkar[1], M.C. Allision[2,3], T. Söhnel[2], C.D. Ling[3], J. Gardner[4], and H.-H. Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [2]School of Chemical Sci-

ences, University of Auckland, Auckland 1142, New Zealand — [3]School of Chemistry, The University of Sydney, Sydney 2006, Australia — [4]Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Menai 2234, Australia

$Fe_4Si_2Sn_7O_{16}$ is a new Fe based kagome system with a $f = \theta/T_N \approx 3.6$. The system consists of alternate stacking of kagome layer formed from edge sharing FeO_6 (S =2) and SnO_6 octahedra and stannate layer $FeSn_6$ (S = 0). $Fe_4Si_2Sn_7O_{16}$ is a classical homologue to a famous kagome compound herbertsmithite, a suitable candidate to realize quanum spin liquid phase. $^{(117/119)}$Sn nuclear magnetic resonance (NMR) allows us to selectively probe the static and dynamic magnetism of different Fe-layers. While the NMR shift vs bulk susceptibility plot follows linear relation down to 10 K confirming the absence of foreign phases in the vicinity of kagome plane, the considerable line broadening below 10 K indicates the distribution of static internal field. NMR spin-lattice/spin relaxation rate $(1/T_1)/(1/T_2)$ reflect the slowing down of spin fluctuations at ∼3 K associated with the static magnetism of Fe-kagome layer. Additionally, $(1/T_1)$ and $(1/T_2)$ temperature dependency show a spin-gap behavior with $\Delta \sim 6.5$ K.
[1] Ling *et al.* Phys. Rev. B 96, 180410(R).

TT 41.7 Tue 12:00 H 3005

NMR investigations on doped kagomé lattice mott insulator $Ga_xCu_{4-x}(OD)_6Cl_2$ — •Ranjith Kumar Kizhake Malayil[1], Pascal Puphal[2], Cornelius Krellner[2], and Michael Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Institute of Physics, Goethe- University Frankfurt, 60438 Frankfurt am Main, Germany

Herbertsmithite ($ZnCu_3(OH)_6Cl_2$),[1] which is reported as a prototype kagome quantum spin liquid (QSL) triggers the search for new QSL materials among its polymorphs. Replacing the divalent Zn by the trivalent Ga was proposed to form a new correlated Dirac-kagome metal combining Dirac electrons, strong interactions, and frustrated magnetism[2]. Polycrystalline samples of $Ga_xCu_{4-x}(OD)_6Cl_2$ were synthesized with Ga-doping level of $0 < x < 1$. We have employed ^{71,69}Ga and ^{2}H nuclear magnetic resonance (NMR) experiments together with bulk studies to explore the ground state properties of $Ga_xCu_{4-x}(OD)_6Cl_2$. Ga-NMR proof a homogeneous Ga distribution and narrow Ga-lines which is typical for Ga-based quantum magnets. Magnetic ordering is found to be suppressed with increasing Ga-concentration similar to that observed for Zn- Herbertsmithite. Spin-lattice relaxation measurement reveals the existence of a spin gap in the excitation spectrum which is increasing linearly with the applied field.
[1] P. Mendels et al., J. Phys. Soc. Jpn. 79, 011001 (2010).
[2] I. Mazin et al., Nature Communications 5, 4261 (2014)

TT 41.8 Tue 12:15 H 3005

Spinon Excitations in Quantum Spin-Liquids Identified by Optical Spectroscopy — Andrej Pustogow[1], Yohei Saito[1], Elena Zhukova[2], Boris Gorshunov[2], Reizo Kato[3], and •Martin Dressel[1] — [1]1. Physikalisches Inst., Universität Stuttgart, Germany — [2]Moscow Inst. Phys. Techn., Dolgoprudny, Moscow Region, Russia — [3]RIKEN, Saitama, Japan

The electrodynamic response of several organic quantum spin-liquids with highly-frustrated triangular lattices has been measured in a wide energy range. Even below the Mott-Hubbard gap, large non-thermal contributions to the optical conductivity are observed in the vicinity of the metal-insulator phase boundary; such metallic quantum fluctuations are most pronounced in κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$.
Only when investigating the more strongly correlated Mott insulator β'-$EtMe_3Sb[Pd(dmit)_2]_2$ at very low frequencies and temperatures, we succeeded identifying an excess conductivity that cannot be explained by the charge response of the correlated electrons. Upon subtracting the smooth power-law background of the Mott-Hubbard band, a broad dome-like mode is identified, delimited by $J \approx 20$ meV at its high-energy end; the low-frequency decrease is consistent with the ω^2 dependence expected for spinons. Due to this fast decay, the effective range of well-defined spinons is confined to the microwave and THz energy ranges. Our findings are in excellent agreement with recent dynamical mean field theory calculations stating that the controversially discussed spinon Fermi surface is damped away upon approaching the Mott metal-insulator transition.

TT 41.9 Tue 12:30 H 3005

Exploration of the quantum spin liquid state in $Ca_{10}Cr_7O_{28}$ — Christian Balz[1,2], •Bella Lake[1,3], ATM Nazmul Islam[1], Ulrich Tutsch[4], Michael Lang[4], Yuji Matsuda[5], Lars Opherden[6,7], Thomas Herrmannsdoefer[6], and Jose A. Rodriguez-Rivera[8] — [1]Helmholtz Zentrum Berlin, Germany — [2]Oak Ridge National Lab, USA — [3]Technical University Berlin, Germany — [4]Goethe University, Germany — [5]Kyoto University, Japan — [6]Helmholtz Zentrum Dresden Rossendorf, Germany — [7]Technical University Dresden, Germany — [8]NIST, MD, USA

$Ca_{10}Cr_7O_{28}$ is a new candidate spin liquid where the magnetic Cr^{5+} ions (S-$\frac{1}{2}$) form breathing Kagome bilayers. Both kagome layers consist of alternating ferromagnetic/antiferromagnetic corner-sharing triangles and the two layers are stacked so that the ferromagnetic triangles lie on top of antiferromagnetic triangles and vice versa. Previous measurements revealed the absence of long-range magnetic order and the presence of persistent spin dynamics in the ground state. Here we present a detailed exploration of the ground state and excitations using magnetisation, heat capacity, thermal conductivity and inelastic neutron scattering. The heat capacity and thermal conductivity are linear in temperature suggesting the presence of a gapless spinon Fermi surface while the excitations are diffuse revealing the presence of spinon continuua. The excitations appear gapless and form a distinct pattern that evolves gradually with energy. Together these results provide strong evidence that $Ca_{10}Cr_7O_{28}$ is a gapless quantum spin liquid. The origins of this spin liquid state will be discussed.

TT 41.10 Tue 12:45 H 3005

Low-temperature spin-liquid phase in a S = 3/2 undistorted triangular lattice: $RbAg_2Cr[VO_4]_2$ — •Angela Möller[1], Joshua Tapp[1], Clarina R. dela Cruz[2], Michaela Bratsch[3], Ngozi E. Amuneke[3], Lars Postulka[4], Bernd Wolf[4], Michael Lang[4], Harald O. Jeschke[5], Roser Valentí[4], and Peter Lemmens[6] — [1]JGU Mainz, D — [2]ORNL, USA — [3]University of Houston, USA — [4]GU Frankfurt, D — [5]Okayama University, Jpn — [6]TU Braunschweig, D

We present a series of distorted and undistorted antiferromagnetic triangular lattice (TL) compounds, $AAg_2Cr[VO_4]_2$ with A = Ag, K, or Rb. The A-site cation induces slight symmetry changes of the $[CrO_6]$ complex and thereby alters the relative orientation of the vanadate with respect to the TL. This aspect of fine-tuning allows for distinct alterations of the magnetic exchange interactions between the Cr^{3+} ($3d^3$) ions, J^{Ag}=3K, J^K=1K, J^{Rb}=0.5K. We observe for the distorted TL collinear antiferromagnetic long-range order at T_N=10K (A = Ag), whereas the high-symmetry cases (A = K, Rb) even evade the theoretically predicted 120° long-range order in zero field down to 0.03K.[1] Our experiments support a spin liquid ground state for the latter compounds which is unconventional for antiferromagnetic TL systems and points towards the relevance of additional competing interaction mechanisms.

This work received support from NSF, ORNL-DOE, Carl-Zeiss Stiftung, and DFG.
[1] J. Tapp et al. Phys. Rev. B 96, 064404 (2017).

TT 42: Charge Order

Time: Tuesday 10:15–13:00 Location: HFT-FT 131

TT 42.1 Tue 10:15 HFT-FT 131

Charge order and Frustration on the triangular lattice - A Monte Carlo Study of the Falicov-Kimball model — •Miguel M. Oliveira[1], Andrey Antipov[3], Pedro Ribeiro[1], and Stefan Kirchner[2] — [1]Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China — [3]Station Q, Microsoft Research, Santa Barbara, California 93106, USA

The Falicov-Kimball model is commonly used as one of the simplest possible models to study the metal-insulator transition. Recently, it has been shown that the half-filled Falicov-Kimball model on the square lattice, above the charge order transition, has a richer phase diagram than originally anticipated [1].

In this talk we present the extension of these results to the triangular lattice. In particular, for 1/3 filling, we find that the high temperature disordered phases are similar to those found for the half-filled square lattice.

At low temperatures and large coupling, the ordered phase has a broken Z_3 symmetry and the transition into this state is of the same universality as the three-state Potts model.

We investigate the possibility that frustration effects in the weak-coupling regime and at low temperatures may destroy the Z_3-broken phase and induce other kinds of ordered or liquid states.

[1] A.Antipov et al PRL **117** 146601 (2016).

TT 42.2 Tue 10:30 HFT-FT 131

Density Matrix Renormalization Group Study of the Two-Dimensional Hubbard Model in Hybrid Real-Momentum Space — •Georg Ehlers and Reinhard M. Noack — Philipps Universität Marburg

We investigate the square-lattice Hubbard model in hybrid real-momentum space using the density matrix renormalization group (DMRG). The variation of the DMRG that we use is formulated for lattices with cylindrical geometry and utilizes the conserved transverse lattice momentum. Compared to the standard real-space algorithm, it achieves a speedup that scales quadratically with the width of the lattice [G. Ehlers et al., Phys. Rev. B 95, 125125 (2017)]. For width-four and width-six cylinders at one-eighth doping and Coulomb interaction strengths U/t=8 and U/t=4, we find a striped ground state. In a combined study with other state-of-the-art numerical methods, we provide strong evidence that the striped state is present in a substantial region of the underdoped regime of the ground-state phase diagram of the two-dimensional Hubbard model. The periodicity and stripe filling of our striped state differs from that found experimentally in hole-doped cuprates, indicating that terms beyond the standard Hubbard model must be included to accurately model high-temperature superconductivity [1].

[1] B.-X. Zheng et al., Science 358, 1155 (2017).

TT 42.3 Tue 10:45 HFT-FT 131

Dynamical manipulation of crystalline symmetry — Tanay Nag, R-J Slager, and •Takashi Oka — Max Planck Institute for Physics of Complex Systems (MPI-PKS), Dresden, Germany

Our main aim is to break a discrete symmetry of honeycomb lattice model by introducing suitable laser field. Unlike the laser field with single frequency that is not able to generate a inversion symmetry breaking on-site momentum independent mass term, a bi-harmonic laser filed with commensurate frequencies can break the C_3 symmetry of the model and lead to a finite charge density wave order. We show that there is a possibility that the CDW shows memory effect (hysteresis). In order to enhance the CDW order, we consider an extended Hubbard interaction implemented through a mean field approach. We explain the synchronization dynamics of CDW in the switch on and switch off region by making resort to a simple toy model namely, Kuramoto model. Furthermore, we show that van Hove singularity in density of states for this model substantially contributes to the dynamics.

TT 42.4 Tue 11:00 HFT-FT 131

Supercooled and hidden electronic phases in thin 1T-TaS_2 — •Quirin Stahl[1], Tobias Ritschel[1,2], Maximilian Kusch[1], Florian Heinsch[1,3], Gaston Garbarino[4], Norman Kretzschmar[4], and Jochen Geck[1] — [1]TU Dresden, Germany — [2]UBC, Vancouver, Canada — [3]HZDR, Germany — [4]ESRF, Grenoble, France

The ultra-fast semiconductor-to-metal transition in nano-thick 1T-TaS_2 crystals induced by femtosecond laser pulses currently attracts a lot of interest [1,2]. In particular, since it is believed that such laser pulses stabilize so-called hidden states, which cannot be reached from thermal equilibrium and which exhibit unique electronic properties. We present a detailed XRD study of nano-thick 1T-TaS_2 single crystals. In a first experiment we studied the charge density wave order in the supercooled state, which has been observed earlier in resistivity measurements[3]. This phase is then compared to the charge density wave order created by a femto-second laser pulse. We find that the supercooled and the hidden electronic phases are identical within the error of the experiment, implying that the hidden state of 1T-TaS_2 is a supercooled NC-CDW state. These results will be discussed in terms of unusual phase ordering kinetics caused by a down-scaling of the sample thickness into the nanometer-regime.

[1] L. Stojchevska *et al.*, Science 334, 177 (2014)
[2] I. Vaskivskyi *et al.*, Science Advances 1, 6 (2015)
[3] M. Yoshida *et al.*, Scientific Reports 4, 7302 (2014)

TT 42.5 Tue 11:15 HFT-FT 131

Temperature-dependence of the three-dimensional band structure of 1*T*-TaS_2 — •Sanjoy K. Mahatha[1], Arlette S. Ngankeu[1], Kevin Guilloy[1], Marco Bianchi[1], Charlotte E. Sanders[1], Kerstin Hanff[2], Kai Rossnagel[2], Jill A. Miwa[1], Christina Breth Nielsen[3], Martin Bremholm[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNANO), Aarhus University, 8000 Aarhus C, Denmark — [2]Institute for Experimental and Applied Physics, Kiel University, Germany — [3]Department of Chemistry, University of Aarhus, Aarhus, Denmark

The 1*T* polymorph of the layered transition metal dichalcogenide compound TaS_2 undergoes a series of temperature-dependent phase transitions consisting of periodic structural distortions and organization of the electrons into regular patterns known as charge density waves (CDW). The different CDW phases vary remarkably in their electronic properties. The commensurate CDW phase of 1*T*-TaS_2 has widely been studied as a quasi-two-dimensional phenomenon that coexists with a Mott insulating state. However, recent theoretical calculations predicted the coexistence of the CDW phase with a nearly one-dimensional metallic dispersion perpendicular to the crystal planes. Our recent angle-resolved photoemission spectroscopy results confirm the existence of a dispersive band which exists for all the different CDW phases at different temperatures. Here, we will give a detailed account of the three dimensional band structure of this highly correlated material.

TT 42.6 Tue 11:30 HFT-FT 131

Zigzag-chain domain walls facilitate metalisation of the Mott insulator on a triangular lattice — Jan Skolimowski[1] and •Rok Žitko[1,2] — [1]Jožef Stefan Institute, Jamova 39, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, Ljubljana, Slovenia

Motivated by the occurrence of a long-lived metastable metallic hidden-state in 1T-TaS_2 that can be induced by optical or voltage pulses and that shows a characteristic mosaic pattern of mesoscale charge-density-wave (CDW) domains separated by a dense web of domain walls, we study how the structural domain walls affect the electron dynamics. We consider the Hubbard model on a triangular lattice as a low-energy effective model describing the narrow electron band formed around the Fermi level in the low-temperature commensurate $\sqrt{13} \times \sqrt{13}$ phase of 1T-TaS_2. Within the effective model a domain wall between two CDW domains leads to a local modification of the hopping constants along a one-dimensional defect line. We study the resulting Hamiltonian using the extension of the dynamical mean-field theory to inhomogeneous systems. We discuss in detail the case where the hopping constants are enhanced and the domain wall metallises. We show that this is facilitated by the fact that in the triangular lattice the domain walls tend to enhance the hopping constants along a connected zigzag line, rather than forming a ladder of dimers which

instead show a band gap. We also discuss the case of multiple domain walls and comment on the relevance of the domain-wall-metallisation scenario for the metallic hidden-state.

15 min. break.

TT 42.7 Tue 12:00 HFT-FT 131

Competition of strong charge and spin fluctuations in monolayer NbS_2 — •Erik van Loon[1], Malte Rösner[2,3], Gunnar Schönhoff[3], Mikhail Katsnelson[1], and Tim Wehling[3] — [1]Radboud Universiteit, Nijmegen, Nederland — [2]University of Southern California, Los Angeles, USA — [3]Universität Bremen, Bremen, Deutschland

Single-layers of transition metal dichalcogenides have rich phase diagrams featuring metallic, insulating and charge/spin density wave phases. Competing interactions lie beneath these competing phases. Theoretical descriptions have so far focussed on the electron-phonon interactions in these materials, whereas the electron-electron interaction has mostly been ignored. In this talk, we show that in NbS_2 the local Coulomb interaction is by itself strong enough to turn the material insulating. Screening by the electron-phonon and the non-local Coulomb interaction restores the metallic phase, leads to a broadening of the electronic spectral function and to a coexistence of strong charge and spin fluctuations. These results are obtained by combining an abinitio determination of the band structure and Coulomb interaction with the Dual Boson approach for the extended Hubbard model.

TT 42.8 Tue 12:15 HFT-FT 131

Three-Dimensional Fermi Surface of $2H$-$NbSe_2$ - Implications for the Mechanism of Charge Density Waves — •Roland Hott[1], Frank Weber[1], Rolf Heid[1], Leonid L. Lev[2], Thorsten Schmitt[2], and Vladimir N. Strocov[2] — [1]Institute for Solid State Physics, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]Paul Scherrer Institut, Swiss Light Source, CH-5232 Villigen PSI, Switzerland

We investigated the three-dimensional electronic structure of the seminal charge-density-wave (CDW) material $2H$-$NbSe_2$ by soft x-ray angle-resolved photoelectron spectroscopy and density-functional theory. Our results reveal the pronounced 3D character of the electronic structure formed in the quasi-two-dimensional layered crystal structure. In particular, we find a strong dispersion along k_z excluding a nesting-driven CDW formation based on experimental data.

TT 42.9 Tue 12:30 HFT-FT 131

The Coherent Response in the Ground State of the Excitonic Insulator Ta_2NiSe_5 — •Minjae Kim[1,2], Parmida Shabestari[1,2], Emily Huang[1,2], Daniel Werdehausen[1,2], Steinn Ymir Agustsson[1,2], Timofei Larkin[1], Alexander Boris[1], Tomohiro Takayama[1,2], Hao Chu[1,2], Hidenori Takagi[1,2], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Germany

The excitonic insulator (EI) is an intriguing phase of condensed excitons undergoing a BEC-type transition. A prominent candidate has been identified in Ta_2NiSe_5 [1]. Ultrafast spectroscopy allows tracing the coherent response of the EI condensate directly in the time domain. Probing the collective electronic response we can identify the Higgs-amplitude mode of the condensate. In addition we find a peculiar coupling of the EI phase to a low frequency phonon mode [2]. We will discuss the transient response on multiple energies scales ranging from the exciton dynamics in the NIR down to the coherent THz response of the gap.

[1] Y.F. Lu et al., Nat. Comm. 8, 14408 (2017).
[2] D. Werdehausen et al., arXiv:1611.01053 (2016).

TT 42.10 Tue 12:45 HFT-FT 131

Nearfield Optical Probe of the Excitonic Insulator Transition in Ta_2NiSe_5 — •Amrit Raj Pokharel[1,2], Heiko Linnenbank[2], Tomohiro Takayama[1,2], Hidenori Takagi[1,2], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]University of Stuttgart

The Excitonic Insulator (EI) is an intriguing phase of condensed excitons that undergo Bose Einstein Condensation (BEC). A prominent solid-state candidate for an EI is Ta_2NiSe_5, which is a quasi-one-dimensional material that undergoes a semiconductor to excitonic insulator phase transition at T_c=328K [1]. Here we investigate the formation of the excitonic gap using Scattering-Scanning Nearfield Optical Microscope (s-SNOM). That allows us tracing the optical response with spatial resolution down to tens of nanometer when the system is driven across T_c by temperature. Probing at different energy scales - in the gap, at the exciton peaks and close to strongly coupled phonons - reveals the nature of the EI transition. We will discuss a homogeneous gap and an inhomogeneous near field pattern on the exciton peak around T_c with respect to the second order nature of the phase transition.

[1] Y.F.Lu, et al. Nat.Com. 8, 14408 (2017).

TT 43: Graphene: Electronic Properties, Structure and Substrate Interaction II (joint session O/TT)

Time: Tuesday 10:30–13:15 Location: MA 043

Invited Talk TT 43.1 Tue 10:30 MA 043

Inside graphene devices — •Clemens Winkelmann[1], Sayanti Samaddar[1], Alessandro De Cecco[1], Hervé Courtois[1], Indra Yudhistira[2], Shaffique Adam[2], Vladimir Prudkovskiy[1,3], Claire Berger[1,3], and Walt de Heer[3] — [1]Univ. Grenoble Alpes / France — [2]NUS / Singapore — [3]Georgia Inst. of Technol. / USA

The electronic transport properties of devices are governed by microscopic physics which can often only be inferred indirectly from the former. By combining in situ transport and scanning probe experiments in graphene-based devices, we directly test the microscopic pictures used for predicting macroscopic transport properties.

The first part focusses on the charge puddles in diffusive graphene on a disordered dielectric substrate. Because of the linear dispersion relation in monolayer graphene, the puddles are predicted to grow near charge neutrality, a markedly distinct property from conventional two-dimensional electron gases. Using STM/STS on a gated single mesoscopic graphene device, we observe the puddles' growth as the Fermi level approaches the Dirac point. Self-consistent screening theory provides a unified description of both the macroscopic transport properties and the microscopically observed charge disorder.

The second part extends the above technique to a system with very little disorder, namely graphene nanoribbons grown on the sidewalls of steps of a SiC substrate. By performing STM (and the related scanning tunneling potentiometry technique) on such nanoribbons driven out of equilibrium, we gain novel insights into the extraordinary transport properties of graphene nanoribbons.

TT 43.2 Tue 11:00 MA 043

Probing bulk and edge transport channels in sidewall graphene nanoribbons by dual-probe spectroscopy — •Johannes Aprojanz[1,2], Stephen Power[3,4], Anti-Pekka Jauho[4], Stephan Roche[3], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Germany — [3]ICREA - Institucio Catalana de Recerca i Estudis Avancats, Barcelona, Spain — [4]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), Lyngby, Denmark

The electronic confinement in graphene nanoribbons (GNR) leads to the formation of subbands as well as topologically protected edge states. GNR epitaxially grown on nanofacets of SiC mesa structures have shown fully spin-polarized ballistic transport signatures for probe spacings larger than 200 nm [1]. By means of a 4-tip STM/SEM contacts with even smaller probe spacings were realized. In this regime sudden jumps to plateaus of multiples of the conductance quantum e^2/h were observed using one blunt tip covering the entire GNR and one sharp tip gradually crossing the ribbon. We attribute these plateaus to edge and bulk transport channels, respectively. Based on tight-binding calculations these findings are explained by transversal electric fields which originate from distinct edge terminations on both sides of the GNR.

[1] Baringhaus et al., Nature **506**, 349 (2014)

TT 43.3 Tue 11:15 MA 043

Polycyclic molecules with geometrical frustration via pyrolysis on a metal — •Alexandre Artaud[1], Laurence Magaud[2], Kitti Ratter[3], Bruno Gilles[3], Valérie Guisset[2], Philippe David[2], Jose I. Martinez[4], Jose A. Martin-Gago[4], Claude Chapelier[5], and Johann Coraux[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Germany — [2]CNRS, Institut Néel, Grenoble, France — [3]Grenoble INP, SIMAP, Grenoble, France — [4]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain — [5]CEA, INAC, PHELIQS, Grenoble, France

The geometry of molecules is a key to several of their properties. In graphene fragments, electron delocalization from one carbon sublattice to the other is frustrated for molecular shapes breaking the balance of sublattices. Optical, electronic, and magnetic properties emerge in this case, but the synthesis of such molecules remains challenging.

Here, a pyrolysis reaction catalysed by the surface of rhenium is investigated using scanning tunneling microscopy and density functional theory. This reaction known to form graphene is found to also yield graphene fragments consisting of well-defined, zigzag-edged polycyclic molecules, some of which have sublattice imbalance. However, they are found in metastable configurations, which is interpreted as a kinetic rather than thermodynamic control of their formation. Hence, metastable molecules are expectedly ubiquitous in graphene growth, and deleterious to achieve perfect graphene. Pyrolysis is conversely a promising route towards molecules with sought-after properties.

TT 43.4 Tue 11:30 MA 043

Partial dislocations in bilayer graphene — •Reena Gupta[1], Heiko Weber[2], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany — [2]Angewandte Physik, FAU Erlangen-Nürnberg, Staudtstrasse 7, 91058 Erlangen, Germany

We study the bernal stacked bilayer in the presence of symmetry lowering networks of partial dislocations. We find that the transport state of the bilayer is essentially determined by the structure of the partial dislocation network, which may result in both a minimal conductivity i.e., the appearance of a pristine bilayer, as well as an insulating phase [1]. We consider both an ideal model of straight partials, which reveals the essential physics, as well as more complex networks of wandering partials. Finally, we examine the topological edge states that exist at the partial dislocation edge, and examine their behaviour in the presence of an applied magnetic field.

[1] S. Shallcross et al., Nature Communications 8, 342 (2017).

TT 43.5 Tue 11:45 MA 043

A topological edge state in the graphene twist bilayer — •Maximilian Fleischmann, Reena Gupta, Dominik Weckbecker, and Sam Shallcross — Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Staudtstrasse 7/B2, 91058 Erlangen, Germany

The edge physics of graphene based systems is well known to be highly sensitive to the atomic structure at the boundary, with localized zero mode edge states found only on zigzag type terminations of the lattice. Here we demonstrate that the graphene twist bilayer supports an additional class of topological edge states, that (i) are found for all edge geometries (and thus are robust against edge roughness), (ii) occur at energies coinciding with twist-induced van Hove singularities in the bulk electronic spectrum and possess an electron density strongly modulated by the moiré lattice. Interestingly, these "moiré edge states" exist only for certain lattice commensurations and thus the edge physics of the twist bilayer is, in dramatic contrast to that of the bulk [1], not uniquely determined by the twist angle.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.

TT 43.6 Tue 12:00 MA 043

Structural study of the graphene/n-Ge(110) interface for nanoelectronic applications — •Julia Tesch[1], Fabian Paschke[1], Marko Wietstruk[2], Stefan Böttcher[2], Mikhail Fonin[1], Elena Voloshina[3], and Yuriy Dedkov[3,1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]SPECS Surface Nano Analysis GmbH, 13355 Berlin, Germany — [3]Department of Physics, Shanghai University, 200444 Shanghai, China

While graphene nanoelectronics show great promise to replace silicon-based technology in the future[1], the fabrication of graphene-based electronic units is accompanied by several drawbacks such as organic residue or metal contamination, defects and other transfer related issues. An alternative route to designing nanoscale device components is presented by epitaxial graphene growth directly on semiconducting substrates.

In order to shed light on the interactions at the graphene-semiconductor interface, we present local and macroscopic studies of graphene/Ge(110) regarding both structural and electronic properties investigated by means of low temperature STM/STS[2] as well as ARPES. The arrangement of dopants is discussed with respect to corrugation, Fermi velocity renormalization and doping level of graphene. Due to only a weak interaction between graphene and Ge(110) substrate, the characteristic linear dispersion of graphene is preserved, making it a viable candidate for device applications.

[1] Westervelt, Science 320, 324 (2008). [2] Tesch *et al.*, Carbon 122, 428 (2017).

TT 43.7 Tue 12:15 MA 043

Landau-level spectroscopy of twisted epitaxial graphene multilayers on a metal substrate — •Sabina Simon[1], Elena Voloshina[2], Julia Tesch[1], Felix Förschner[1], Vivien Enenkel[1], Charlotte Herbig[3], Timo Knispel[3], Alexander Tries[4], Jörg Kröger[4], Yuriy Dedkov[1,2], and Mikhail Fonin[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Physics Department, Shanghai University, Shanghai 200444, China — [3]Institute of Physics II, University of Köln, 50937 Cologne, Germany — [4]Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to its potential in the development of new generation technologies, graphene remains the focus of many theoretical and experimental studies, principally when considering high-quality, large-scale epitaxial growth. In this work we investigate multilayered graphene systems epitaxially grown on Ir(111). Large patches of graphene twisted layers of high quality are fabricated upon atomic carbon intercalation underneath a continuous graphene sheet. By means of scanning tunneling spectroscopy in magnetic filed we study the evolution of the Landau-level spectra reflecting the variation of local electronic properties of the top graphene layer. We show that bilayers with large twist angles as well as twisted trilayers exhibit the electronic properties characteristic for a pristine graphene monolayer, pointing towards an effective decoupling of the top layer from the metal substrate. Complementary, we investigate changes in electronic properties of twisted graphene induced by subsequent alkali metal intercalation.

TT 43.8 Tue 12:30 MA 043

Strong spin-orbit interaction in graphene/WSe_2 probed at local scale — •Mikhail Fonin[1], Felix Förschner[1], Fabian Paschke[1], Lena Stoppel[1], Julia Tesch[1], Yuriy Dedkov[2,1], and Andor Kormányos[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Department of Physics, Shanghai University, 200444 Shanghai, China

Deposition on transition metal dechalcogenide substrates allow to considerably modify the strength of spin-orbit interaction (SOI) in graphene, as shown in recent magnetotransport experiments [1,2]. Here we investigate structure and electronic properties of graphene on tungsten diselenide (WSe_2) by means of scanning tunneling microscopy and spectroscopy. In external magnetic field local spectroscopic measurements reveal pronounced Landau level sequences on graphene/WSe_2. Detailed analysis of the obtained tunneling spectra shows that each Landau level is split into subpeaks, where the splitting strength grows with increasing magnetic fields. We attribute the splittings to the manifestation of substrate induced SOI in graphene. A comparison of the experimental splitting strengths with the those yielded by a spin-dependent low-energy effective Hamiltonian allows the determination of the SOI coupling constants for the Rashba term and the so-called spin-valley coupling term. Furthermore, we map the real space fluctuations of the SOI coupling strength which correlate with the variations of local electronic potential.

[1] Z. Wang *et al.*, Nature Comm. **6**, 8339 (2015). [2] Z. Wang *et al.* Phys. Rev. X **6**, 041020 (2016).

TT 43.9 Tue 12:45 MA 043

Origin of the band gap in Bi-intercalated graphene on Ir(111) — •Maxim Krivenkov[1,2], Dmitry Marchenko[1], Evangelos Golias[1], Jaime Sánchez-Barriga[1], Oliver Rader[1], and Andrei Varykhalov[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Albert-Einstein-Str. 15, D-12489 Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

We report a study of the structural and electronic properties of epitaxial graphene on Ir(111) intercalated with Bi. A novel structural phase of intercalated Bi was observed which is remarkably different from the phase reported earlier by Warmuth et al. [1]. This novel phase is more dense and, as seen by angle resolved photoemission spectroscopy, provides a quasifreestanding graphene with a very small band gap (∼180 meV) and nearly ideal band structure without band replicas and electronic hybridization with the substrate. Furthermore, we demonstrate the possibility of fine tuning (±30 meV) of the band gap width in the Dirac cone by varying concentration of Bi.

To determine a possible origin of the observed band gap in Dirac point, we analyze the effect of structural corrugation on graphene band structure as well as interference effects in photoemission from graphene. The band gap was concluded to be of trivial nature and is ascribed to the breaking of sublattice symmetry of graphene.

[1] Warmuth et al. in Phys. Rev. B 93, 165437 (2016)

TT 43.10 Tue 13:00 MA 043

Extremely flat band in bilayer graphene on silicon carbide — •Dmitry Marchenko[1], Daniil Evtushinsky[1], Vagelis Golias[1], Andrei Varykhalov[1], Thomas Seyller[2], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie GmbH — [2]Technische Universitat Chemnitz

In the present work we discover by angle-resolved photoemission an extremely flat band forming a strong 2D-extended van Hove singularity near the K point in bilayer graphene on SiC. We present a novel model for flat band formation in bilayer graphene and other bipartite lattices. Our finding implies that we can expect strong propensity towards a superconducting transition with high critical temperature.

TT 44: Focus Session: Frontiers of Electronic-Structure Theory: Correlated Electron Materials III (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Tuesday 10:30–13:00 Location: HL 001

TT 44.1 Tue 10:30 HL 001

Control and prediction of molecular crystal properties by multilevel strategies — •Jan Gerit Brandenburg — London Centre for Nanotechnology, Department of Physics and Astronomy, University College London, 20 Gordon Street, London, U.K.

Computational material science is a dynamic and thriving area of modern scientific research. Approaches based on the fundamental laws of quantum mechanics are now integral to almost any materials design initiative in academia and industry, underpinning efforts such as the Materials Genome initiative or the computational crystal structure prediction [1]. I will present a hierarchy of quantum chemical methods designed for this purpose, in particular targeting molecular crystals and their property prediction. The methods range from high-level diffusion Monte-Carlo (DMC) to London dispersion inclusive DFT, and thus, cover many orders of magnitudes in computational efficiency [2,3]. I will demonstrate the application to the 6^{th} blind test for organic crystal structure prediction. Comparisons to other state-of-the-art methods indicate both success and remaining challenges in the recent method developments [4].

[1] S. L. Price and J. G. Brandenburg, *Molecular Crystal Structure Prediction*; Elsevier Australia, **2017**.

[2] A. Zen, J. G. Brandenburg, J. Klimeš, A. Tkatchenko, D. Alfè, A. Michaelides, **2017**, *submitted.*

[3] J. G. Brandenburg, E. Caldeweyher, S. Grimme, *Phys. Chem. Chem. Phys.* **2016**, *18*, 15519.

[4] A. M. Reilly, et al. *Acta. Cryst. B* **2016**, *72*, 439.

TT 44.2 Tue 11:00 HL 001

Advances in first-principles and model spin Hamiltonian simulations of point defects in semiconductors for quantum sensors and computing — •Viktor Ivády — Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden — Wigner Research Center for Physics, Konkoly-Thege Miklós út 29-33, 1121 Budapest, Hungary

First principles simulations play a key role in understanding the physics of point defects in semiconductors, while model spin Hamiltonian approaches are traditionally used to interpret experimental spin dependent observations and describe the spin dynamics of point defects. The development of novel point defect applications, such as quantum bit (qubit) and single photon emitter applications for quantum information processing and quantum sensing, requires detailed understanding of spin-related couplings and addressability of localized defects states in the bath of delocalized electrons that calls for further development and implementation of theoretical tools. Here, I report on my contribution to this field that covers 1) first principles studies for identification of point defect based qubits and single photon emitters , 2) method development for the description of point defects with correlated electron states, 3) implementation of zero-field-splitting calculation for point defect based qubits, 4) development of model spin Hamiltonian approaches for the simulation of optical dynamic nuclear polarization process (ODNP) of point defects, and 5) spin dynamic simulation of existing point defect qubits. As an outlook, I discuss the requirements toward fully-ab initio point defect spin dynamic simulations.

TT 44.3 Tue 11:30 HL 001

Recent advances in first-principles modelling of correlated magnetic materials — •Yaroslav Kvashnin — Department of physics and astronomy, Uppsala University, BOX 516, 75120 Uppsala

Most of modern first-principles electronic structure studies of correlated materials are based on a combination of density functional theory and dynamical mean field theory (DFT+DMFT).

Addressing magnetic materials within DFT+DMFT has certain peculiarities. There are two recipes one can follow: either to account for magnetism within the DFT functional or to introduce it entirely within the self-energy. Both approaches have their flaws and advantages, which are well-known for DFT+U, but are not often discussed for DFT+DMFT. In my talk I will present a systematic comparison of the two methods and demonstrate the evidences favouring the use of non-polarised functionals.

Next, I will demonstrate how the obtained electronic structure information can be used to simulate finite-temperature magnetic properties in real materials. I employ a so-called two-step approach. First, I map the system on a Heisenberg model and extract the effective exchange parameters Jij's from DFT+DMFT. Then the atomistic spin dynamics simulations are used to simulate magnon spectra and predict the magnetic ordering temperatures.

I will demonstrate the power of such an approach by showing a direct comparison with available experimental data for a wide range of different materials.

TT 44.4 Tue 12:00 HL 001

A first-principles approach to hot-electron-induced ultrafast dynamics at metal surfaces — •Reinhard J. Maurer — Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL Coventry, UK

Low-lying electronic excitations in metals, so-called hot electrons, couple efficiently to molecular adsorbate motion. In doing so, they give rise to a number of curious experimental observations. This includes picosecond-scale energy loss of molecular adsorbate vibration, highly inelastic atomic and molecular scattering from metal surfaces, and light-assisted molecular desorption and chemical transformations, recently coined "hot-electron chemistry". In this talk, I will present a first-principles treatment of hot-electron-induced molecular dynamics based on Density Functional Theory that correctly captures the magnitude and mode-specificity of hot-electron mediated adsorbate-substrate energy transfer [1]. Utilizing our efficient all-electron local-orbital implementation of hot-electron-induced frictional forces based on Time-

Dependent Perturbation Theory, [2] I will show how we correctly capture vibrational relaxation in large-scale metal-mounted molecular catalysts as well as the energy loss and coupled electron-nuclear dynamics of small molecular adsorbates in both thermal and laser-heated conditions. [3] We scrutinize our approach in comparison to recent Sum-Frequency Generation (SFG) spectroscopy and molecular beam scattering experiments. [1] Phys. Rev. Lett. 116, 217601 (2016) ; [2] Phys. Rev. B 94, 115432 (2017); [3] Phys. Rev. Lett. 118, 256001 (2017);

TT 44.5 Tue 12:30 HL 001

Temperature effects in spin-orbit physics from first principles — •Bartomeu Monserrat — University of Cambridge, UK — Rutgers University, USA

The spin-orbit interaction drives a number of physical phenomena, including the band inversion in topological insulators and the spin splitting of electronic bands in inversion asymmetric crystals. In this work, we study the effects of finite temperature on such spin-orbit physics, including both thermal expansion and electron-phonon coupling effects [PRB 92, 184301 (2015)].

First, we describe the temperature dependence of the inverted gap in topological insulators. We find that increasing temperature reduces the topological gap in the Bi2Se3 family of materials, and we predict a temperature-induced topological phase transition in Sb2Se3 [PRL 117, 226801 (2016)].

Second, we study the temperature dependence of the spin splitting of electronic bands in both inversion symmetric and asymmetric crystals. We predict a dynamical spin splitting in centrosymmetric crystals and characterise the associated phenomenology in the cubic perovskite CsPbCl3 [arXiv:1711.06274]. In inversion asymmetric crystals, exemplified by the bismuth tellurohalides, we find that increasing temperature suppresses the static spin splitting arising from the Rashba effect [PRM 1, 054201 (2017)].

TT 45: Nano- and Optomechanics

Time: Tuesday 11:45–13:00 Location: H 0110

TT 45.1 Tue 11:45 H 0110

Nanomechanical characterization of the Kondo charge dynamics in a carbon nanotube — Karl J. G. Götz, Daniel R. Schmid, Felix J. Schupp, Peter L. Stiller, Christoph Strunk, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Suspended single wall carbon nanotubes are at cryogenic temperatures both extraordinary nanomechanical systems and clean and defect-free single electron devices. By measuring the gate voltage dependence of the transversal vibration frequency, the evolution of the charge on a quantum dot embedded in the nanotube can be evaluated.

We apply this technique to the limit of strong Kondo correlations between a nanotube quantum dot and its contacts. The current through the nanotube displays a clear odd-even pattern, with a zero-bias conductance anomaly at odd electron number. The charge on the quantum dot, however, shows no such odd-even pattern, and can be well modeled via sequential tunneling only. We conclude that the Kondo current is carried via virtual occupation of the quantum dot alone, without impact on the vibration. This is in excellent agreement with recent results coupling a nanotube to a coplanar waveguide resonator.

In addition, the simultaneous detection of charge and current signal allows us to compare the gate potentials where on one hand the current is maximal and on the other hand the charge in the quantum dot increases. Here, a distinct relative shift is observed, which decreases logarithmically with temperature, displaying the typical scaling of the Kondo effect.

TT 45.2 Tue 12:00 H 0110

Nano-electromechanics with High Impedance Superconducting Microwave Resonators and Aluminum Strings — •L. Rosenzweig[1,2], D. Schwienbacher[1,2,3], P. Schmidt[1,2,3], M. Pernpeintner[1,2,3], C. Utschick[1,2], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meißner-Insitut, Garching, Germany — [2]Physik-Departement, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

In optomechanics the interaction of light with a tailored phononic state is studied. Replacing optical cavities by superconducting microwave resonators defines the subfield of nano-electromechanics. These circuits benefit from high-Q microwave resonators and nanometer-sized mechanical resonators. A key challenge is the realization of a large electromechanical coupling exceeding the damping rate of the microwave cavity.

We present a hybrid system consisting of a high impedance superconducting microwave and a mechanical string resonator. Using finite element modeling, we discuss how the capacative electromechanical coupling rate (g_0) scales with the system geometry and how high impedance resonators allow to enhance g_0 compared to 50 Ω resonators. We show experimental data and compare the results to simulations. Moreover, high impedance resonators are compatible with superconducting qubits and provide hereby a pathway towards the preparation of quantum states in mechnical resonators.

TT 45.3 Tue 12:15 H 0110

Inductively Coupled Nano-Electromechanics in Flux Tunable Superconducting Resonators — •C. Utschick[1,2], P. Schmidt[1,2,3], D. Schwienbacher[1,2,3], L. Rosenzweig[1,2], N. Segercrantz[1,2], F. Deppe[1,2,3], A. Marx[1,2], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meißner-Insitut, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Nanosystems Initiative Munich, München, Germany

The field of cavity electromechanics provides a platform to study the light matter interaction on a quantum level. To observe quantum mechanical effects a strong photon-phonon coupling is desired, preferably exceeding the microwave (MW) resonator decay.

In this talk we present a hybrid system consisting of a magnetic field tunable superconducting MW resonator based on a dc-SQUID, where the latter encloses a nanomechanical string resonator. Here, the nanomechanical string displacement couples inductively to the MW resonator by changing the area of the dc-SQUID loop. The parameters of the system offer an inherently large photon-phonon coupling on the single excitation level and estimates for optimized parameters suggest a coupling rate on par with the decay rate of the MW resonator. We discuss the optomechanical coupling strength, present the device layout including its fabrication and show experimental data of the mechanical element and the superconducting circuit.

TT 45.4 Tue 12:30 H 0110

Magnetoelasticity of CoFe thin films — •Daniel Schwienbacher[1,2,3], Matthias Pernpeintner[1,2,3], Mathias Weiler[1,2], Eric R.J Edwards[4], Hans Nembach[4,5], Justin M. Shaw[4], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Germany — [2]Physik-Department, Technische Universität München, Germany — [3]Nanosystems Initiative Munich (NIM), Germany — [4]National Institute for Standards and Technology, Boulder, CO, USA — [5]JILA,University of Colorado, CO, USA

Ultra-low magnetic damping materials are essential for spintronic applications. Schoen *et al.*[1] recently discovered ultra-low magnetic damping in a metallic CoFe thin film. Magnetoelastic properties are known to critically affect spintronic devices, however, they are difficult to quantify in thin films. Here, we use SiN nanostring resonators loaded with CoFe thin films for measuring the magnetoelastic properties and find a saturation magnetostriction coefficient of $\lambda = (-27.2 \pm 4.1) \times 10^{-6}$ for 10 nm thick $Co_{25}Fe_{75}$ films. This opens exciting perspectives for combining magnetoelastics with ultra-low damping materials.

[1] Schoen et al., Nature Physics **12**, 839 (2016)

TT 45.5 Tue 12:45 H 0110

Multistability in vibrational lasing of a nanomechanical resonator — •Mattia Mantovani[1], Andrew Armour[2], Wolfgang Belzig[1], and Gianluca Rastelli[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, United Kingdom

We study the nonequilibrium dynamics of a nanomechanical resonator, realized by a suspended carbon nanotube in contact with two ferromagnetic leads. The nanotube hosts a quantum dot with two spin levels, which are coupled to the vibrational flexural modes via spin-vibration interaction [1-3]. We show that the system encodes a single-atom laser [4] in which the mechanical vibration plays the role of the cavity with frequency equal to the Zeeman splitting of the two levels. The lasing state can be achieved in the experimental range of the parameters for the spin-vibration coupling strength and magnetic polarization of the leads. Moreover, such a system has unique features which distinguish it from the single-atom model. In particular, we find regions with multistability of the resonator that are reflected in the zero-frequency current noise through the quantum dot.

[1] P. Stadler et al., Phys. Rev. Lett. 113, 047201 (2014).
[2] P. Stadler et al., Phys. Rev. B 91, 085432 (2015).
[3] A. Pályi et al., Phys. Rev. Lett. 108, 206811 (2012).
[4] Y. Mu, M. Savage, Phys. Rev. A 46, 5944 (1992).

TT 46: Poster Session: Graphene (joint session O/TT)

Time: Tuesday 18:15–20:30 Location: Poster A

TT 46.1 Tue 18:15 Poster A

The effects of defects and disorder on the electronic structure of graphene — •Piotr Kot[1], Jonathan Parnell[2], Sina Habibian[2], Pavel Ostrovsky[1], and Christian Ast[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of British Columbia, Vancouver, Canada

We use a real-space nearest neighbor tight-binding model to study the effect of defects on the band dispersion of graphene. We find that defects in graphene either generally preserve the canonical band structure, or disrupt it by separating the two cones creating an "elongated" Dirac point. This second structure greatly resembles the band dispersion of experimentally measured epitaxial graphene. By using a self-consistent T-matrix approximation we find the reason why defects create two distinctly different band structures, by showing that point defects are either resonant or non-resonant in graphene. Adding all these pieces together, we conclude on the cause of "elongation" in epitaxial graphene and the nature of the electronic structure in the "elongated" region finding that this region can not be considered a gap.

TT 46.2 Tue 18:15 Poster A

Spin and charge transport in quasi-freestanding epitaxial graphene grown by CVD — •Jantje Schommartz[1,2], Alexey Kaverzin[2], Christoph Tegenkamp[1], and Bart J. van Wees[2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland — [2]Physics of Nanodevices, University of Groningen, Netherlands

A promising route for the synthesis of homogeneous large-area graphene, suitable for standard device fabrication techniques, is the epitaxial growth of graphene on SiC. In the present work the growth is achieved by chemical vapor deposition (CVD) by using a hydrocarbon precursor for the carbon deposition on the Si-face of the SiC wafer. We study the quasi-freestanding epitaxial CVD graphene (CVD- QFEG) grown on 6H-SiC(0001) by contacting it with ferromagnetic Cobalt electrodes made by electron-beam lithography technique. By standard lock-in techniques we address the charge and spin transport properties independently by local and non-local measurement geometries. To the best of our knowledge, we detect for the first time spin signatures in transport measurements on CVD-QFEG. This study shows that the CVD-QFEG reveals striking differences in spin and charge transport properties compared to CVD epitaxial graphene. We attribute this to the influence of localized states arising from the buffer layer consistent with the measurements performed on epitaxial graphene grown by sublimation.

TT 46.3 Tue 18:15 Poster A

Preparation and characterization of high quality stacks of graphene/h-BN/graphite picked up by a mica substrate — •Michael Weimer[1], Tjorven Johnsen[1], Sayanti Samaddar[1], Peter Nemes-Incze[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [2]Centre of Energy Research, Institute of Technical Physics and Materials Science, Nanotechnology Department, 2D NanoFab ERC Research Group, Budapest, 1525, POB 49, Hungary

Graphene on h-BN provides a highly mobile two-dimensional electron system (2DES) which can be characterized by scanning tunneling microscopy (STM). In combination with transport experiments, a comparison of global and local properties of the sample is feasible. Such combination requires an ultra clean graphene surface and at least two electrical contacts. Therefore we present a dry and polymer free preparation technique by using a mica substrate. We exfoliate graphite on mica and subsequently pick up h-BN and graphene from a SiO_2/Si chip one after another. Shadow mask evaporation of gold provides clean contacting. Omitting wet chemical methods and polymers enables ultra clean surfaces with low impurity concentration.

TT 46.4 Tue 18:15 Poster A

Effect of the carbon 1s core hole on the polarized x-ray spectra of HOPG - theory and experiment — •Dominik Legut[1], Christine Jansing[2], Hans-Christoph Mertins[2], Andreas Gaupp[2], Peter M. Oppeneer[3], Heiko Timmers[4], and Hud Wahab[4] — [1]IT4Innovations Center, VSB-TU Ostrava, 17.listopadu 15, CZ 70833 Ostrava, Czech Republic — [2]FH Mnster, Stegerwaldstr. 39, D-48565 Steinfurt, Germany — [3]Dept. of Physics and Astronomy, Box 530, S-751 21 Uppsala, Sweden — [4]Univ. of New South Wales Canberra, Australia

Bandstructure calculations using the WIEN2K code have been performed to study the polarized x-ray reflection spectra of highly oriented pyrolytic graphite (HOPG). Varying the amount of the included 1s core hole we find that the DFT calculations provide good agreement with experimentally obtained x-ray spectra [1]. The change of x-ray polarization upon reflection of linearly polarized synchrotron radiation can be become as huge as a birefringent rotation of polarization plane of up to 140°, and the polarization changes from linear to nearly fully circular polarization. The best calculated results are obtained for a partial core hole per excitation. The distinct contributions from the A and B sites of HOPG to the spectra are discussed as well.

Refereces: 1. C. Jansing et al, PRB 94, 045422 (2016).

This work was supported by CSF grant No. 17-27790S and Path to Exascale project No. CZ.02.1.01/0.0/0.0 /16_013/0001791.

TT 46.5 Tue 18:15 Poster A

Polycyclic molecules with geometrical frustration via pyrolysis on a metal — •Alexandre Artaud[1], Laurence Magaud[2], Kitti Ratter[3], Bruno Gilles[3], Valérie Guisset[2], Philippe David[2], Jose I. Martinez[4], Jose A. Martin-Gago[4], Claude Chapelier[5], and Johann Coraux[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts Universität zu Kiel, Germany — [2]CNRS, Institut Néel, Grenoble, France — [3]Grenoble INP, SIMAP, Grenoble, France — [4]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid-CSIC, Madrid, Spain — [5]CEA, INAC, PHELIQS, Grenoble, France

The geometry of molecules is a key to several of their properties. In graphene fragments, electron delocalization from one carbon sublattice to the other is frustrated for molecular shapes breaking the balance of sublattices. Optical, electronic, and magnetic properties emerge in this case, but the synthesis of such molecules remains challenging.

Here, a pyrolysis reaction catalysed by the surface of rhenium is investigated using scanning tunneling microscopy and density functional theory. This reaction known to form graphene is found to also yield graphene fragments consisting of well-defined, zigzag-edged polycyclic molecules, some of which have sublattice imbalance. However, they are found in metastable configurations, which is interpreted as a kinetic rather than thermodynamic control of their formation. Hence, metastable molecules are expectedly ubiquitous in graphene growth, and deleterious to achieve perfect graphene. Pyrolysis is conversely a promising route towards molecules with sought-after properties.

TT 46.6 Tue 18:15 Poster A

Scanning Tunneling Microscopy and spectroscopy of Au islands on graphene/Rh(111) — •Anne Holtsch and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken

Using scanning probe techniques we investigated how graphene (gr) electronically interacts with substrates in the presence of metallic islands on top of the gr layer. In the case of rhodium as a substrate, the band structure is significantly altered with respect to freestanding graphene due to the hybridization of its d orbital with the pz orbital of gr [1]. Using scanning tunneling spectroscopy (STS) the influence of Au Islands on top of the gr was investigated. The islands were deposited by in-situ evaporation. Subsequently their relative orientation with respect to the gr lattice was observed by scanning tunneling microscopy (STM). The STS measurements on and in the vicinity of the islands show locally varying electronic properties of the system. The presence of gold induces the opening of a band gap. At the same time there is an increase in conductivity, compared to the conductivities of gold and gr. Measurements show that the increase in conductivity is restricted to that area of the islands which adjoins to the gr. In this case both gr and gold contribute to a increase of the measured tunnel current.

[1] A. Holtsch, T. Euwens, B. Uder, S. Grandthyll, F. Müller, and U. Hartmann, Surf. Sci. 668 (2018) 107.

TT 46.7 Tue 18:15 Poster A

Landau quantization in a graphene monolayer on WSe_2 and $NbSe_2$ — •Felix Förschner[1], Lena Stoppel[1], Fabian Paschke[1], Julia Tesch[1], Yuriy Dedkov[2,1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Deutschland — [2]Department of Physics, Shanghai University, 200444 Shanghai, China

By depositing graphene on transition metal dichalcogenides (TMDs), it is possible to alter the electronic properties of graphene [1]. Here we focus on the fabrication of graphene on WSe_2 and $NbSe_2$, which was successfully performed by an adapted wet chemical transfer process. By means of low-temperature scanning tunneling microscopy we investigate the atomic structure of graphene and observe different Moiré structures indicating a successful transfer of graphene onto the TMD. In an external magnetic field, Landau level sequences are observed giving access to the electronic properties of graphene, i.e. doping level, Fermi velocity etc. Detailed analysis of the obtained tunneling spectra shows that each Landau level is split into subpeaks, where the pronounced splitting strength grows with increasing magnetic field. The magnitude of the observed splitting indicates an enhanced spin-orbit interaction strength in graphene due to the presence of the TMD substrate.

[1] Z. Wang *et al.*, Nature Comm. **6**, 8339 (2015).

TT 46.8 Tue 18:15 Poster A

Dislocations in bilayer graphene — •Florian Wullschläger, Konstantin Weber, and Bernd Meyer — Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg

Dislocations, i.e. one-dimensional line defects, are the main carriers of plastic deformation in 3D crystalline solids. In a recent TEM study it was shown that dislocations even exist in materials as thin as two graphene layers [1]. Using atomistic simulations based on the registry-dependent potential of Kolmogorov and Crespi [2] we show that the properties of dislocations in quasi-2D crystals differ significantly from their 3D counterparts. The step components of the dislocations give rise to a pronounced buckling of the bilayer in order to release strain energy. All dislocations split into equally-spaced partials due to the absence of a stacking fault energy, a peculiar property of bilayer graphene. Finally, in 2D materials the strain energy induced by a dislocation does not diverge with sample size as in 3D, but remains finite. In addition to this structural characterization of 2D dislocations we will show first results on how dislocations move in bilayer graphene and how they are pinned at lattice defects.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H.B. Weber, B. Meyer, E. Spiecker, Nature **505** (2014) 533.
[2] A. Kolmogorov, V. Crespi, Phys. Rev. B **71** (2005) 235415.

TT 46.9 Tue 18:15 Poster A

Microscopic investigations of graphene-nickel interactions — •Philip Schädlich, Florian Speck, Adrian Schütze, and Thomas Seyller — Professur für Technische Physik, TU Chemnitz, Reichenhainer Straße 70, D-09126 Chemnitz

In order to realize possible applications of graphene in electronics, it is important to understand the properties of graphene - metal contact interfaces. In this study we investigate the impact of nickel as possible contact material on the underlying graphene.

Graphene samples are grown by sublimation of Si atoms from a 6H-SiC(0001) substrate in Ar atmosphere at ambient pressure [1]. The local graphene coverage is probed by photoemission electron microscopy as well as low-energy electron microscopy (LEEM) and reflectivity (LEER) spectra. The deposition process of nickel is monitored *in-situ* via LEEM. After deposition, LEER spectra indicate a change of the work function in the covered areas while the characteristic interlayer states [2] stay unchanged. The morphology of the deposited nickel layer is revealed by atomic force microscopy, while the thickness was determined by x-ray photoemission spectroscopy. Angle-resolved photoemission spectroscopy confirms an unchanged electronic band structure with the Dirac point located 0.4 eV below the Fermi energy, which is close to values found for bare monolayer graphene on the 6H-SiC(0001) surface.

[1] K. V. Emtsev et al., Nature Materials 8, 203 (2009).
[2] N. Srivastava et al. Phys. Rev. B 87, 245414 (2013).

TT 46.10 Tue 18:15 Poster A

Development of a high-dimensional neural network potential for hydrogen atoms at graphene. — •Sebastian Wille[1,2], Marvin Kammler[2], Martín L. Paleico[3], Jörg Behler[3], Alec M. Wodtke[1,2], and Alexander Kandratsenka[2] — [1]Institute for Physical Chemistry, Georg-August University Göttingen, Germany — [2]Department of Dynamics at Surfaces, Max Planck Institute for Biophysical Chemistry, Göttingen, Germany — [3]Theoretical Chemistry, Georg-August University Göttingen, Germany

To fully understand atom-surface interactions, the availability of an accurate full-dimensional potential energy surface (PES) is crucial. High-dimensional neural network potentials have been shown to provide very accurate PESs for a wide range of systems. Here, we develop a neural network potential for H-atom scattering from a graphene sheet. We fit the potential to density functional theory energies calculated on-the-fly in *ab initio* molecular dynamics simulations. We find that the procedure can reliably describe H at graphene, which makes it possible to effectively simulate the scattering for this system in a large range of incidence conditions.

TT 46.11 Tue 18:15 Poster A

Influence of atomic-scale dopants on the transport properties of graphene on SiC — •Anna Sinterhauf[1,2], Philip Willke[1], Georg Traeger[1], Davood Momeni Pakdehi[3], Klaus Pierz[3], Hans Werner Schumacher[3], Hans Hofsäss[4], and Martin Wenderoth[1,2] — [1]IV. Physikalisches Institut, Universität Göttingen, Germany — [2]International Center for Advanced Studies of Energy Conversion (ICASEC), Universität Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt Braunschweig, Germany — [4]II. Physikalisches Institut, Universität Göttingen, Germany

Tailoring the electronic structure of graphene by substitutional doping often additionally changes its transport properties. In order to study the impact of atomic-scale dopants on electron transport, graphene samples were prepared by polymer-assisted sublimation growth (PASG) [1] and doped with nitrogen atoms by low energy ion beam implantation [2]. Using highly resolved scanning tunneling microscopy and potentiometry, we determined the dopant density as well as the local sheet resistance on the nanometer scale. Moreover, the defect resistance at substrate steps was evaluated. Subsequently, the mobility and the mean free path length were estimated and compared for pristine and nitrogen doped PASG graphene. Furthermore, we were able to quantify the impact of nitrogen dopants on the charge transport, which introduce an additional short-range scattering process along with long-range Coulomb scattering. [1] Kruskopf et al., 2D Materials 3, 041002, 2016 [2] Willke et al., Nano Lett. 15(8), 2015

TT 46.12 Tue 18:15 Poster A

Variation of the local transport properties of epitaxial graphene caused by the stacking order of 6H-SiC — •Georg Traeger[1], Anna Sinterhauf[1,2], Davood Momeni Pakdehi[3], Philip Schädlich[5], Florian Speck[5], Johannes Aprojanz[4,5], Thomas Seyller[5], Hans-Werner Schumacher[3], Christoph Tegenkamp[4,5], Klaus Pierz[3], and Martin Wenderoth[1,2] — [1]IV. Physical Institute, University of Göttingen, Göttingen, Germany — [2]Internatonal Center for Advanced Studies of Energy Con-

version (ICASEC), University of Göttingen, Göttingen, Germany — [3]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [4]Institute for Solid State Physics, University of Hannover, Hannoner, Germany — [5]Institute of Physics, Chemnitz, Chemnitz, Germany

We present a scanning tunneling potentiometer (STP) study on graphene on silicon carbide (6H-SiC(0001)) grown by polymer assisted sublimation growth (PASG). The high homogeneity of the buffer layer, grown by PASG allows for an investigation of the substrate graphene interaction. [1] Highly resolved STP measurements revealed two distinct sheet resistances, which occur in a characteristic pattern. We identified this pattern with the 6H stacking sequence of the substrate and assigned the graphene terraces to different substrate terminations. Park et al. found that these terminations have different polarization charges [2]. According to this findings, we attribute the termination with the highest polarization charge to the graphene sheet with the highest conductivity.

[1] Pakdehi et al., Submitted [2] Park et al., Phys. Rev. B, 1995

TT 46.13 Tue 18:15 Poster A

Ru - mediated growth of graphene on SiC for radiation sensing application — •Rajesh Kumar Chellappan, Simon Cooil, Marina Jorge, Håkon Røst, and Justin Wells — Center for Quantum Spintronics, Norwegian University of Science and Technology, Norway

Graphene has been proposed as a suitable candidate for photo/radiation sensors primarily because of its exceptional electronic properties. However, this advantage has been difficult to realize because of the problems associated with the preparation of high quality graphene on dielectric/semiconductor substrates. Therefore, this study focuses on addressing epitaxial ruthenium mediated graphene growth on silicon carbide and the subsequent interface oxidation using soft X-ray photoemission spectroscopy (SXPS). The growth of graphene and formation of ruthenium silicide was investigated by systematic annealing of ruthenium (~1nm) deposited on silicon carbide samples in vacuum at temperatures ranging from 450°C to 700°C. The interlayer oxidation was achieved by exposing the sample at 460°C to oxygen partial pressure of 9.5*10-7 mbar for 1 hour to form a graphene/dielectric/silicon carbide device structure.

TT 47: Frustrated Magnets - Iridates and Fe-based Materials

Time: Wednesday 9:30–12:45 Location: H 0104

TT 47.1 Wed 9:30 H 0104

Dimer formation in hyperhoneycomb iridate β-Li_2IrO_3 under pressure — •Aleksandra Krajewska[1,2], Tomohiro Takayama[1,2], Alexandra Gibbs[3], Craig Bull[3], and Hidenori Takagi[1,2] — [1]1 Institut für Funktionelle Materie und Quantentechnologien, University of Stuttgart, Germany — [2]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [3]ISIS Facility, Rutherford Appleton Laboratory, Didcot, UK

Honeycomb-based iridates α, β-A_2IrO_3 (A = Li, Na) are attracting attention because the magnetic coupling between $J_{\text{eff}} = 1/2$ isospins renders bond-dependent ferromagnetic interaction, providing a possible route for Kitaev quantum spin liquid (QSL). However, these materials order at low temperatures due to the presence of other magnetic couplings. β-Li_2IrO_3 shows order below 38 K. With increasing pressure, the magnetic order vanishes above 2 GPa and structural transition occurs at around 4 GPa. The driving force of the structural transition and the relevance to the QSL behaviour remains unclear. We studied the crystal structure of β-Li_2IrO_3 under pressure in detail by neutron diffraction. Above 4 GPa one of the Ir-Ir distances in the hyperhoneycomb network becomes much shorter than the others. The difference between them is 15%, similar to that in honeycomb Li_2RuO_3 with spin-singlet dimers, suggesting dimer formation in β-Li_2IrO_3. We argue that the lattice tuning by pressure modifies the balance of multiple magnetic couplings and leads to the likely destruction of $J_{\text{eff}} = 1/2$ as a consequence of dimerisation.

TT 47.2 Wed 9:45 H 0104

Coexistence of static and dynamic magnetism in pressurized β-Li_2IrO_3 — •Mayukh Majumder[1], Rudra Sekhar Manna[1], Gediminas Simutis[2], Jean-Christophe Orain[2], Tusharkanti Dey[1], Friedrich Freund[1], Rustem Khasanov[2], Pabitra Kumar Biswas[3], Alexander Tsirlin[1], and Philipp Gegenwart[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]PSI, Villigen, Switzerland — [3]ISIS, Rutherford Appleton Laboratory, United Kingdom

Frustrated systems with Kitaev-type exchanges show long-range magnetic ordering instead of quantum spin liquid state because of the presence of other exchanges. Interestingly, theoretical studies suggest the possibility of tuning β-Li_2IrO_3 towards a QSL state by applying pressure. In order to establish the temperature-pressure phase diagram in β-Li_2IrO_3 we have used magnetization, thermal expansion, magnetostriction and μSR measurements. Our comprehensive study established - i) a weak increase of ordering temperature (T_{MO}) up to the pressure of about 14 kbar without showing any detectable change in the magnetic moment and in the nature of ordered state compared to ambient pressure, ii) above 14 kbar, T_{MO} sharply drops showing a first-order like behavior, iii) magnetic phase separation occurs above 14 kbar where static and dynamic spins coexist.

TT 47.3 Wed 10:00 H 0104

NMR studies on the single crystalline Na_2IrO_3: A model system to realize Kitaev interaction — •R. Sarkar[1], Z. Mei[2], A. Ruiz[3,4], H.-H. Klauss[1], J. G. Analytis[3,4], and N. J. Curro[2] — [1]Institute of Solid State and Materials Physics, Technical University of Dresden, 01062 Dresden, Germany — [2]Department of Physics, University of California, Davis, California 95616, USA — [3]Department of Physics, University of California, Berkeley, California 94720, USA — [4]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

We present results of ^{23}Na nuclear magnetic resonance (NMR) measurements on single crystalline Na_2IrO_3, a possible candidate to realize Kitaev spin model on the honeycomb lattice. The NMR shifts ($^{23}K(\%)$), that is the measure of local susceptibility, have been studied in two crystallographic orientations. The NMR shifts reflect strong anisotropic behavior similar to the bulk susceptibility. However, below a temperature $T^* \sim 50$ K, the shift deviates from the bulk susceptibility. This anomalous behavior may be related to the exchange anisotropic bond interaction connected to the magnetic frustration. In contrast to the Knight shift, the spin-lattice relaxation rate $^{23}(1/T_1)$ is isotropic in the paramagnetic state and exhibits a strong peak at T_N. Deep in the ordered state, $^{23}(T_1T)^{-1}$ approaches a constant value as a function of temperature, suggesting the presence of significant dynamics and/or the band of excitations associated with the close proximity of quantum spin liquid ground state of Na_2IrO_3.

TT 47.4 Wed 10:15 H 0104

Tuning the Magnetism in Honeycomb Magnets — •Sebastian Selter[1], Esther Jarossay[1,2], Anja U. B. Wolter[1], Saicharan Aswartham[1], and Bernd Buechner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We present a magnetic phase diagram of $Na_2(Ir_{1-x}Pt_x)O_3$, where the magnetic order is systematically suppressed by Pt substitution. Further, preliminary data on crystal growth and magnetic behavior of $Na_2Co_2TeO_6$ and $Na_3Co_2SbO_6$ will be discussed.

Na_2IrO_3 possess a frustrated honeycomb lattice, similar to $RuCl_3$ (Ir, Ru: d^5) and $Na_2Co_2TeO_6$ and $Na_3Co_2SbO_6$ (Co: d^7). These compounds are proposed to be the best suited candidates to host a Quantum spin liquid (QSL) state. However, all these compounds show a zig-zag antiferromagnetic order at low temperatures, still indicating strong bond dependent Kitaev-type interactions. Recent experiments have shown that this magnetic order is extremely fragile. In Na_2IrO_3 already 5% of Ru substitution on the Ir site is sufficient to suppress the magnetic order, while $RuCl_3$ shows a field induced QSL state.

We address the question, how the magnetic ground state of Na_2IrO_3 is affected by dilution of the magnetic Ir honeycomb lattice with nonmagnetic Pt.

TT 47.5 Wed 10:30 H 0104

Robust spin liquid state in honeycomb iridate $D_3LiIr_2O_6$ against large isotope effect — •Tomohiro Takayama[1,2], Kentaro Kitagawa[3], Yosuke Matsumoto[1], Kenji Ishii[4], Sebastian

Bette[1], Robert Dinnebier[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Insitute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Stuttgart, Germany — [3]University of Tokyo, Tokyo, Japan — [4]QST SPring-8, Hyogo, Japan

Honeycomb iridates recently appeared as a possible materialization of Kitaev spin liquid. All hitherto-known candidate materials display a magnetic order at low temperatures likely due to the presence of additional magnetic interactions. We recently succeeded in realizing a quantum spin liquid state in proton-exchanged honeycomb iridate $H_3LiIr_2O_6$. $H_3LiIr_2O_6$ shows a large negative Weiss temperature θ_{CW} ∼ -105 K, and it is not clear yet whether the Kitaev coupling is indeed a prime driving force for the spin liquid state or not.

We also synthesized an isotropic compound $D_3LiIr_2O_6$. Although $D_3LiIr_2O_6$ crystallizes basically in the same crystal structure with $H_3LiIr_2O_6$, it shows a large structural isotope effect with the elongated *c*-axis. This results in a substantial change in magnetic couplings; the antiferromagnetic couplings are enhanced as evidenced by θ_{CW} ∼ -168 K. Nevertheless, $D_3LiIr_2O_6$ retains a spin-liquid state. We will discuss the differences from $H_3LiIr_2O_6$ and details of their spin-liquid state.

TT 47.6 Wed 10:45 H 0104

Synthesis and magnetic properties of Double Perovskites with Ir(IV)-states — •Michael Vogl[1], Anja Wolter[1], Sabine Wurmehl[1], Saicharan Aswartham[1], and Bernd Büchner[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW Dresden — [2]Technische Universität Dresden

The magnetism of strongly spin-orbit coupled 5d-systems is a rapidly evolving topic with many open questions. In particular, Iridates are in focus for theoretical and experimental investigations.

The Double Perovskite structure, with the general notation $A_2BB'O_6$, allows the tuning of magnetic properties by doping and incorporation of various magnetic ions and sublattices. In general, Double Perovskite Iridates offer the possibility to study the magnetic exchange interaction of spin-orbit coupled Ir-ions in detail. Furthermore the B-sublattice of a Double Perovskite can be viewed as a geometrically frustrated fcc-lattice. Hence, the magnetism of these materials also touches the intriguing field of frustrated magnetism.

In this talk we present new Double Perovskite Iridates. We focus on the realization of a fcc-lattice of Ir(IV) within the Double Perovskite structure. Furthermore the interactions of Ir(IV) with rare earth ions on the A-site is examined. Particularly interesting properties were found for Nd_2ZnIrO_6. In this contribution, we present a magnetic phase diagram of this compound.

TT 47.7 Wed 11:00 H 0104

Magnetic ordering in the mixed valent iridate $Ba_3LuIr_2O_9$ — •Tusharkanti Dey[1], Mayukh Majumder[1], Jean-Christophe Orain[2], Anatoliy Senyshyn[3], Philipp Gegenwart[1], and Alexander Tsirlin[1] — [1]EP-VI, EKM, University of Augsburg, Germany — [2]Paul Scherrer Institut, Villigen PSI, Switzerland — [3]FRM II, TU Munich, Germany

Mixed valent iridates with the general formula $Ba_3MIr_2O_9$ (M is a trivalent ion) contain face-sharing Ir_2O_9 bi-octahedra with Ir-Ir dimers along the crystallographic c-axis. In these materials, Ir has a single crystallographic site with an average charge state of +4.5. The two Ir sites within the dimer share 9 electrons among them resulting in S=1/2 moments per dimer [1]. These dimers form a triangular lattice in the crystallographic ab-plane and a buckled honeycomb lattice between the neighboring planes. We have recently synthesized polycrystalline samples of $Ba_3M^{3+}Ir_2^{4.5+}O_9$ (M=In,Lu) and studied their structural and magnetic properties. In this presentation, we will discuss the results of our neutron diffraction, magnetic susceptibility, heat capacity and μSR measurements suggesting magnetically ordered ground state for $Ba_3LuIr_2O_9$ below 5.5 K and compare with the sister compound $Ba_3InIr_2O_9$ showing persistent spin dynamics and the absence of long range ordering down to 20 mK [1].
[1] T. Dey *et. al.*, Phys. Rev. B **96**, 174411 (2017)

15 min. break.

TT 47.8 Wed 11:30 H 0104

Low temperature heat capacity measurements on the mixed-valence iridate $Ba_3InIr_2O_9$ — •Sebastian Bachus, Yoshifumi Tokiwa, Tusharkanti Dey, Mayukh Majumder, Alexander Tsirlin, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Frustrated magnetism can give rise to new exotic states. A prominent example are quantum spin liquids (QSL) which show no ordering of their magnetic moments even at zero temperature. Promising candidates for a QSL ground state are materials with highly frustrated magnetic moments e.g. on a kagomé or triangular lattice.
Recently the family of mixed-valence iridates has been proposed as an alternative material class for the search of QSL. One example is $Ba_3InIr_2O_9$, where mixed-valence Ir_2O_9 dimers with $Ir^{4.5+}$ are formed, sharing one unpaired electron per dimer [1]. Here, we report low temperature measurements of heat capacity. Our data show no long-range ordering as well as continuos excitations down to at least 80 mK, which strongly indicates a gapless QSL ground state. This work has been funded by the German Science Foundation through TRR 80.
[1] T. Dey *et al.*, Phys. Rev. B 96, 174411 (2017).

TT 47.9 Wed 11:45 H 0104

Magnetism in the fcc lattices of K_2IrX_6 (X=Cl, Br) crystals: Candidate j_{eff}=1/2 Mott insulators — •Nazir Khan[1], Danil A. Prishchenko[2], Vladimir G. Mazurenko[2], Anton Jesche[1], and Alexander A. Tsirlin[1] — [1]EP VI, EKM, Augsburg University, 86159 Augsburg, Germany — [2]Ural Federal University, Mira Str. 19, 620002 Ekaterinburg, Russia

Potassium hexahaxoiridates $K_2Ir^{4+}X_6$ (X= Cl, Br) are fascinating systems to explore the physics of spin-orbit coupled j_{eff}=1/2 moments on the geometrically frustrated fcc lattice. The structural symmetry of the system and the spin-orbit coupling in the Ir^{4+} ions allow different anisotropic exchanges besides the isotropic Heisenberg exchange (J_H) such as the Kitaev (J_K) and off-diagonal (J_γ) exchanges to determine its magnetic ground state. Transport measurement shows highly insulating electronic nature with charge gaps of 0.7 eV and 1.0 eV for the K_2IrCl_6 and K_2IrBr_6 compounds, respectively. Magnetization and heat capacity measurements show paramagnetic to antiferromagnetic phase transitions with Néel temperatures T_N= 3.1 K and 10.2 K for the K_2IrCl_6 and K_2IrBr_6 crystals, respectively, with effective moments close to that predicted theoretically for the j_{eff}=1/2 moment. The field dependence of the magnetization along different crystallographic directions suggests intricate nature of the exchange interactions. The structural and the magneto-electronic phase diagrams show strong dependence on the nature of the halogen ion X^- (Cl^- and Br^-). Magnetism in K_2IrCl_6 has been discussed in terms of a Heisenberg-Kitaev model.

TT 47.10 Wed 12:00 H 0104

The magnetic phase diagram and short-range magnetic order in γ-Li_2FeSiO_4 — •Martin Jonak[1], Fabian Billert[1], Sisi Gu[1,2], Christoph Neef[1], Waldemar Hergett[1], Johannes Werner[1], Changhyun Koo[1], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, University of Heidelberg, Heidelberg, Germany — [2]University of Science and Technology of China, Hefei, China

We report thermal expansion, specific heat, and high-frequency electron spin resonance (HF-ESR) studies up to 17 T, as well as pulsed-field magnetisation data on a γ-Li_2FeSiO_4 (space group *Pmnb*) single crystal. The data imply the onset of long-range antiferromagnetic order at T_N = 17.0(5) K. The uniaxial pressure dependencies are derived from our uniaxial thermal expansion data. At low temperatures, the saturation field for B||easy axis amounts to 33 T. In addition, there are several field-induced anomalies suggesting competing magnetic phases. The antiferromagnetic resonance modes exhibit significant zero-field splitting associated with magnetic anisotropy. At higher temperatures, the HF-ESR data imply the evolution of local magnetic fields at least up to 100 K, and are accompanied by sizeable magnetostriction well above T_N.

TT 47.11 Wed 12:15 H 0104

Interplay of structure and magnetism in frustrated intermetallic AFe_4X_2 systems — Inga Kraft[1,2], Katharina Weber[1,2], Christoph Bergmann[1], Christoph Geibel[1], and •Helge Rosner[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Technical University of Dresden

Due to their complex and versatile behavior frustrated systems present great experimental and theoretical challenges. Even slight perturbations induce instabilities in such systems and prompt the emergence of unusual phenomena. The intermetallic AFe_4X_2 compounds (A=Sc,Y,Lu,Zr; X=Si,Ge) are suggested to cover the whole regime from frustrated AFM order up to an AFM quantum critical point.

Our DFT calculations exhibit a strong interplay of structure and magnetism. However, according to our calculations, the structural and the magnetic phase transition can be considered as independent in reasonably good approximation. We discuss the influence of the A and X site atoms on the strength of magnetic interactions and the size of structural distortion.

TT 47.12 Wed 12:30 H 0104

Role of single-ion anisotropy in Fe^{3+}-based frustrated magnets — •Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Transition-metal ions with the half-filled d-shell and the high-spin d^5 electronic configuration are magnetically nearly isotropic. Here, using density-functional calculations juxtaposed with the experimental data from thermodynamic measurements and neutron diffraction, I will argue that such d^5 ions still feature a non-negligible single-ion anisotropy that prevails over intersite anisotropy terms and drives multiple magnetic transitions in frustrated magnets based on Fe^{3+}. The talk will cover Fe-based pyroxene compounds, where frustrated interchain interactions trigger a collinear spin-density-wave phase separating the ground-state helical order from the paramagnetic state. I will further report the sequence of magnetic transitions in the Cairo antiferromagnet $Bi_4Fe_5O_{13}F$, where competing single-ion anisotropies introduce two flavors of orthogonal order separated by a collinear phase. Despite their small size, typically less than 1% of the isotropic exchange couplings, the single-ion terms play pivotal role for the magnetically ordered states of Fe^{3+} compounds.

TT 48: Focus Session: Exploiting Spintronics for Unconventional Computing (joint session MA/TT)

Over the past century, the miniaturization of electronics has improved commensurately to the growth in computational power following an empirical relationship known as "Moore's law", an observation that microprocessor performance doubles every 18 months. It has now become clear that this trend will unlikely continue in the future due to limits both in the downscaling of transistors as well as the fundamental throughput of data between CPU and memory elements in traditional Von Neumann computer architectures. A completely new path forward has however been offered by bioinspired approaches to computation which attempt to capture the intrinsic parallelism and energy efficiency exhibited by the animal brain. The past two decades have in fact seen the flourishing of digital machine learning and deep neural network techniques to process data intensive tasks ranging from image recognition to AI development. The next frontier will consist of further optimizing these approaches by designing physical devices capable of implementing these functional principles analogically. Advances in nanomagnetism and spintronics have assembled a versatile toolbox of electrically controllable materials and phenomena whose applications not only integrate seamlessly within current CMOS architectures but also present a radical new horizon for the evolution of device construction and development. The goal of this focus session is to construct a comprehensive picture of the state-of-the-art of spintronic applications to unconventional computing paradigms such as Boltzmann Machines, Neural Network, Probabilistic and Reservoir Computing. The talks will bring together leading scientist in the rapidly evolving field of spintronic computing to highlight the roles that thermally susceptible magnetization dynamics, exotic magnetic textures, frustrated systems and spin waves can play in shaping the computing devices of tomorrow.

Organized by: Daniele Pinna, Karin Everschor-Sitte (U. Mainz)

Time: Wednesday 9:30–12:15 Location: H 1012

Invited Talk TT 48.1 Wed 9:30 H 1012

Control of Mesoscopic Magnetism for Computation — •Laura Heyderman — Laboratory for Mesoscopic Systems, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — Laboratory for Multiscale Materials Experiments, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

To exploit mesoscopic magnetism in computation, it is necessary to control the magnetic states with an external stimulus. In hybrid mesoscopic structures with two different ferromagnetic layers, the static and dynamic behaviour results from the mutual imprint of the magnetic domain configurations, which can be exploited to create a nanoscale switch for the magnetisation [1]. With multiferroic composites, an electric field can be used to induce uniform magnetization rotation in single domain submicron ferromagnetic islands grown on ferroelectric single crystal [2]. In artificial spin ice [3], which are arrays of coupled nanomagnets, emergent magnetic monopoles can be manipulated in a magnetic field [4]. For device applications, the additional control can be gained by modifying the anisotropy of the individual magnets. Such anisotropy engineering can also be used to control the chirality of vortex states in hexagonal rings of nanomagnets [5]. Finally, one can modify the geometry of an artificial spin ice to display dynamic chirality where the average magnetization rotates in unique sense during thermal relaxation [6]. [1] M. Buzzi et al. PRL (2013) [2] P. Wohlhüter et al. Nat. Commun. (2015) [3] L.J. Heyderman and R.L. Stamps, JPCM (2013) [4] E. Mengotti et al. Nature Phys. (2011) [5] R. Chopdekar et al. New J. Phys (2013) [6] S. Gliga et al. Nat. Mater. (2017)

TT 48.2 Wed 10:00 H 1012

Phase domain nucleation and growth investigated in nanofabricated FeRh — •Rowan Temple[1], Jamie Massey[1], Trevor Almeida[2], Kayla Fallon[2], Stephen McVitie[2], Thomas Moore[1], and Christopher Marrows[1] — [1]University of Leeds, Leeds, UK — [2]University of Glasgow, Glasgow, UK

The binary alloy FeRh with B2 (CsCl) chemical ordering displays a magnetostructural phase transition at an unusually high temperature of 350 K. Heating through this point the material undergoes an antiferromagnetic (AF) to ferromagnetic (FM) transition, this is accompanied by a 1% volume expansion in the crystal lattice. Being thermodynamically first order in nature, the transition is hysteretic with metastable states coexisting within the material close to the transition temperature. Using nanofabricated epitaxially grown films of FeRh we have examined the effects of rapid thermal heating of this material beyond its equilibrium state. We find decay into equilibrium state is exponential independent of temperature, commensurate with a purely nucleation rather than domain growth driven transition. We have further investigated size dependence of the transition through PEEM imaging and find edge nucleations are key to the transition in a patterned device and lower the expected transition temperature. This understanding will be used to enable the use of patterned FeRh for unconventional computing techniques.

Invited Talk TT 48.3 Wed 10:15 H 1012

Spin waves for unconventional computing and data processing — •Philipp Pirro, Thomas Brächer, and Andrii Chumak — Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Straße 56, 67663 Kaiserslautern

Spin waves, the collective excitations of the spin lattice of a magnetic material and their quanta, magnons, show a large variety of linear and nonlinear wave phenomena. They constitute a flow of spin angular momentum which opens a new sub-field of spintronics: magnon spintronics, where information is transferred and processed using magnons including a coupling to electron-based spintronic circuits.

In my presentation, I will first review different computing approaches based on spin waves and discuss the advantages and challenges of an interference-based logic. Next, I will present a selection of the experimentally realized macroscopic prototypes for spin-wave based logic like the majority gate and the magnon transistor. A downscaling of more than three orders of magnitude of these prototypes is required to compete with conventional CMOS technology. Therefore, I will discuss new features associated with the miniaturization like strong quantization effects as well as ways to interconnect to conventional spintronic circuits. Exemplarily, I will present different nanoscopic magnonic devices which use linear and nonlinear effects like magnonic wake-up receivers and nano-transistors.

15 minutes break

Invited Talk TT 48.4 Wed 11:00 H 1012

p-bits, p-transistors and p-circuits — •Kerem Camsari — Purdue University

Conventional logic/memory devices are built out of deterministic units such as MOS transistors, or nanomagnets with energy barriers in excess of 40 kT. We show that unstable, stochastic units which we call "p-bits" can be interconnected to create correlations that implement Boolean functions with impressive accuracy, comparable to digital circuits. They are also "invertible", a unique property that is absent in digital circuits. In the direct mode, the input is clamped, and the network provides the correct output. In the inverted mode, the output is clamped, and the network fluctuates among all possible inputs that are consistent with that output. We present an implementation of such a p-bit using existing technology. The results for this hardware implementation agree with those from a universal model for p-bits, showing that p-bits need not be magnet based: any transistor-like tunable random bit generator should be suitable. We present an algorithm for designing a bi-directional p-bit network that implements a given truth table. We then show such bi-directional units, such as Full Adders, can be interconnected in a directed manner to implement 32-bit addition, that correlate hundreds of stochastic p-bits. We also show that despite the directed interconnections, invertibility is largely preserved. This combination of digital accuracy and logical invertibility is enabled by the hybrid design using bidirectional BM units to construct circuits with directed inter-unit connections.

TT 48.5 Wed 11:30 H 1012

Thermally excited skyrmion motion for probabilistic computing — •Jakub Zázvorka[1], Daniel Heinze[1], Kai Litzius[1,2,3], Samridh Jaiswal[1,4], Sascha Kromin[1], Niklas Keil[1], and Mathias Kläui[1,4] — [1]Johannes Gutenberg University Mainz, Institute of Physics, Mainz, Germany — [2]Max Plank Institute for Intelligent Systems, Stuttgart, Germany — [3]Graduate School of Excellence "Materials Science in Mainz", Mainz, Germany — [4]Singulus Technologies AG, Kahl am Main, Germany

A key problem for probabilistic computing is that cascading gates propagate undesired correlations. Therefore, one needs to reshuffle the signals to keep them uncorrelated. While for many non-conventional computing approaches non-magnetic implementations are most promising, for building a "reshuffler", skyrmions might be ideally suited due to the low footprint and low power compared to e.g. CMOS implementations [1]. We have studied a Ta-based material where we can stabilize skyrmions and controllably nucleate and displace them by current pulses due to spin-orbit torques. We find topologically non-trivial N=1 skyrmions that move with the application of current pulses. At zero applied current, we find thermally activated skyrmion motion. We track the trajectories of skyrmions and from the dependence of their mean-square-displacement (MSD) on time, we can identify motion by diffusion and obtain the diffusion constant. There is a strong dependence of the skyrmion diffusion parameter on temperature and the skyrmion size. Finally, we patterned the reshuffler geometry and ascertain its performance. [1] D. Pinna et al., arXiv:1701.07750, 2017.

Invited Talk TT 48.6 Wed 11:45 H 1012

Bits and Brains: New materials and brain-inspired concepts for low energy information processing — •Theo Rasing — Radboud University, Nijmegen, the Netherlands

Data is the fuel of the new digital economy that has stimulated a whole new class of innovative technologies and businesses. While data has become an indispensable part of modern society, the rate at which data is generated is exploding. This is not only pushing our current technologies to their limits, but also that of our energy production: our ICT and data centers already consume around 5% of the world electricity production and with an annual increase of 7%, this is rapidly becoming unsustainable. In stark contrast, the human brain, with its intricate architecture combining both processing and storing of information, only consumes about 10 Watt of energy while having a similar capacity as a supercomputer consuming around 10 Megawatt. We have created a consortium of condensed matter, material and neuro scientists with the aim to develop materials and concepts that mimic the efficiency of the brain by combining local processing and storage, using adaptable physical interactions that can implement learning algorithms.

TT 49: Superconductivity: Superconducting Electronics I

Time: Wednesday 9:30–13:00 Location: H 2053

Invited Talk TT 49.1 Wed 9:30 H 2053

Parametric Amplification in Josephson Circuits with Non-Centrosymmetric Nonlinearity — •Alexander Zorin, Marat Khabipov, Judith Felgner, and Ralf Dolata — Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

The superconducting technology enabling passive components with extremely low losses and Josephson elements with large nonlinearity makes it possible to engineer various networks possessing remarkable properties for propagating microwaves. We show that nonlinearity of the transmission line based on one-dimensional array of inductively-shunted Josephson junctions, i.e. serially connected rf-SQUIDs, can be effectively controlled by external magnetic flux with crossover from Kerr-like (centrosymmetric) nonlinearity to the pure $\chi^{(2)}$-type, i.e. non-centrosymmetric nonlinearity [1]. The later property, much like in quantum optics with materials having broken inversion symmetry, gives rise to the important effects including second harmonic generation, sum and difference frequency generation, and parametric amplification of microwave light. Due to excellent phase matching, which is possible in this transmission line in a wide frequency range, large parametric gain of traveling microwaves with ultimately quantum-limited performance can be achieved. Recent experiments performed with Nb trilayer circuits [2] have confirmed the validity of our concept and shown great promise for operation in the single-photon regime.

[1] A. B. Zorin, Phys. Rev. Applied **6**, 034006 (2016).
[2] A. B. Zorin, M. Khabipov, J. Dietel, R. Dolata, arXiv:1705.02859.

TT 49.2 Wed 10:00 H 2053

Design of a non-degenerate parametric amplifier based on two coupled Josephson junction arrays — •Ivan Takmakov[1,2], Patrick Winkel[1], Luca Planat[2], Natalia Maleeva[1], Kirill Borisov[1], Alexey V. Ustinov[1,4], Wolfgang Wernsdorfer[1,2,3], Ioan M. Pop[1], and Nicolas Roch[2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France — [3]Institute for Nanotechnology, Karlsruhe Institute for Technology — [4]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

We present the design of a parametric amplifier which consists of two identical, capacitively coupled Josephson junction array resonators, referred to as Dimer Josephson Junction Array Amplifier (DJJAA). If

design parameters are chosen appropriately, the Josephson Junction array resonators exhibit a dispersion relation with a linear regime including several eigenmodes. Due to the shared coupling capacitance between the arrays, their spectra hybridize to symmetric and antisymmetric pairs of modes, with a level splitting up to several hundreds of MHz. By applying a strong pump tone in-between a pair of hybridized modes we predict non-degenerate amplification, with an instantaneous bandwidth up to 50 MHz and a dynamic range well above the single photon regime. By utilizing several eigenmodes of the same system our approach potentially allows to cover a much larger band of operation.

TT 49.3 Wed 10:15 H 2053

Optical lithography implementation of a non-degenerate parametric amplifier based on two coupled Josephson junction arrays — •Patrick Winkel[1], Ivan Takmakov[1,2], Luca Planat[2], Nataliya Maleeva[1], Kiril Borisov[1], Alexey V. Ustinov[1,4], Wolfgang Wernsdorfer[1,2,3], Nicolas Roch[2], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut Néel, CNRS and Université Joseph Fourier, Grenoble, France — [3]Institute for Nanotechnology, Karlsruhe Institute of Technology — [4]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

We present the implementation of a parametric amplifier which consists of two identical, capacitively coupled Josephson junction array resonators, referred to as Dimer Josephson Junction Array Amplifier (DJJAA). In accordance to our theoretical model we observe non-degenerate amplification in excess of 20 dB, instantaneous bandwidth of approx. 10 MHz and dynamic range exceeding the single-photon regime. The field dependent critical current of the junctions, implemented in the shape of SQUIDs, allows for over 1 GHz frequency tunability. All structures are fabricated using standard two step optical lithography, making the DJJAA fabrication procedure easily accessible to a wide community.

TT 49.4 Wed 10:30 H 2053

Ex vivo continuous Overhauser nuclear dynamic polarization in a SQUID-based ultralow-field magnetic resonance imaging system — •Paul Fehling[1], Rebekka Bernard[1], Rolf Pohmann[1], Matthias Rudolph[1,2], Dieter Koelle[2], Reinhold Kleiner[2], Klaus Scheffler[1], and Kai Buckenmaier[1] — [1]Max Planck Institut for Biological Cybernetics, Max Planck Ring 11, 72076 Tübingen, Germany — [2]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

Overhauser Dynamic Nuclear Polarization (ODNP) is a hyperpolarization method for magnetic resonance measurements. The polarization of free radicals is transferred to ^{1}H using HF pulses, thus enhancing the ^{1}H signal. Only at UltraLow Fields (ULF) below 10 mT the corresponding HF pulse frequencies are low enough to penetrate large sample volumes, making continuous *in vivo* hyperpolarization possible. Since conventional Faraday coils are not sensitive enough at ULF, a SQUID-based detector is employed as the centerpiece of the ULF-MRI Scanner. With a superconducting second order gradiometric pickup coil the SQUID enables measurements with a sensitivity below $1\,\mathrm{fT}/\sqrt{\mathrm{Hz}}$. First proof-of-principle *ex vivo* images using ODNP enhanced, SQUID based ULF-MRI have been acquired successfully. This is an important step in the direction of a combined ULF MRI and magnetoencephalography system.

TT 49.5 Wed 10:45 H 2053

Nonlinear rf-SQUID metamaterials: two-tone spectroscopy and parametric effects beyond the Duffing regime — •Egor I. Kiselev[1,2], Alexander S. Averkin[2], Mikhail Fistul[4,3], and Alexey V. Ustinov[2,3] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]National University of Science and Technology "MISIS", Moscow, Russia — [4]Center for Theoretical Physics of Complex Systems, Daejeon, Republic of Korea

An experimental and theoretical study of the response of an rf-SQUID metamaterial to strong driving by means of two-tone resonant spectroscopy is presented. The superconducting metamaterial consists of an array of non-hysteretic rf-SQUIDs. We have observed pronounced oscillations of the intrinsic resonance frequency of the meta-atoms with the power of the driving tone. The shapes of these oscillations vary with the frequencies of the driving and probe signals. The response to the probe signal shows remarkable features such as parametric instabilities and sidebands and allows the direct imaging of a bistability. Our theoretical analysis is based on the classical nonlinear dynamics of rf-SQUIDs and in good agreement with experimental observations. We also present first results on parametric amplification by means of an rf-SQUID metamaterial beyond the Duffing regime.

TT 49.6 Wed 11:00 H 2053

Reconstructing Josephson current-phase relations from intermodulation spectroscopy — •Thomas Weissl, Shan W. Jolin, Per-Anders Thorén, Riccardo Borgani, Daniel Forchheimer, and David B. Haviland — KTH- Royal Institute of Technology, Stockholm, Sweden

Two pump tones driving a nonlinear system intermodulate, creating response at integer linear combinations of the their frequencies. With appropriate choice of the pumping frequencies, it is possible to measure not only the amplitudes, but also the phases of these intermodulation products, which depend on the detailed form of the nonlinearity that generates them. We present a method based on pseudo-inversion of a 'mixing matrix' built from the intermodulation response, to reconstruct the non-linear current-phase relation of a superconducting weak link [1,2]. The intermodulation spectra of a Nb-coplanar waveguide resonator with an engineered weak-link was measured as a function of drive amplitude, and the method was applied to obtain the coefficients of a Taylor expansion of the current-phase relation. The method allows for precision characterization of nonlinearities in microwave crcuits without the need of DC connections.

[1] Hutter et al., PRL 104, 050801 (2010).
[2] Platz et. al., Beilstein J. Nanotechnol. 4, 352360 (2013)

15 min. break.

TT 49.7 Wed 11:30 H 2053

Improved quasiparticle thermalization for hybrid single-electron turnstiles — •Joonas Peltonen[1], Dmitry Golubev[1], Antti Moisio[1], Ville Maisi[1], Matthias Meschke[1], Jaw-Shen Tsai[2,3], and Jukka Pekola[1] — [1]Department of Applied Physics, Aalto University School of Science, Espoo, Finland — [2]RIKEN Center for Emergent Matter Science, Wako, Saitama, Japan — [3]Department of Physics, Tokyo University of Science, Kagurazaka, Tokyo, Japan

To advance towards metrologically useful current quantization accuracy in a turnstile based on a single-electron transistor with superconducting aluminium electrodes and a normal metallic island, low density of both residual and drive-induced quasiparticles in the superconducting leads is required. We present measurement results from devices where the thickness of the Al electrodes has been increased by an order of magnitude compared to the maximum allowed by the conventional fabrication process [1]. We further discuss recent experiments where the quasiparticle density at the turnstile junctions is actively lowered by running a current through a nearby voltage-biased tunnel junction between two superconductors with differing energy gaps.

[1] J. T. Peltonen, A. Moisio, V. F. Maisi, M. Meschke, J. S. Tsai, and J. P. Pekola, 1709.09832 (2017).

TT 49.8 Wed 11:45 H 2053

Ultrasensitive Microwave Detector — •Mikko Möttönen[1], Joonas Govenius[1], Roope Kokkoniemi[1], Visa Vesterinen[1,2], Dibyendu Hazra[1], Marton Gunyho[1], Russell E. Lake[1,3], and Kuan Yen Tan[1,4] — [1]QCD Labs, Department of Applied Physics, Aalto University, Aalto, Finland — [2]VTT Technical Research Centre of Finland Ltd, VTT, Finland — [3]NIST, Boulder, Colorado, USA — [4]CQC2T, University of New South Wales, Australia

Intense development of nanobolometers has taken place for well more than a decade with the aim to reach NEP = 1e-20 W/rtHz which is required, for example, in effcient measurements of the cosmic terahertz spectrum in space. Furthermore, observation of single photons at increasingly long wavelengths is a long-standing effort [1]. We present a microwave nanobolometer based on proximity Josephson junctions. Using positive electrothermal feedback, we show that we can achieve a single-shot detection fidelity of 0.56 for 1.1-zJ pulses of 8.4-GHz photons [2]. This is more than an order of magnitude improvement over the previous thermal detectors. Importantly, we also observe that we can reach a sensitivity of NEP = 2e-20 W/rtHz with our detector in the linear continuous mode. This was achieved using a Josephson parametric amplifier in the detector readout chain [3]. In the future, ultrasensitive bolometers and thermometers are expected to play an important role in quantum information processing and quantum ther-

modynamics.
[1] K. Inomata et al., Nat. Commun. 7, 12303 (2016).
[2] J. Govenius et al., Phys. Rev. Lett. 117, 030802 (2016).
[3] V. Vesterinen et al. , Supercond. Sci. Technol. 30, 085001 (2017).

TT 49.9 Wed 12:00 H 2053

Development of a novel calorimetry setup based on metallic paramagnetic temperature sensors — •Andreas Reifenberger, Matthew Herbst, Sebastian Kempf, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, D-69120 Heidelberg

For the measurement of the specific heat of superconducting mg-sized metallic glass samples in the temperature range down to 10 mK we have developed a new microfabricated platform. It addresses challenging aspects of setups of this kind such as the thermal contact between sample and platform, the necessary thermometer resolution, and an addenda heat capacity exceeding that of the samples of interest (typically nJ/K at 20 mK). Our setup allows us to use the relaxation method, where the thermal relaxation following a well defined heat pulse is monitored to extract the specific heat. The sample platform ($5 \times 5\,\mathrm{mm}^2$) includes a microstructured paramagnetic Ag:Er temperature sensor, which is read out by a dc-SQUID via a superconducting pickup loop. In this way, a relative temperature precision of $30\,\mathrm{nK}/\sqrt{\mathrm{Hz}}$ can be reached, while the addenda heat capacity falls well below 0.5 nJ/K for $T < 300$ mK. A gold-coated mounting area ($4.4 \times 3\,\mathrm{mm}^2$) is included to improve the thermal contact between sample and platform. The performance of our setup is presented and discussed.

TT 49.10 Wed 12:15 H 2053

Dc-SQUID readout with high dynamic range and intrinsic frequency-domain multiplexing capability — •Sebastian Kempf, Daniel Richter, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

As a consequence of their periodic flux-to-voltage characteristic direct-current superconducting quantum devices (dc-SQUIDs) are intrinsically non-linear devices. The linear flux range of a dc-SQUID is therefore rather small and in most cases a flux-locked loop (FLL) is used both to increase the dynamic range and to linearize the output signal of the SQUID system. However, for FLL operation the requirements on the digitizer sampling the SQUID signal as well as on the readout electronics are challenging. In addition, individual feedback wires have to be routed to the SQUID setting often a practical limit to the implementation of massive multi-channel SQUID systems.

Within this context we present a novel approach for reading out dc-SQUIDs that provides an easy solution for linearizing the SQUID output signal and for increasing the dynamic range. At the same time it intrinsically allows for implementing frequency-domain multiplexing. In relies on applying a periodic sawtooth-shaped magnetic flux signal to the SQUID. The signal amplitude and repetition rate are chosen such that the input signal is transduced into a phase shift of the related SQUID characteristic. We discuss the basics as well as a comprehensive suitability study of our approach and demonstrate the intrinsic multiplexing capability using a customized multiplexer device.

TT 49.11 Wed 12:30 H 2053

Advanced nanoSQUIDs based on sub-micron trilayer Nb/HfTi/Nb Josephson junctions — •Julian Linek[1], Aaron Koser[1], Benedikt Müller[1], Katrin Meyer[1], Maria José Martínez-Pérez[2], Thomas Weimann[3], Oliver Kieler[3], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza and Fundación ARAID, Zaragoza, Spain — [3]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

We report on the development and performance of advanced Nb nanoSQUIDs for magnetization reversal studies on individual magnetic nanoparticles (MNPs). The nanoSQUIDs are based on trilayer high critical current density Nb/HfTi/Nb Josephson junctions. This offers the unique advantage of combining the realization of SQUIDs with very small loop inductance and hence extremely low flux noise, with a superconductor multilayer approach that offers the fabrication of complex devices with significantly increased functionality for various applications. One example is the recently developed 3-axis vector nanoSQUID [1]. Here, we present the performance of improved vector nanoSQUIDs and first attempts to simultaneously detect at 4.2 K in applied magnetic fields up to a few 100 mT all three orthogonal components of the magnetic moment of individual Co MNPs deposited onto our devices by focused electron beam deposition.
[1] M.J. Martínez-Pérez *et al.*, ACS Nano **10**, 8308 (2016)

TT 49.12 Wed 12:45 H 2053

An argon ion beam milling process for native AlO_x layers enabling coherent superconducting contacts — Lukas Grünhaupt[1], Uwe von Lüpke[1], •Daria Gusenkova[1], Sebastian T. Skacel[1], Nataliya Maleeva[1], Steffen Schlör[1], Alexander Bilmes[1], Hannes Rotzinger[1], Alexey V Ustinov[1,2], Martin Weides[1,3], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, 119049 Moscow, Russia — [3]Physikalisches Institut, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

We present an argon ion beam milling process to remove the native oxide layer forming on aluminum thin films due to their exposure to atmosphere in between lithographic steps [1]. Our cleaning process enables integration of complex superconducting quantum circuits without compromising their coherence properties. From measurements of the internal quality factors of superconducting microwave resonators, we place an upper bound on the residual resistance of an ion beam milled contact of $50\ \Omega \cdot \mu\mathrm{m}^2$ at a frequency of 4.5 GHz. Resonators for which only 6% of the total foot-print in areas of high magnetic field was exposed to the ion beam milling showed quality factors above 10^6 in the single photon regime, and no degradation compared to single layer samples.
[1] L. Grünhaupt et al., Applied Physics Letters, 111, 072601 (2017).

TT 50: Quantum-Critical Phenomena I

Time: Wednesday 9:30–13:00 Location: H 3005

TT 50.1 Wed 9:30 H 3005

Uniaxial stress tuning of geometrical frustration in a Kondo lattice — R. Küchler[1,2], C. Stingl[2], Y. Tokiwa[2], M.S. Kim[3], T. Takabatake[3], and •P. Gegenwart[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [3]Department of Quantum Matter, ADSM, Hiroshima University, Higashi-Hiroshima, 739-8530, Japan

Hexagonal CeRhSn with paramagnetic $4f$ moments on a distorted Kagome lattice displays zero-field quantum critical behavior related to geometrical frustration [1]. We report high-resolution thermal expansion and magnetostriction measurements under multiextreme conditions such as uniaxial stress up to 200 MPa, temperatures down to 0.1 K and magnetic fields up to 10 T. Under uniaxial stress along the a-direction, quantum criticality disappears and a complex magnetic phase diagram arises with a sequence of phases below 1.2 K and fields between 0 and 3 T ($\| a$). Since the Kondo coupling increases with stress, which alone would stabilize paramagnetic behavior in CeRhSn, the observed order arises from the release of geometrical frustration by in-plane stress.
[1] Y. Tokiwa, C. Stingl, M.-S. Kim, T. Takabatake, and P. Gegenwart, Sci. Adv. 1, e1500001(2015).

TT 50.2 Wed 9:45 H 3005

Close proximity of FeSe to a magnetic quantum critical point as revealed by high-resolution μSR measurements — •Vadim Grinenko[1,2], Rajib Sarkar[1], Philipp Materne[1], Sirko Kamusella[1], Aichi Yamashita[3], Yoshihiko Takano[3], Yue Sun[4], Tsuyoshi Tamegai[4], Dmitriy Efremov[2], Stefan-Ludwig Drechsler[2], Jean-Christophe Orain[5], Tatsuo Goko[5], Robert Scheuermann[5], Hubertus Luetkens[5], and Hans-Henning Klauss[1] — [1]Institute for Solid State and Material Physics, TU Dres-

den, 01069 Dresden, Germany — [2]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [3]National Institute for Materials Science (NIMS), Tsukuba, Ibaraki, 305-0047 JAPAN, Japan — [4]Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan — [5]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute (PSI), CH-5232 Villigen, Switzerland

We investigated FeSe single crystals using high-field (up to 9.5 T) muon spin rotation (μSR) measurements. We observed that the muon spin depolarization rate follows a critical behavior $\Lambda^2 \propto T^{-3/4}$ in the temperature range $T_s \gtrsim T \gtrsim 10$ K. The scaling between Λ^2 and the NMR $1/T_1T$ suggests that $\Lambda \propto 1/T_2$ spin-spin relaxation rate. The observed non-Fermi liquid behavior with a cutoff at $T^* \sim 10$ K indicates that FeSe is close to a magnetic quantum critical point. The μSR Knight shift and the bulk susceptibility linearly scale at high temperatures but deviate from this behavior below T^* where the Knight shift exhibits a kink. Our analysis shows a reduction of the density of states crossing the region near T^* maybe related to a Lifshitz transition.

TT 50.3 Wed 10:00 H 3005

Detailed study of the transverse susceptibility of the model magnet $LiHoF_4$ — •Felix Rucker[1], Christopher Duvinage[1], Steffen Säubert[1,2], Robert Georgii[2], Andreas Wendl[1], and Christian Pfleiderer[1] — [1]Technische Universität München, Physik-Department, Lehrstuhl für Topologie korrelierter Systeme — [2]Heinz Maier-Leibnitz Zentrum, TUM, Garching, Germany

The low temperature properties of $LiHoF_4$, representing a model system for a magnetic field tuned quantum phase transition, have been investigated for over two decades. Despite recent experimental and theoretical efforts, details of the experimentally inferred magnetic phase diagram remain inconsistent with theoretical predictions. In our study, we revisit magnetic transverse susceptibility measurements at low temperatures. We find evidence for the influence of the hyperfine coupling on the magnetic transverse susceptibility, yielding insights to the dynamic properties of the quantum phase transition.

TT 50.4 Wed 10:15 H 3005

Antiferromagnetic correlations in ferromagnetic $YbNi_4P_2$ — •Zita Huesges[1], Stefan Lucas[2], Kristin Kliemt[3], Cornelius Krellner[3], Astrid Schneidewind[4], and Oliver Stockert[2] — [1]Helmholtz-Zentrum Berlin GmbH — [2]MPI Chemische Physik fester Stoffe, Dresden — [3]Goethe-Universität Frankfurt am Main — [4]Forschungszentrum Jülich GmbH, Outstation MLZ

$YbNi_4P_2$ is one of the very few heavy-fermion compounds that shows ferromagnetic order at very low temperature. The Curie temperature, only 150 mK in the pure compound, can be suppressed to zero by As substitution on the P site. Upon substitution, the transition stays second order, thus leading to a ferromagnetic quantum critical point. While the *c*-axis is the magnetic easy axis in the paramagnetic phase, magnetic order occurs with the moments aligned in the *ab*-plane.

To gain microscopic insights into this unusual behaviour, we have performed inelastic neutron scattering (INS) experiments at the triple-axis spectrometers PANDA (MLZ) and FLEXX (HZB). Large single crystals have recently become available due to progress in sample preparation. Remarkably, we observe an INS signal at low-Q antiferromagnetic positions. The signal appears to be quasi-elastic, it is present at much higher temperatures than T_C, and it shows no signature of a moment-reorientation. This indicates that only a fraction of the magnetic moment participates in the low-temperature ferromagnetic order, while antiferromagnetic correlations are present in a broader temperature range.

TT 50.5 Wed 10:30 H 3005

Fermi surface studies of $YbNi_4P_2$ — •Sven Friedemann[1], Alix McCollam[2], Gertrud Zwicknagl[3], Kristin Kliemt[4], and Cornelius Krellner[4] — [1]HH Wills Laboratory, University of Bristol, UK — [2]High Field Magnet Laboratory, University of Radboud, Nijmegen, NL — [3]Institut für Mathematische Physik, TU Braunschweig, Braunschweig, Germany — [4]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a rare example of a heavy-fermion compound with ferromagnetic (FM) order. Moreover, FM order can be suppressed and a FM quantum critical point (QCP) can be accessed if phosphorous is partially substituted by arsenic [1]. The presence of a FM QCP makes $YbNi_4P_2$ unique as FM QCPs are avoided in most systems through a change of the transition to 1st order or through an intervening antiferromagnetic phase. The preservation of the FM QCP is theoretically suggested to be due to an effective one-dimensional electronic structure. Here, we present quantum oscillation measurements performed at high magnetic fields and low temperatures. We compare the angular dependency of the observed frequencies with predictions from band structure calculations treating the f electrons as core electrons and with predictions from fully renormalised band structure calculations.

[1] A. Steppke et al., Science, **339**, 933 (2013).

TT 50.6 Wed 10:45 H 3005

Characterization of substituted $YbNi_4P_2$ single crystals — •Kristin Kliemt[1], Paul Denck[1], Philipp Ross[1], Jacintha Banda[2], Sandra Hamann[2], Alexander Steppke[2], Sven Friedemann[3], Manuel Brando[2], and Cornelius Krellner[1] — [1]Goethe-University Frankfurt, Institute of Physics, 60438 Frankfurt, Germany — [2]MPI CPfS, 01187 Dresden, Germany — [3]University of Bristol, Bristol, United Kingdom

The tetragonal compound $YbNi_4P_2$ has a low Curie temperature, $T_C = 0.17$ K, which can be further suppressed by substituting P by As and the rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at $x \approx 0.1$ [1,2]. Here, we present the characterization of $YbNi_4(P_{1-x}As_x)_2$ single crystals [3,4] with As concentrations $0 \leq x \leq 1$ by electrical transport, heat capacity and magnetization measurements. We also discuss the effect on the magnetic ordering temperature of a substitution at the Yb site by hafnium and scandium.

[1] C. Krellner et al., New J. Phys. **13**, 103014 (2011)
[2] A. Steppke et al., Science **339**, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth **449**, 129 (2016)
[4] K. Kliemt, C. Krellner, J. Phys.: Conf. Series **807**, 032005 (2017)

TT 50.7 Wed 11:00 H 3005

High field NMR near the field induced quantum phase transition in $CeRhIn_5$ — •Guilherme G. Lesseux[1,2], Taisuke Hattori[3], Hironori Sakai[3], Yo Tokunaga[3], Shinsaku Kambe[3], Philip Kuhns[4], Arneil Reyes[4], Pascoal J. G. Pagliuso[1], and Ricardo R. Urbano[1] — [1]"Gleb Wataghin" Institute of Physics - University of Campinas, Campinas, Brazil — [2]1. Physikalisches Institut - Universität Stuttgart, Stuttgart, Germany — [3]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki, Japan — [4]National High Magnetic Field Laboratoy - Florida State University, Tallahassee, USA

We report on the first low temperature and high field ^{115}In NMR measurements on $CeRhIn_5$ through its magnetic field induced transition at $B^* \sim 30$ T (0.5 K) near the quantum critical point at $B_{c0} \sim 50$ T. With the magnetic field applied along *c*-axis and within the limit of the signal-to-noise ratio, no remarkable change of the spectral shape of the planar In(1) signal was observed in the range $2\ \mathrm{T} < B||c < 39$ T, indicating no significant change of the magnetic structure. Moreover, the formal shift for the In(1) transitions was found to be virtually constant from the lowest measured field (2 T) up to 29 T although its value revealed a noticeable change through 30 T. Our results are the first microscopic evidence of the high field induced Fermi surface reconstruction in $CeRhIn_5$ suggested in previous reports based on quantum oscillations.

15 min. break.

Invited Talk TT 50.8 Wed 11:30 H 3005

Critical Phonon Softening Near a Structural Instability at $T = 0$ — •Oliver Stockert — Max-Planck-Institut CPfS, Dresden

While lots of studies have focused on magnetic quantum critical points, remarkably little is known about structural instabilities occurring at $T = 0$. Technological improvements made it recently possible to observe low-energy phonons and phonon softening by high-resolution inelastic x-ray scattering (IXS) with energy resolution of about 1 meV, i.e. quite similar to inelastic neutron scattering (INS). We have studied in detail the lattice dynamics in the quantum critical charge density wave system $Lu(Pt_{1-x}Pd_x)_2In$ [1] using both INS and high-resolution IXS. Superconductivity in this system displays a pronounced maximum of the transition temperature in the vicinity of the structural quantum criticality at $x_c \approx 0.6$ [1]. We were able to trace the softening of the critical phonon modes down to energies of < 0.5 meV using INS and even IXS. Importantly, the results of both methods match, showing the capabilities of IXS. The precise information on the temperature evolution of the critical modes provided by these experiments is essential to get an understanding of the unusual properties observed in such

quantum critical systems, e.g. for the emergence of unconventional superconductivity.
[1] T. Gruner et al., Nature Phys. **13**, 967 (2017).
*In collaboration with T. Gruner, S. Lucas, Z. Huesges, K. Kaneko, S. Tsutsui, K. Schmalzl, M. Koza, A. Hoser, M. Reehuis, C. Geibel.

TT 50.9 Wed 12:00 H 3005

Pressure dependent entropy of the partially frustrated heavy-fermion system $CePd_{1-x}Ni_xAl$ — •Sebastian Kuntz[1], Kai Grube[1], Chien-Lung Huang[2], Veronika Fritsch[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, United States — [3]Experimentalphysik VI, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany

In CePdAl one third of the Ce moments are geometrically frustrated and do not participate in the antiferromagnetic long-range order below $T_N = 2.7$ K. By replacing Pd with isoelectronic, but smaller Ni atoms, the magnetic order can be suppressed at a Ni concentration of $x = 0.14$ [1]. We measured the thermal expansion of $x = 0$, 0.05 and 0.14 single crystals in magnetic fields up to $B = 14$ T to obtain the uniaxial pressure dependences of the entropy $S(T)$ and the ordering temperature T_N. The results will be compared with magnetization measurements of CePdAl under hydrostatic pressure. The impact of external and chemical pressure on the geometric frustration and the Kondo effect will be discussed.
[1] A. Sakai *et al.*, Phys. Rev. B 94, 22045(R) (2016).

TT 50.10 Wed 12:15 H 3005

Investigation of a field induced magnetic transition in the low-dimensional magnet $BiCoPO_5$ — •Margarita Iakovleva[1,2], Evgeniia Vavilova[2], Hans-Joachim Grafe[1], Alexey Alfonsov[1], Bernd Büchner[1], Yurii Skourski[3], Ramesh Nath[4], and Vladislav Kataev[1] — [1]IFW Dresden, Dresden, 01069, Germany — [2]KPhTI, Kazan, 420029, Russia — [3]HZDR, Dresden, 01328, Germany — [4]IISER, Kerala, 695016, India

The frustrated dimeric chain compound $BiCoPO_5$ orders antiferromagnetically at $T_N = 11$ K. Application of an external magnetic field reduces the transition temperature down to T = 0 K at field of $H_C \approx 15.3$ T [1], which according to theory could be a signature of field driven quantum phase transition [2]. Here we present an investigation of the title compound by means of magnetometry, high-field/frequency electron spin resonance (HF-ESR) and nuclear magnetic resonance (NMR) techniques. The high-field magnetization measurements show no saturation of the magnetic moment up to the highest magnetic field of 60 T. Low-temperature HF-ESR measurements reveal several field-dependent resonance modes. The ^{31}P NMR relaxation rates measured at 9 T exhibit a peak at T = 8 K corresponding to the AFM order. Remarkably, at a magnetic field of 15 T the T-dependence of the relaxation rates shows a contrasting gapped behavior that could indicate the emergence of a new quantum disordered phase of $BiCoPO_5$ with gapped spin excitations above H_C.
[1] E. Mathews, et. al., Solid State Commu. 154, 56 (2013)
[2] Rong-Gen Cai, et. al., Phys. Rev. D 92, 086001 (2015)

TT 50.11 Wed 12:30 H 3005

High-pressure fermiology of the metallised Mott insulator NiS_2 — •Jordan Baglo[1], Konstantin Semeniuk[1], Hui Chang[1], Xiaoye Chen[1], Pascal Reiss[1], HongEn Tan[1], Patricia Alireza[1], Audrey Grockowiak[2], William Coniglio[2], Stanley Tozer[2], Alix McCollam[3], Inge Leermakers[3], Sven Friedemann[4], Monika Gamza[5], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]NHMFL, Tallahassee, Florida, USA — [3]HFML, Nijmegen, The Netherlands — [4]HH Wills Laboratory, University of Bristol, UK — [5]Jeremiah Horrocks Institute, University of Central Lancashire, UK

The Mott metal-to-insulator transition continues to be an active topic of investigation; various mechanisms have been proposed, but the precise nature of the transition remains an open question. In many such systems under study, filling (via chemical doping) is used as a tuning parameter, but the resultant disorder hinders the use of sensitive quantum oscillation techniques to study Fermi surface properties. In the prototypical Mott insulator NiS_2, one can instead use pressure to cleanly tune the ratio U/t of onsite Coulomb repulsion to kinetic energy. We will present our most recent quantum oscillation measurements of NiS_2 under hydrostatic pressures from near the Mott transition at ∼30 kbar up to 115 kbar. We find that the Fermi surface remains nearly unchanged on approaching Mott localisation, whereas the effective mass is strongly renormalised – in qualitative agreement with the Brinkman-Rice picture.

TT 50.12 Wed 12:45 H 3005

Quantum criticality in the spin-1/2 Heisenberg chain system CuPzN — Oliver Breunig[1], Markus Garst[2,3], Andreas Klümper[4], Jens Rohrkamp[1], Mark M. Turnbull[5], and •Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Germany — [3]Institut für Theoretische Physik, Universität Dresden, Germany — [4]Fachbereich C Physik, Bergische Universität Wuppertal, Germany — [5]Carlson School of Chemistry, Clark University, Worcester, USA

The magnetic insulator copper pyrazine dinitrate (CuPzN) is one of the best experimental realizations of the Heisenberg spin-1/2 chain model. Its weak antiferromagnetic coupling J of about 10 K provides a unique opportunity for a quantitative comparison between theory and experiment. Here, we study thermodynamic properties with a particular focus on the magnetic-field induced quantum phase transition at 14 T [1]. Thermal expansion, magnetostriction, specific heat, magnetization and magnetocaloric measurements almost perfectly agree with predictions from exact Bethe-Ansatz results. On approaching the critical field, thermodynamics obeys the quantum critical scaling behavior expected from effective field theory. In particular, the magnetic-field and pressure dependent Grüneisen parameters diverge in a characteristic manner. Our study instructively illustrates fundamental principles of quantum critical thermodynamics and also reveals the influence of corrections to scaling.

Funded by the DFG via FOR 960, FOR2316, CRC1143, and CRC1238.
[1] O. Breunig et al., arxiv1709.00274 (Sci. Adv., to appear).

TT 51: Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)

Time: Wednesday 9:30–13:00 Location: H 3010

Invited Talk TT 51.1 Wed 9:30 H 3010

Electronic Squeezing of Pumped Phonons: Negative U and Transient Superconductivity — •Dante M. Kennes[1], Eli Y. Wilner[1], David R. Reichman[2], and Andrew J. Millis[1] — [1]Department of Physics, Columbia University, New York, New York 10027, USA — [2]Department of Chemistry, Columbia University, New York, New York 10027, USA

Advances in light sources and time resolved spectroscopy have made it possible to excite specific atomic vibrations in solids and to observe the resulting changes in electronic properties but the mechanism by which phonon excitation causes qualitative changes in electronic properties, is still under debate. Here, we show that the dominant symmetry-allowed coupling between electron density and dipole active modes implies an electron density-dependent squeezing of the phonon state which provides an attractive contribution to the electron-electron interaction, independent of the sign of the bare electron-phonon coupling and with a magnitude proportional to the degree of laser-induced phonon excitation. Reasonable excitation amplitudes lead to non-negligible attractive interactions that may cause significant transient changes in electronic properties including superconductivity. The mechanism is generically applicable to a wide range of systems, offering a promising route to manipulating and controlling electronic phase behavior in novel materials. Building on these results we analyze the nonequilbrium response of the electronic system and discuss implications for experimentally accessible observables, such as optical conductivity.

TT 51.2 Wed 10:00 H 3010

Photoinduced non-thermal insulator-to-metal transition in NbO_2 epitaxial thin films — •Rakesh Rana[1], John Klopf[1],

Joerg Grenzer[1], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany

The ultrafast insulator-to-metal transition in the correlated oxides such as vanadium dioxide (VO_2) has been extensively explored for its rich physics and potential applications. In this regard, its isovalent counterpart niobium dioxide (NbO_2) with considerably higher transition temperature (T_C = 1080 K) can be envisaged as a potential alternative. We have performed time-resolved optical pump-terahertz (THz) probe measurements on NbO_2 epitaxial thin-film at room temperature. The onset of the THz conductivity is followed by an exponential decay on a timescale of 400 fs. The photoinduced change in THz transmission at later delay times exhibits an excitation threshold of 17.5 mJ/cm^2. Notably, in contrast to VO_2, the pump energy required for the switching into a metastable metallic state is smaller than the energy necessary for heating NbO_2 up to T_C providing strong evidence for the non-thermal character of the photo induced insulator-to-metal transition in this system. The transient optical conductivity in the metastable state can be modelled using the Drude model confirming its metallic character.

TT 51.3 Wed 10:15 H 3010

Emergent CDW order in a 1D correlated electron system with underlying magnetic microstructure — Thomas Köhler, Sebastian Paeckel, and •Salvatore Manmana — Institut f. Theoretische Physik, U. Göttingen

We address the question of charge density wave order (CDW) emerging in a nonequilibrium situation in the course of a photo excitation. Using time-dependent matrix product states (tMPS), we model a pump excitation using Peierls substitution in a Hubbard chain at quarter filling, which is in the presence of an alternating magnetic background field. This magnetic microstructure is obtained for a 1D toy-manganate system, in which the t_{2g} electrons form a frozen lattice of Zener polarons, but do not participate in the charge transport. We investigate the interplay of the magnetic microstructure and the Hubbard U term for the dynamics of the system and discuss possible realizations with ultracold atoms on optical lattices.

We acknowledge financial support by DFG through research unit FOR1807 (project P7) and SFB/CRC1073 (project B03).

TT 51.4 Wed 10:30 H 3010

Non-monotonic response and light-cone freezing in gapless-to-(partially) gapped quantum quenches of fermionic systems — •Sergio Porta[1,2], Filippo Maria Gambetta[1,2], Niccolò Traverso Ziani[3], Dante Marvin Kennes[4], Maura Sassetti[1,2], and Fabio Cavaliere[1,2] — [1]Dipartimento di Fisica, Università di Genova, Genova, 16146 Italy — [2]SPIN-CNR, Genova, 16146 Italy — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [4]Department of Physics, Columbia University, New York, NY 10027, USA

The properties of prototypical examples of one-dimensional fermionic systems undergoing a sudden quantum quench from a gapless state to a (partially) gapped state are analyzed. By means of a Generalized Gibbs Ensemble analysis or by numerical solutions in the interacting cases, we observe an anomalous, non-monotonic response of steady state correlation functions as a function of the strength of the mechanism opening the gap. In order to interpret this result, we calculate the full dynamical evolution of these correlation functions, which shows a freezing of the propagation of the quench information (light cone) for large quenches. We argue that this freezing is responsible for the non-monotonous behaviour of observables. In continuum non-interacting models, this freezing can be traced back to a Klein-Gordon equation in the presence of a source term. We conclude by arguing in favour of the robustness of the phenomenon in the cases of non-sudden quenches and higher dimensionality.
[1] arXiv:1708.09320

TT 51.5 Wed 10:45 H 3010

The non-equilibrium Peierls transition in thermodynamic unbalanced system — •Pedro Ribeiro[1] and Stefan Kirchner[2] — [1]Affiliation: CeFEMA, Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, Zhejiang 310058, China

Spin- and charge density waves are a common phenomenon in condensed matter physics. Charge density waves were predicted by R. Peierls who showed that due to the electron-phonon coupling a one-dimensional lattice may become unstable and undergoes a transition into an ordered. Away from thermal equilibrium, much less is known about this transition. In this talk, we address the fate of this instability under non-equilibrium conditions created by imposing a finite voltage across the system. In particular, we explore the possibility of changing the ordering wave vector away from its equilibrium position by a finite voltage drop across the system.

TT 51.6 Wed 11:00 H 3010

Photoinduced absorptions inside the Mott gap in the two-dimensional extended Hubbard model — Kazuya Shinjo and •Takami Tohyama — Department of Applied Physics, Tokyo University of Science, Tokyo 125-8585, Japan

We theoretically investigate pump-probe optical responses in the two-dimensional extended Hubbard model describing cuprates by using a time-dependent Lanczos method. At half filling, pumping generates photoinduced absorptions inside the Mott gap. A part of low-energy absorptions is attributed to the independent propagation of photoinduced holons and doublons. The spectral weight just below the Mott gap increases with decreasing the on-site Coulomb interaction U. We find that the next-nearest-neighbor Coulomb interaction V1 enhances this U dependence, indicating the presence of biexcitonic contributions formed by two holon-doublon pairs. Photopumping in hole-doped systems also induces spectral weights below remnant Mott-gap excitations, being consistent with recent experiments. The induced weights are less sensitive to V1 and may be related to the formation of a biexcitonic state in the presence of hole carriers.

15 min. break.

TT 51.7 Wed 11:30 H 3010

Multiple particle-hole pair creation in the Fermi-Hubbard model — •Friedemann Queisser, Nicolai ten Brinke, Uwe Bovensiepen, and Ralf Schützhold — Fakultät für Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany

We study the Fermi-Hubbard model in the strongly correlated Mott phase under the influence of a harmonically oscillating hopping rate $J(t) = J_0 + 4Jcos(\omega t)$. If ω is near an integer multiple of the gap we find higher-order resonances where multiple particle-hole pairs are created. The creation of these pairs depends crucially on the specific form of the underlying lattice geometry. We discuss the microscopic mechanism for multiple pair creation in small lattices.
[1] N. ten Brinke, M. Ligges, U. Bovensiepen and R. Schützhold, *Phys. Rev. B* **95**, 195123 (2017)

TT 51.8 Wed 11:45 H 3010

Nonequilibrium gas-liquid transition in the driven-dissipative photonic lattice — Matteo Biondi[1], Gianni Blatter[1], Hakan Tureci[2], and •Sebastian Schmidt[1] — [1]ETH Zurich, Institute for Theoretical Physics, Switzerland — [2]Princeton University, Department of Electrical Engineering, USA

We study the nonequilibrium steady state of the driven-dissipative Bose-Hubbard model with Kerr nonlinearity. Employing a mean-field decoupling for the intercavity hopping J, we find that the steep crossover between low and high photon-density states inherited from the single cavity transforms into a gas-liquid bistability at large cavity-coupling J. We formulate a van der Waals-like gas-liquid phenomenology for this nonequilibrium setting and determine the relevant phase diagrams, including a new type of diagram where a lobe-shaped boundary separates smooth crossovers from sharp, hysteretic transitions. Calculating quantum trajectories for a one-dimensional system, we provide insights into the microscopic origin of this many-body bistability.

TT 51.9 Wed 12:00 H 3010

Frustration-induced quasi-long-range order in a photonic system — •Matteo Biondi, Gianni Blatter, and Sebastian Schmidt — Institut für Theoretische Physik, Wolfgang-Pauli-Str. 27 8093 Zürich Switzerland

We investigate the interplay of geometric frustration and interactions in a nonequilibrium photonic lattice system exhibiting a photonic flat band as described by the driven-dissipative Bose-Hubbard model. We propose how to engineer quasi-long-range order in a quasi one-dimensional frustrated system by pumping the photonic lattice inco-

herently. Using a filter qubit to modulate the bandwidth of the pump, we demonstrate how to obtain a quasi-pure density-wave state of photons characterized by a polynomial decay of density-density correlations. We provide analytic results together with finite-size simulations of the Lindblad master equation using exact diagonalization and propose a state-of-the-art photonic realization of our system within cavity QED.

[1] M. Biondi, G. Blatter and S. Schmidt, in preparation.
[2] M. Biondi, E. v. Nieuwenburg, G. Blatter, S. Huber, and S. Schmidt, PRL 115, 143601 (2015).
[3] F. Baboux, L. Ge, T. Jacqmin, M. Biondi, E. Galopin, A. Lemaitre, L. Le Gratiet, I. Sagnes, S. Schmidt, H. E. Türeci, A. Amo and J. Bloch, PRL 116, 066402 (2016).

TT 51.10 Wed 12:15 H 3010

Thermalization of isolated Bose-Einstein condensates by dynamical heat bath generation — •Anna Posazhennikova[1], Mauricio Trujillo-Martinez[2], and Johann Kroha[2] — [1]Royal Holloway University of London, Egham, Surrey, UK — [2]Physikalisches Institut, Universität Bonn, Germany

If and how an isolated quantum system thermalizes despite its unitary time evolution is a long-standing, open problem of many-body physics. The eigenstate thermalization hypothesis (ETH) postulates that thermalization happens at the level of individual eigenstates of a system's Hamiltonian. However, the ETH requires stringent conditions to be validated, and it does not address how the thermal state is reached dynamically from an initial non-equilibrium state. We consider a Bose-Einstein condensate (BEC) trapped in a double-well potential with an initial population imbalance. We find that the system thermalizes although the initial conditions violate the ETH requirements. We identify three dynamical regimes. After an initial regime of undamped Josephson oscillations, the subsystem of incoherent excitations or quasiparticles (QP) becomes strongly coupled to the BEC subsystem by means of a dynamically generated, parametric resonance. When the energy stored in the QP system reaches its maximum, the number of QPs becomes effectively constant, and the system enters a quasi-hydrodynamic regime where the two subsystems are weakly coupled. In this final regime the BEC acts as a grand-canonical heat reservoir for the QP system (and vice versa), resulting in thermalization. We term this mechanism dynamical bath generation (DBG).

TT 51.11 Wed 12:30 H 3010

State engineering and out of equilibrium dynamics of spin models with cold bosonic atoms — •Araceli Venegas-Gomez and Andrew John Daley — University of Strathclyde, Glasgow, UK

The macroscopic control over cold atoms in optical lattices offers an excellent platform to study the out-of-equilibrium behaviour of strongly correlated systems, such as spin models, which are usually motivated by solid state physics. This offers us opportunities to study fundamental properties away from equilibrium and to probe states of the spin models, as well as providing tools to prepare states of lower temperature and entropy. We theoretically investigate a generalised Bose-Hubbard model for two-component bosonic atoms in an optical lattice, exploring the dynamics in corresponding spin-1/2 and spin-1 models. Investigating the magnetically ordered quantum states that can be engineered, we develop adiabatic state preparation techniques to achieve states with very low entropy starting from a known occupation number of particles per site. We explore this process, and ways to use non-equilibrium dynamics to probe the resulting states, using numerical methods based on tensor networks, focussing on parameters accessible in current experiments.

TT 51.12 Wed 12:45 H 3010

Reconstructing quantum states of cold atomic quantum simulators from non-equilibrium dynamics — •Marek Gluza[1], Thomas Schweigler[2], Bernhard Rauer[2], Christian Krumnow[1], Joerg Schmiedmayer[2], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria

Systems of ultra-cold atoms on atom chips provide an architecture to probe aspects of out-of-equilibrium quantum many-body physics including equilibration, thermalization and pre-thermalization. We present a novel tomographic reconstruction method for these quantum simulators allowing to access the expectation value of quadrature operators which are inaccessible from direct measurements but capture crucial characteristics of the elementary excitations of cold atomic systems. Specifically, we use interferometric data of non-equilibrium phase fluctuations to reconstruct the covariance matrix – including density fluctuations – of eigenmodes of the corresponding mean-field models. Experimentally, we observe quench dynamics in the non-interacting regime of particles in harmonic or box potentials. Formally, we use that one can efficiently keep track of the evolution and employ signal processing and semi-definite programming to perform a reliable reconstruction of covariance matrices. This method opens a new window into the study of dynamical quantum simulators – an insight that we exploit and discuss at the hand of several examples, including Gaussifying quantum many-body dynamics.

TT 52: Superconductivity: Fe-based Superconductors - FeSe and LiFeAs

Time: Wednesday 9:30–13:00 Location: HFT-FT 101

TT 52.1 Wed 9:30 HFT-FT 101

Interfacial phonons in the single unit cell of FeSe grown on $SrTiO_3$(001) — •Dominik Rau[1], Tobias Engelhardt[2], Jasmin Jandke[2], Fang Yang[2], Endre Barta[2], Wulf Wulfhekel[2], and Khalil Zakeri Lori[1] — [1]Heisenberg Spin-dynamics Group, Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

Among all Fe-based superconductors a single unit cell of FeSe on $SrTiO_3$ exhibits the highest transition temperature T_c. Despite the intensive research, the physical origins of the observed high T_c and the role of the interfacial phonons in superconductivity are still highly under debate. Utilizing high-resolution electron energy-loss spectroscopy we probe the phonon spectrum in a unit cell of FeSe epitaxially grown on Nb-doped $SrTiO_3$(001). The Fuchs–Kliewer interfacial phonons are observed to appear at energies of 57 and 91.5 meV near the zone center. Both modes exhibit a weak dispersion while increasing the wave vector from $\overline{\Gamma}$ towards the zone boundary ($\overline{X}$-point). The intrinsic linewidth of the higher energy phonon mode is about 11.5 meV at the $\overline{\Gamma}$-point and remains nearly constant over a large fraction of the Brillouin zone. The nearly momentum-independent phonon lifetime excludes particularly strong electron–phonon coupling near the zone center. This observation indicates that other bosonic excitations, e.g. those of electronic origin, should play an important role in the formation of Cooper pairs and superconductivity in this system. This work has been supported by DFG through the Heisenberg Programme ZA 902/3-1 and DFG Grant Wu 349/12-1 and by the Alexander von Humboldt Foundation.

TT 52.2 Wed 9:45 HFT-FT 101

Interface high temperature superconductivity in FeSe/TiO_2 — •Lili Wang and Qikun Xue — Tsinghua University, Beijing, China

The discovery of high temperature superconductivity with a superconducting gap of 20 meV in monolayer FeSe films epitaxially grown on $SrTiO_3$ substrate has stimulated tremendous interest in superconductivity community, for it opens new avenue for both raising superconducting transition temperature and understanding the pairing mechanism of unconventional high temperature superconductivity. In this talk, I will present the experimental progress on interface enhanced superconductivity in FeSe/TiO_2 interfaces, studied by scanning tunneling microscopy/spectroscopy, angle-resolved photoemission spectroscopy and transport experiments. Then I will discuss the roles of interfaces, such as charge transfer and electron-phonon coupling, inferred from those studies.

[1] Q.-Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012).
[2] W.-H. Zhang et al., Chin. Phys. Lett. 31, 017401 (2014).
[3] C. J. Tang et al., Phys. Rev. B 93, 020507(R) (2016).
[4] G. Y. Zhou et al., Appl. Phys. Lett. 108, 202603 (2016).
[5] H. Ding et al., Phys. Rev. Lett. 117, 067001 (2016).
[6] H. M. Zhang et al., Nature Communs. 8 214 (2017).

TT 52.3 Wed 10:00 HFT-FT 101

Response of the Structural Transition of FeSe under Uniaxial Stress — •Jack Bartlett[1,2], Alexander Steppke[1], Suguru Hosoi[3], Takasada Shibauchi[3], Andrew Mackenzie[1,2], and Clifford Hicks[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Nöthnitzerstr. 40, Dresden, 01187, Germany — [2]University of St Andrews, School of Physics and Astronomy, St Andrews KY16 9SS, United Kingdom — [3]University of Tokyo, Department of Advanced Materials Science, Kashiwa, Chiba 277-8561, Japan

FeSe is unique as an iron-based superconductor due to its simple structure, and lack of magnetic order at ambient pressure, which offers an opportunity to disentangle the interplay of structural, magnetic and orbital degrees of freedom. Additionally, this material undergoes a structural phase transition at $T_s \sim 90$ K, in which the lattice changes symmetry from tetragonal to orthorhombic. Uniaxial stress is a conjugate field to this transition, and therefore one naively expects an increase in the transition temperature and a broadening of the transition under uniaxial stress. We observe an unexpected suppression of T_s under both compressive and tensile stress, as well as a dramatic broadening of the transition. We discuss these results in the context of orbital-selective physics.

TT 52.4 Wed 10:15 HFT-FT 101

Gap anisotropy in FeSe from ARPES — •Yevhen Kushnirenko[1], Alexander Fedorov[1], Erik Haubold[1], Timur Kim[2], Thomas Wolf[3], Saicharan Aswartham[1], Bernd Büchner[1], and Sergey Borisenko[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Diamond Light Source, Didcot OX11 0DE, United Kingdom — [3]Institut für Festkörperphysik, Karlsruhe Institute for Technology, Karlsruhe 76021, Germany

There were plenty of attempts to measure superconducting gap in FeSe and related SC using different techniques: tunneling spectroscopy, photoemission spectroscopy, specific heat. But the consensus on a size and symmetry of the SC gap has not been reached. ARPES is only one technique, in which it is possible to measure SC gap in a certain part of momentum space directly. Because of this ARPES is a key tool for solving this complicated problem. Here we present results of our investigation of the superconducting gap anisotropy in FeSe using angle-resolved photoemission spectroscopy. We have measured the superconducting gap for both electron- and hole-like pockets for different kz positions. The gaps on both pockets are considerably anisotropic. Such gap anisotropy can possibly be explained in terms of orbital-selective pairing.

TT 52.5 Wed 10:30 HFT-FT 101

Evolution of the Fermi surface across a clean nematic quantum phase transition in $FeSe_{1-x}S_x$ — •Pascal Reiss[1], David Graf[2], Amir A. Haghighirad[3], and Amalia I. Coldea[1] — [1]Clarendon Laboratory, Oxford University, UK — [2]NHMFL, Tallahassee, USA — [3]IFP, Karlsruhe Institute of Technology, GER

The interplay between superconductivity and long-range electronic orders is an intensely studied subject. Iron-based superconductors offer a fruitful field to investigate the role of magnetic order, however the concomitant instability towards nematic (orbital) order requires to be disentangled. For this purpose, the isoelectronic doping series $FeSe_{1-x}S_x$ is ideally suited. Undoped FeSe displays nematic but no long-range magnetic order, and becomes superconducting below 9 K. Applied pressure suppresses the nematic transition towards 0 K, but the nematic quantum phase transition is masked by an emerging magnetic phase stabilising superconductivity up to 37 K [1].

With sulphur doping, magnetic order is quickly suppressed, and the nematic quantum phase transition is unmasked [2,3]. We will present transport and TDO measurements as a function of pressure and fields up to 45 T, and – for the first time – we will follow the evolution of the Fermi surface and the strength of electronic correlations across a nematic quantum phase transition.

We acknowledge funding from the EPSRC UK (EP/I004475/1), the NSF and the State of Florida.

[1] S. Medvedev *et al.*, Nat. Mater. (2009)
[2] K. Matsuura *et al.*, Nat. Commun. (2017)
[3] L. Xiang *et al.*, PRB (2017)

TT 52.6 Wed 10:45 HFT-FT 101

Domain Imaging Across the Magneto-Structural Phase Transition in $Fe_{1+y}Te$ — •Jonas Warmuth[1], Martin Bremholm[2], Philip Hofmann[2], Jens Wiebe[1], and Roland Wiesendanger[1] — [1]Dept. of Physics, Hamburg University, Germany — [2]Depts. of Chemistry and Physics, Aarhus University, Denmark

The investigation of the magnetic phase transitions in the parent compounds of Fe-based superconductors is essential for understanding the pairing mechanism in the related superconducting compounds [1,2]. Here, we present a real space spin-resolved scanning tunneling microscopy investigation of the surface of $Fe_{1+y}Te$ single crystals with different excess Fe contents, y, which are continuously driven through the magnetic phase transition. For $Fe_{1.08}Te$, the transition into the low-temperature monoclinic commensurate antiferromagnetic phase [3] is accompanied by the sudden emergence of ordering into four rotational domains with different orientations of the monoclinic structure and of the antiferromagnetic order, showing how structural and magnetic order are intertwined. In the low-temperature phase of $Fe_{1.12}Te$ one type of the domain boundaries disappears, and the transition into the paramagnetic phase gets rather broad, which is assigned to the formation of a mixture of orthorhombic and monoclinic phases [4].

[1] Paglione, J. *et al*, Nature Physics **6**, 645-658 (2010)
[2] Stewart, G. R. *et al*, Reviews of Modern Physics **83**, 1589 (2011)
[3] Hänke, T. *et al*, Nature Communications **8**, 13939 (2017)
[4] Koz, C. *et al*, Physical Review B **88**, 094509 (2013)

TT 52.7 Wed 11:00 HFT-FT 101

evidence of orbital selective cooper pairing within surface unit cell of FeSe — •Fang Yang[1], Jasmin Jandke[1], Peter Adelmann[2], Markus Klug[3], Thomas Wolf[2], Jörg Schmalian[3], and Wulf Wulfhekel[1] — [1]Physikalisches institut, KIT, Karlsruhe, Germany — [2]Institut für Festkörperphysik, KIT, Karlsruhe, Germany — [3]Institut für Theorie der Kondensierten Materie, KIT, Karlsruhe, Germany

Numerous attempts have been made to demonstrate the multi-band nature of superconductivity in bulk FeSe in the nematic phase. To investigate this multi-band character, we determined the electronic density of states at the surface of FeSe with high energy and spatial resolution using a 40 mK dilution STM. A high spatial resolution was achieved using an STM tip with electronic p-states, which not only gives a higher lateral resolution compared to an s-state tip but also is sensitive to the surface symmetry. With this, we were able to resolve the superconducting gap of all five bands cutting the Fermi energy and, in combination with the high lateral resolution, the spatial distribution of the intensity of the quasiparticle peaks within the unit cell. By comparison with the expected d-orbital wave functions, we propose that different gaps are of particular orbital nature.

15 min. break.

TT 52.8 Wed 11:30 HFT-FT 101

Structural component of an incipient ordering mode — •Sahana Roessler[1], Alexander A. Tsirlin[2], Marco Scavini[3], Cevriye Koz[1], Ulrich Schwarz[1], Ulrich K. Roessler[4], and Steffen Wirth[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Experimental Physics VI, University of Augsburg, Germany — [3]Chemistry Department, University of Milan, Milano, Italy — [4]IFW-Dresden, Institute for Solid State Research, D-01171 Dresden, Germany

The binary compound FeSe is a multiband superconductor with fascinating properties. Unlike other Fe-based superconductors, the transition from tetragonal ($P4/nmm$) to orthorhombic ($Cmme$) structure in FeSe at $T_s \approx 87$ K at ambient pressure is not accompanied by a long-range magnetic order and the leading order parameter of the phase transition is attributed to an electronic origin. Upon further reducing temperature, two energy scales at temperatures $T^* \approx 75$ K and $T^{**} \approx 20$ K have been identified based on anomalies observed in the Hall effect, magnetotransport, thermal conductivity, and scanning tunneling spectroscopy [1]. Here we show, using a pair distribution function analysis, a local Fe-Fe atomic distortion with short-range correlations occurring at T^{**}. Thus, incipient ordering in FeSe occurs as a precursor state to superconductivity and is reminiscent of behavior found in several high-T_c cuprates [2].

[1] S. Rößler *et al.*, Phys. Rev. B 92, 060505(R) (2015).
[2] E. Fradkin and S. A. Kivelson, Nature Phys. 8, 864 (2012).

TT 52.9 Wed 11:45 HFT-FT 101

Unconventional pairing versus phonon mediated superconductivity in single FeSe layers — •Jasmin Jandke[1], Fang Yang[1], Patrik Hlobil[2], Tobias Engelhardt[1], Chunlei Gao[3],

Jörg Schmalian[2,4], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, KIT, 76131 Karlsruhe, Germany — [2]Institut für Theorie der Kondensierten Materie, KIT, 76131 Karlsruhe, Germany — [3]State Key Laboratory of Surface Physics and Department of Physics, Fudan University Shanghai 200433, China — [4]Institut für Festörperphysik, KIT, 76344 Karlsruhe, Germany

Both conventional [1] and unconventional [2] mechanisms have been discussed for a single layer FeSe films on $SrTiO_3$ showing a T_c of 60-100 K [3,4], i.e. an order of magnitude larger than in bulk FeSe. Here we report a direct measurement of the electron-boson coupling in FeSe on $SrTiO_3$ using inelastic tunneling spectroscopy. We exclude strong electron-phonon coupling except for places near structural domain boundaries in the FeSe layer. Instead, the bosonic excitation spectrum is shown to be fully gapped below T_c in agreement with an electronic pairing mechanism. By deconvolution of the experimental data, we were able to reconstruct the electron-boson coupling function, which shows beside a gap a characteristic peak at the expected resonance mode energy of paramagnons.

[1] J. J. Lee et al., Nature, 515, 245 (2014)
[2] B. Li et al., J. Appl. Phys. 115, 193907 (2014)
[3] Q.-Y. Wang et al., Chin. Phys. Lett. 29, 037402 (2012)
[4] J.-F. Ge et al., Nat. Mat., 14, 285 (2015)

TT 52.10 Wed 12:00 HFT-FT 101

Interplay of structural properties and magnetic disorder in FeSe: Density-functional theory calculations — •Felix Lochner[1,2], Ilya Eremin[2], Jörg Neugebauer[1], and Tilmann Hickel[1] — [1]Max-Planck-Institut für Eisenforschung, Düsseldorf, Deutschland — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Deutschland

We calculate the effect of local magnetic moments and particularly their paramagnetic disorder on the normal state of a prototype iron-based superconductor FeSe. For this purpose the spin-space averaging approach [1] for density functional theory (DFT) calculations is applied.

Here, we analyze the structural parameters of FeSe, the impact on the electronic properties as well as the interplay of electronic and phononic degrees of freedom in the paramagnetic state. In contrast to original non-magnetic DFT calculations [2], the results in the paramagnetic state agree after relaxation with experimentally observed lattice parameters with an error less than 5%. Based on this achievement a DFT based understanding of the mechanisms underlying the superconducting behavior and driving the nematic transition of FeSe seems now to be feasible.

[1] F. Körmann, A. Dick, B. Grabowski, T. Hickel, J. Neugebauer, Phys. Rev. B 85, 125104 (2012).
[2] L. Boeri, M. Calandra, I. I. Mazin, O. V. Dolgov, and F. Mauri Phys. Rev. B 82, 020506(R) (2010)

TT 52.11 Wed 12:15 HFT-FT 101

Electron-boson interaction of LiFeAs revealed by resonantly enhanced Friedel oscillations: Experiment — Zhixiang Sun[1], Pranab Kumar Nag[1], Steffen Sykora[1], Jose M. Guevara[1], Rhea Kappenberger[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2,3], and •Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

For rationalizing the Cooper pairing mechanism in a superconductor, it is central to identify bosons interacting with the conduction electrons. We determine the energy and momentum characteristics of such bosons in LiFeAs by exploiting the boson-assisted resonant amplification of Friedel oscillations by Fourier transform scanning tunneling spectroscopy (FT-STS). We show that the FT-STS signatures of the bosonic states survive in the normal state, and, moreover, that they are in perfect agreement with well-known strong above-gap anomalies in independently measured tunneling spectra at the very same energy. Thus, the small-momentum bosonic modes are promising candidates for providing the pairing interaction in LiFeAs.

TT 52.12 Wed 12:30 HFT-FT 101

Nematic fluctuations in Li doped NaFeAs — •Jose M. Guevara[1], Zhixiang Sun[1], Steffen Sykora[1], Chanhee Kim[2], Aga Shahee[2], Dilipkumar Bhoi[2], Kee Hoon Kim[2], Bernd Büchner[1], and Christian Hess[1] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]CeNSCMR, Department of Physics and Astronomy, Seoul National University, Seoul 151-747, South Korea

In strongly correlated electronic systems, the electronic distribution favors local variations, often forming patterns that break the rotational symmetry of the crystal. Nematicity has special relevance in systems where competiton of different phases plays an important role, and has been observed in the most prominent families of high temperature superconductors, i.e. cuprates and iron-pnictides. The Li doped NaFeAs samples allows a new approach to explore nematicity in Iron-pnictides, given the strong differences of the phase diagram in the parents compounds, NaFeAs and LiFeAs.

In our work, we measure 3%, 4% and 5% Li doped NaFeAs samples, where longe range order is suppressed, with a low temperature scanning tunneling microscope. We visualize the real-space distribution of the nematic fluctuations, which are found to ubiquitously exist, from the superconducting state to the normal state at higher temperatures.

TT 52.13 Wed 12:45 HFT-FT 101

Electron-boson interaction of LiFeAs revealed by resonantly enhanced Friedel oscillations: Theory — •Steffen Sykora[1], Zhixiang Sun[1], Pranab Kumar Nag[1], Jose M. Guevara[1], Rhea Kappenberger[1], Sabine Wurmehl[1,2], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

We present a new experimental/theoretical approach to determine bosonic modes by investigating resonantly enhanced Friedel oscillations caused by a coupling of conduction electrons to the bosons. Upon focusing on the unconventional superconductor LiFeAs we show that under particular conditions the impurity scattering potential is strongly renormalized leading to enhanced signals in the quasiparticle interference. For this a simplified model of electron-boson coupling in the presence of one single impurity is solved by a many-particle renormalization method. Comparing our theoretical results with Fourier transform scanning tunneling spectroscopy data we reveal for LiFeAs bosonic states at particular momentum and energy. The bosonic modes are promising candidates for providing the pairing interaction in LiFeAs.

TT 53: Quantum Impurities and Kondo Physics

Time: Wednesday 9:30–11:15 Location: HFT-FT 131

TT 53.1 Wed 9:30 HFT-FT 131

Quench dynamics in correlated quantum dots coupled to ferromagnetic leads — •Kacper Wrześniewski and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Poznan, Poland.

We investigate the quantum quench dynamics in the single impurity Anderson model with ferromagnetic leads. The real-time evolution at finite temperatures is calculated by means of the time-dependent numerical renormalization group method in the matrix product states framework. In order to suppress the band discretization effects, we use the z-averaging trick and apply an appropriate broadening of data in collected frequency space, which is then Fourier-transformed to the real-time domain.

We study the system's response to two different types of quantum quenches: The first one relies on a sudden shift of the dot's energy level, while the second one is performed in the coupling strength to the leads. We analyze the charge and spin dynamics by calculating the time-dependent expectation values of local variables, such as the impurity's occupation number and its magnetization. We determine the time-dependence of a ferromagnetic-contact-induced exchange field and predict its nonmonotonic build-up. The influence of temperature and quench magnitude on the considered dynamics is also thoroughly discussed.

TT 53.2 Wed 9:45 HFT-FT 131

A pseudogap Anderson impurity model as a continuum limit of a generalized integrable Hubbard model — •Yahya Öz and Andreas Klümper — Bergische Universität Wuppertal

Starting from the integrable Hubbard model by use of Shastry's R-matrix we add an impurity on the lattice. Furthermore, we modify the dispersion relation and hence the density of states of the host characteristic for a pseudogap system. For the thermodynamics of this lattice model we derive a finite set of non-linear integral equations (NLIE) of convolution type. Applying a suitable continuum limit to this integrable lattice model we obtain a pseudogap Anderson impurity model (pAIM). This AIM has vanishing density of states at the Fermi energy with a tunable exponent ($\rho \simeq |\epsilon|^r$). In this way, the new integrable lattice impurity model with interacting host interacting with an impurity yields a new impurity model in the continuum with a non-interacting host that still interacts with the impurity. We describe the screening of the impurity moment. The Hamiltonian of the new pseudogap Anderson impurity model is explicitly specified.

TT 53.3 Wed 10:00 HFT-FT 131

The role of impurities in model correlated fermionic systems — •Banhi Chatterjee[1,2], Jan Skolimowski[1,3], and Krzysztof Byczuk[1] — [1]Institute of Theoretical Physics, Warsaw University, Warsaw, Poland — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [3]Jozef Stefan Institute, Ljubljana, Slovenia

The role of impurities and resulting Friedel Oscillations (FO) in the Fermi liquid phase, Mott insulating phase, and at the Mott transition is studied in fermionic lattice models at zero temperature. We consider the case of two impurities which is aimed to simulate the effect of defects and dopants in real lattices. A comparative picture with the single impurity case is also presented. Electronic correlations are accounted for by including the local self-energy term from the homogeneous dynamical mean-field theory calculations. Interference effects due to the additional impurity on FO is seen which reduces with the interaction and also the relative distance between the impurities. The position of interference maxima and minima are not changed by the interactions. In the metallic phase the amplitudes of FO are damped with increasing the interactions while the period remains unchanged at half-filling. FO almost disappear close to the Mott transition and completely beyond it in all the cases. The screening effects, quantified by the screening charge are discussed. The effects of interference on the spectral functions are also shown.

TT 53.4 Wed 10:15 HFT-FT 131

Numerical Renormalization Group study of Gate Induced Kondo Screening in Graphene — •Daniel May[1], Kira Deltenre[1], Anika Henke[1], Jinhai Mao[2], Yuhang Jiang[2], Po-Wei Lo[3,4], Guohong Li[2], Guang-Yu Guo[3,4], Frithjof Anders[1], and Eva Y. Andrei[2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, Germany — [2]Rutgers University, Department of Physics and Astronomy, USA — [3]National Taiwan University, Department of Physics, Taiwan — [4]National Center for Theoretical Sciences, Physics Division, Taiwan

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries. When graphene's honeycomb lattice is disrupted by single atom vacancies a gate voltage dependent Kondo effect may emerge. We present numerical renormalization group (NRG) calculations for a realistic two-orbital model consisting of a local σ orbital and a localized π orbital induced by the vacancy. Depending on the graphene curvature in the vicinity of the vacancy, we determine three different regimes. The re-entrance regime is characterized by a conventional Kondo effect (p doping), a breakdown of the Kondo peak close to the Dirac point $|\mu| \to 0$, and a underscreened Kondo (n doping) where the π band is screening the magnetic moment of the σ orbital. Changing the hybridization between impurity and band drives the system into a regime where Kondo screening is present for either strong n or p doping.

TT 53.5 Wed 10:30 HFT-FT 131

Restoring the Varma-Jones quantum critical point in absence of local particle-hole symmetry — •Fabian Eickhoff[1], Benedikt Lechtenberg[2], and Frithjof Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund — [2]Department of Physics, Kyoto University, Kyoto 606-8502, Japan

The quantum critical point (QCP) in two impurity model established by Varma and Jones marks the transition between an RKKY driven impurity singlet and a extended Kondo singlet and is generically destroyed by particle-hole symmetry breaking. We derive an effective low energy description for the two-impurity Anderson model and extract the marginal relevant operator that drives the system away from the QCP. By adding an additional electron tunneling term with an analytically calculated strength, we prove the restoration of the Varma-Jones QCP using Wilson's numerical renormalization group approach. We show that the antiferromagnetic contribution to the RKKY interaction is given by an analytic function of this hopping amplitude. We analyse the strength and directionality of the RKKY interaction in different spatial dimensions.

TT 53.6 Wed 10:45 HFT-FT 131

Dimensional crossover in molecular Kondo systems — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Advances in scanning tunneling microscopy allow nowadays for the atomically precise engineering of Kondo nanosystems ranging from a single impurity to lattice Kondo situations with a dominant Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction between the individual magnetic atoms. Here, starting with a single magnetic impurity deposited on the metallic surface, we perform auxiliary-field quantum Monte Carlo simulations of the Kondo lattice model and elucidate necessary conditions for the emergence of the Kondo lattice behavior in a nanosystem composed of a few magnetic atoms only.

TT 53.7 Wed 11:00 HFT-FT 131

Two-stage Kondo effect in the presence of induced pairing in T-shaped double quantum dots — •Krzysztof Wójcik[1,2] and Ireneusz Weymann[2] — [1]Institute of Physics, Polish Academy of Sciences, 60-197 Poznań, Poland — [2]Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland

In this contribution the transport properties of a T-shaped double quantum dot (QD) proximized by a superconductor (SC) are discussed. In particular, the linear response conductance and the Seebeck coefficient, calculated by means of the numerical renormalization group method, are analyzed. In the absence of SC and for relatively small inter-dot hopping matrix element, the two-stage Kondo screening is known to be present in the system [1]. We show that, generally, the effects of coupling of only one QD to SC may be qualitatively understood as a consequence of effective reduction of the Coulomb interactions. In particular, the dependence of the Kondo temperature corresponding to

the two-stage Kondo screening on the coupling to SC lead is explained in this way. Similarly, one can describe the quantum phase transition between the Kondo-like state and the state characterized by the local density of states dominated by the Andreev bound states. However, the coupling of both QDs to SC results in creation and destruction of nonlocal pairs, which tends to additionally enhance the formation of total Kondo singlet. The consequences for transport properties in such a scenario are discussed.

[1] P. S. Cornaglia, D. R. Grempel, Phys. Rev. B **71**, 075305 (2005).

TT 54: Focus Session: Chaos and Correlation in Quantum Matter (joint session DY/TT)

The irreversibility of dynamics of complex systems ("emergent arrow of time") has been a point of controversy lasting over a century. At its heart lies the seeming contradiction between the intrinsic reversibility of the microscopic laws of nature and the manifestly time-irreversible behavior of macroscopic phenomena. Chaos plays a crucial role in resolving this paradox. The past decade has seen a great revival of interest in this question concerning the foundations of quantum statistical mechanics and how chaos arises in quantum manybody systems. It has been driven by theoretical findings involving the long sought demonstration that many-body localization (MBL) exists as well as the derivation of exact bounds on chaos. On the experimental side, significant advances have been made in the study of cold atomic gases which provide examples of closed macroscopic quantum systems for which the foundational questions of quantum statistical mechanics are especially relevant. The focus session will summarize recent advances in this very active field of studies.

Coordinators: Frank Pollmann, David Luitz

Time: Wednesday 9:30–12:15 Location: EB 107

Invited Talk TT 54.1 Wed 9:30 EB 107

Computing quantum thermalization dynamics: from quantum chaos to emergent hydrodynamics — •Ehud Altman — Department of Physics, University of California, Berkeley, CA 94720

Computing the dynamics of strongly interacting quantum systems presents a fundamental challenge due to the growth of entanglement entropy in time. In the first part of the talk I will describe a new approach that overcomes this obstruction and captures chaotic dynamics and emergent hydrodynamic transport of quantum systems. Our scheme utilizes the time dependent variational principle with matrix product states to truncate "non-useful" entanglement, while retaining crucial information on local observables. In the second part of the talk I will offer a new viewpoint on the relation between quantum and classical chaos in many body systems, using a classical version of the Sachdev-Ye-Kitaev model as an example. Chaos in this model can be understood as arising from diverging geodesics on a SO(N) manifold equipped with a random metric with locally negative curvature. The quantum bound on chaos arises from a *chaotic mobility edge* in the classical Lyapunov spectrum, separating the lower part of the spectrum for which a classical chaos picture applies from the higher part of the spectrum for which quantum interference effects are strong enough to kill classical chaos. This edge corresponds to a curvature scale of the order of the de Broglie wavelength.

TT 54.2 Wed 10:00 EB 107

Hydrodynamics of operator spreading from random circuits — •Tibor Rakovszky[1], Curt von Keyserlingk[2], Shivaji Sondhi[3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]University of Birmingham, School of Physics & Astronomy, B15 2TT, UK — [3]Department of Physics, Princeton University, Princeton, New Jersey 08544, USA

In this talk we use random local unitary circuits to gain insight into the scrambling of quantum information in many-body systems. For a circuit with no conserved quantities we show that the average spreading of operators obeys an exact "hydrodynamic" description, in terms of a biased diffusion equation, and discuss the consequences for out-of-time ordered correlators (OTOCs) and entanglement growth. We conjecture that a similar effective description should hold in more generic ergodic systems, a claim supported by numerical results. Furthermore, we consider random circuits with a U(1) symmetry and discuss the interplay between the hydrodynamics of the conserved charge and that of operator spreading, leading to the appearance of long-time power law tails in out-of-time-ordered correlators. We also discuss the behavior of OTOCs at different chemical potentials, an analogous quantity to the finite temperature OTOCs discussed in the literature, and find that their initial spreading is slowed down when the chemical potential is large.

TT 54.3 Wed 10:15 EB 107

Out-Of-Time-Ordered Correlators in Chaotic and Critical Many-Body Systems: Path Interference and Scrambling Times — •Josef Rammensee, Benjamin Geiger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Out-of-time-ordered correlators $\langle[\hat{V},\hat{W}(t)]^\dagger[\hat{V},\hat{W}(t)]\rangle$ have been identified to be highly suitable tools to identify the onset of chaos in many-body quantum systems[1]. Contrary to already known indicators, the unusual time ordering of the operators is able to directly capture the local hyperbolic nature of the classical counterpart. One expects an exponential increase at short times with a rate related to classical Lyapunov exponents. Numerical studies in chaotic systems[2] indicate a saturation after the time scale for the classical-to-quantum-crossover, known as Ehrenfest or scrambling time. Our numerical studies show, that many-body criticality mimics this behaviour of chaotic systems, however with an exponent given by the local instability rate. We provide insight into the physical origin of the exponential growth and the saturation by using semiclassical methods based on the Van-Vleck-propagator for single- and many-body systems[3]. We show that the notion of interfering classical trajectories is well suited to provide a quantitative picture and we explicitly discuss the emergence of the Lyapunov exponent, resp. instability rates and the relevant time scales.

[1] J. Maldacena *et al.*, JHEP 2016:106 (2016)
[2] E. B. Rozenbaum *et al.*, PRL **118**, 086801 (2017)
[3] T. Engl, J. Dujardin, A. Argüelles *et al.*, PRL **112**, 140403 (2014)

TT 54.4 Wed 10:30 EB 107

Out of time order correlators from the time dependent variational principle — •Kevin Hemery, Frank Pollmann, and David Luitz — Department of Physics, T42, Technische Universität Muenchen, James-Franck-Strasse 1, D-85748 Garching, Germany

Out of time order correlators (OTOCs), which measure the spreading of information in quantum systems, have drawn a lot of attention recently. However, the numerical calculation of OTOCs is extremely challenging, which renders the verification of theoretical predictions difficult. We tackle this problem within the Schroedinger picture in combination with a matrix-product state formulation of the time dependent variational principle (TDVP). First, we benchmark this technique by comparing the results with exact Krylov space time evolution results for small chains. Second, we calculate the OTOCs for system sizes which are unreachable by exact methods and analyze the hydrodynamic spreading of the light cone front.

TT 54.5 Wed 10:45 EB 107

Out-of-time-ordered correlation functions in the O(N) model — •Alexander Schuckert[1] and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Institute for Advanced Study, Technical University of Munich,

85748 Garching, Germany

In classical systems, chaos can be characterized by the sensitivity of the particles' trajectories with respect to small deviations in the initial state. An exponential growth in time then marks chaotic behavior. Recently, it has been proposed that certain out-of-time-ordered correlation functions (OTOCs) may be a suitable extension to characterize chaos in quantum many-body systems. OTOCs also probe the scrambling of quantum information across the system and thereby provide a direct connection between an information theoretic measure and chaotic dynamics. We calculate the time evolution of OTOCs in an O(N) symmetric scalar field theory at high temperatures using non-perturbative expansion techniques. Apart from the Lyapunov exponent quantifying a potential exponential growth of chaos, we are also interested in the emergent time scales of information propagation, including light-cone and butterfly velocities.

15 min. break

Invited Talk TT 54.6 Wed 11:15 EB 107

Quantum Thermalization Dynamics: From Information Scrambling to Emergent Hydrodynamics — •Michael Knap — Department of Physics and Institute for Advanced Study, Technical University of Munich, 85748 Garching, Germany

Generic, clean quantum many-body systems approach a thermal equilibrium after a long time evolution. In order to reach a global equilibrium, conserved quantities have to be transported across the whole system which is a rather slow process governed by diffusion. By contrast, the scrambling of quantum information is ballistic and hence can be characterized by a "butterfly" velocity. One way of describing the propagation of quantum information is to study out-of-time ordered (OTO) correlation functions, which are unconventional correlation functions with time arguments that are not time ordered. Using matrix-product-state based numerical simulations, we compute such correlators at high temperatures in a one-dimensional Bose-Hubbard model and in generic spin-models, where well defined quasi-particles cease to exist [1]. Finally, we will discuss ways of experimentally characterizing these unconventional OTO correlation functions in synthetic quantum matter.

[1] A. Bohrdt, C. B. Mendl, M. Endres, M. Knap, New J. Phys. 19, 063001 (2017).

TT 54.7 Wed 11:45 EB 107

Entanglement Entropy in SYK — •Renato Miguel Alves Dantas[1], Daniele Trapin[1], Paul McClarty[1], Piotr Surówka[1], and Masudul Haque[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Str. 38, 01187 Dresden — [2]Department of Theoretical Physics, Maynooth University, Co. Kildare, Ireland

Eigenstates of interacting systems far from the ground state are now recognized as important for understanding non-equilibrium phenomena. We present a study of the entanglement in eigenstates of zero-dimensional fermionic models with random interactions. We consider both chaotic and integrable versions of these Sachdev-Ye-Kitaev models, respectively having quartic and quadratic couplings.

TT 54.8 Wed 12:00 EB 107

What is the right theory of transverse Anderson localization of light? — •Walter Schirmacher[1,3,4], Behnam Abaie[2], Arash Mafi[2], Giancarlo Ruocco[3,4], and Marco Leonetti[3,4] — [1]Universität Mainz — [2]Univ. New Mexico, USA — [3]Istituto Italiano di Technologia, Roma, Italy — [4]Universit'a La Sapienza, Roma, Italy

Anderson localization of light is traditionally described in analogy to electrons in a random potential. Within this description, the random potential depends on the wavelength of the incident light. For transverse Anderson localization this leads to the prediction that the distribution of localization lengths – and hence its average – strongly depends on the wavelength. In an alternative description, in terms of a spatially fluctuating electric modulus, this is not the case. Here, we report on an experimentum crucis in order to investigate the validity of the two conflicting theories using optical samples exhibiting transverse Anderson localization. We do not find any dependence of the observed average localization radii on the light wavelength. We conclude that the modulus-type description is the correct one and not the potential-type one. We corroborate this by showing that in the derivation of the traditional, potential-type theory a term in the wave equation has been tacitly neglected. In our new modulus-type theory the wave equation is exact. We check the consistency of the new theory with our data using the nonlinear sigma model. We comment on the consequences for the general case of three-dimensional disorder.

TT 55: Multiferroic Oxide Thin Films and Heterostructures I (joint session KFM/TT/MA)

Organizers: César Magén - University of Zaragoza, Aragón (Spain); Kathrin Dörr - Martin-Luther-Universität Halle-Wittenberg - Halle

Multiferroic oxide thin films and magnetoelectrically coupled oxide heterostructures are among the most attractive topics in the field of Complex Oxides. Within this extensive family of compounds, which are characterized by an unprecedented wealth of physical phenomena upon subtle variations of the structure or chemistry, multiferroics stand out due to the exciting novel physics underlying the coexistence and coupling of multiple ferroic orders. This exotic behavior bestows inherent multifunctionality upon these systems (either single-phase or heterostructure multiferroics), providing strong potential for future nanoelectronic devices.

Time: Wednesday 9:30–12:45 Location: EMH 225

Invited Talk TT 55.1 Wed 9:30 EMH 225

Oxygen vacancy controlled functionalities at interfaces of multiferroic tunnel junctions. — •Jacobo Santamaria — GFMC. Universidad Complutense 28040 Madrid

Oxygen vacancies are the most common defect in oxide perovskite oxides. Important applications are associated to their controlled generation and transport in electrochemical energy (fuel cells and batteries) and memory (memristors) devices. At interfaces oxygen vacancies can accumulate under the action of external electric fields and, especially in nanostructures be the source of novel, yet unreported, functionalities. Here we demonstrate the dynamic control of the vacancy profile in the nanometer thick barrier of a ferroelectric tunnel junction. Oxygen vacancies generated at an electrochemically active electrode accumulate towards the asymmetric interfaces of a ferroelectric tunnel barrier under the action of an external electric field and their ensuing doping effect modify the stability of ferroelectric polarization. I will further show that oxygen vacancies in a ferroelectric tunnel barrier may stabilize unexpected domain structures which control the tunneling transport providing a major step forward towards the new concept *The Wall is the Device* , to exploit the electronic properties of domain walls for ferroelectric tunnel barriers with new functionalities.

TT 55.2 Wed 10:00 EMH 225

Structure and Magnetism of the Co/PZT/LSMO Interface — •Holger Meyerheim[1], Arthur Ernst[2], Katayoon Mohseni[1], Andrey Polyakov[1], Nathalie Jedrecy[3], Andy Quindeau[1], Victor Antonov[1], Manuel Valvidares[4], Hari Vasili[4], and Pierluigi Gargiani[4] — [1]MPI f. Mikrostrukturphysik, D-06120 Halle — [2]Inst. für Th. Physik, JKU, A-4040 Linz, Austria — [3]INSP, UPMC-Sorbonne Univ., 75005 Paris, France — [4]Alba, 08290 Cerdanyola del Vallés, Spain

Using surface x-ray diffraction, x-ray absorption fine structure and x-ray circular dichroism (XMCD) experiments we have studied the geometric and magnetic properties of the Co/Pb($Ti_{0.8}Zr_{0.2}$)O_3 interface. Co deposition in submonolayer amounts on the 2 unit cells thick (Ti,Zr)O_2 terminated Pb ($Ti_{0.8}Zr_{0.2}$)O_3 (PZT) layer leads to

the formation of a perovskite type structure with Co-O distances of approximately 2.0 Å (octahedral) and 2.8 Å (cubic) in addition to a metallic Co-Co correlation near 2.4 Å. Co-$L_{2,3}$-XMCD spectra also reveal different Co environments, especially two Co-O contributions (A) and (B) related to the octahedral coordination (m=2.69μ_B) and the cubic coordination (m=2.33 μ_B). The XMCD analysis also evidences an anti-FM oriented induced moment at the PZT top layer Ti site (m=-0.005μ_B) related to the negative tunneling electro resistance effect. This result supports the "hybridization model" suggested by D.Pantel et al., Nat. Mat. 11, 289 (2012).
Support by SFB 762 (TP A5) is acknowledged. We thank E. Fonda (Samba at Soleil) and the ALBA staff for help during the experiments.

TT 55.3 Wed 10:15 EMH 225

Interfacial mechanisms in magneto-electric bismuth iron garnet thin films — •Laura Bocher[1], Adrien Teurtrie[1,2], Elena Popova[2], Odile Stéphan[1], Alexandre Gloter[1], and Niels Keller[2] — [1]Laboratoire de Physique des Solides - UMR 8502 CNRS, Université Paris-Sud, Orsay, FR — [2]Groupe d'Etude de la Matière Condensée - UMR8635 CNRS, UVSQ, Université Paris-Saclay, FR

Bismuth iron garnet (BIG) is ferrimagnetic with a relatively high magnetization (1600 G at 300 K), a magnetic ordering temperature from 650 K, and a giant Faraday rotation [1]. More recently, we evidenced a strong magneto-electric coupling at 300 K and above in BIG thin films opening new perspectives for an electric control of the magnetization [2]. However BIG can solely be elaborated in thin film form using non-equilibrium growth techniques and no bulk reference exists for conventional investigations. Hence precise knowledge on the atomic and electronic structures of BIG thin films remains a key challenge to understand better their structure-property relationships.

Here we will shed light on BIG thin films using advanced electron spectro-microscopy techniques, i.e. Cs-STEM/EELS, to identify how its cubic structure can accommodate locally different lattice mismatches through a variety of relaxation mechanisms and verify down to the scale of the atomic columns any possible cation interdiffusion and/or electronic reconstruction at the film/substrate interface [3].

[1] M. Deb, et al. J. Phys. D 45 (2012) 455001. [2] E. Popova et al. APL 110 (2017) 142404. [3] E. Popova et al. JAP 121 (2017) 115304

TT 55.4 Wed 10:30 EMH 225

Nonlinear spin-lattice coupling in EuTiO3: novel two-dimensional magneto-optical device for light modulation — •Annette Bussmann-Holder[1], Krystian Rolder[2], and Jürgen Köhler[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]2Institute of Physics, University of Silesia, ul. Uniwersytecka 4, 40-007 Katowice, Poland

EuTiO3 is antiferromagnetic at low temperature, namely below TN=5.7K. In the high temperature paramagnetic phase the strongly nonlinear coupling between the lattice and the nominally silent Eu 4f7 spins induces magnetic correlations which become apparent in muon spin rotation experiments and more recently in birefringence measurements in an external magnetic field. It is shown here, that high quality films of insulating EuTiO3 deposited on a thin SrTiO3 substrate are versatile tools for light modulation. The operating temperature is close to room temperature and admits multiple device engineering. By using small magnetic fields birefringence of the samples can be switched off and on. Similarly, rotation of the sample in the field can modify its birefringence Δn. In addition, Δn can be increased by a factor of 4 in very modest fields with simultaneously enhancing the operating temperature by almost 100K. The results can be understood in terms of paramagnon phonon interaction where spin activity is achieved via the local spin-phonon double-well potential.

TT 55.5 Wed 10:45 EMH 225

Complexity in the structural and magnetic properties of almost multiferroic EuTiO3 thin films — Zurab Guguchia[1], Zaher Salman[2], •Hugo Keller[3], Krystian Roleder[4], Jürgen Köhler[5], and Annette Bussmann-Holder[5] — [1]Department of Physics, Columbia University, New York, New York 10027, USA — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [3]Physik-Institut der Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [4]Institute of Physics, University of Silesia, ul. Uniwersytecka 4, PL-40-007 Katowice, Poland — [5]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

In a number of recent publications hidden magnetic properties at high temperatures have been reported for EuTiO3 (ETO), which orders antiferromagnetically below TN=5.7K. In addition, structural phase transitions have been discovered which correlate with the magnetic responses and can be tuned by a magnetic field. In order to identify the magnetic properties of ETO at temperatures well above TN, low-energy muon-spin rotation (μSR) experiments have been performed on thin films of ETO which exhibit all properties observed in bulk materials and are thus well suited to conclude about the magnetic order of the bulk. The μSR data reveal anomalies at 282 and 200 K related to the structural phase transitions in accordance with birefringence results. In addition, a transition to some kind of magnetic order below 100 K was observed as previously indirectly deduced from conductivity and dielectric constant measurements.

TT 55.6 Wed 11:00 EMH 225

Surface reconstructions and related local properties of a $BiFeO_3$ thin film — •Pengxiang Xu[1] and Lei Jin[2] — [1]Institute for Theoretical Physics, ETH Zurich — [2]Peter Grünberg Institute (PGI-5), Forschungszentrum Juelich

Coupling between lattice and order parameters, such as polarization in ferroelectrics and/or polarity in polar structures, has a strong impact on surface relaxation and reconstruction. However, up to now, surface structures that involve the termination of both matrix polarization and polar atomic planes have received little attention, particularly on the atomic scale. Here, we study surface structures on a $BiFeO_3$ thin film using atomic-resolution scanning transmission electron microscopy and spectroscopy. Two types of surface structure are found, depending on the polarisation of the underlying ferroelectric domain. On domains that have an upward polarisation component, a layer with an Aurivillius-Bi_2O_2-like structural unit is observed. Dramatic changes in local properties are measured directly below the surface layer. On domains that have a downward polarisation component, no reconstructions are visible. Calculations based on ab initio density functional theory reproduce the results and are used to interpret the formation of the surface structures.

15 min. break

TT 55.7 Wed 11:30 EMH 225

Domain engineering in BFO films — •Yeseul Yun[1,2], Niranjan Ramakrishnegowda[1,2], David Knoche[1,2], Daesung Park[1,2], and Akash Bhatnagar[1,2] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany — [2]Martin Luther Universität Halle-Wittenberg, Halle (Saale, Germany)

Multiferroic materials have attracted great attention due to their unusual physical properties and potential in device applications. The lead-free bismuth ferrite ($BiFeO_3$) is one of the most promising candidates. The domain structure plays a crucial role in determining ferroelectric and magnetic properties. Domains and domain walls can be modulated by parameters such as epitaxial strain, film thickness, substrate termination and presence of conductive layers.

In this study, we investigate the role of plume-related characteristics in obtaining long range order of ferroelastic domains in $BiFeO_3$ films. BFO/LSMO hetero-structures were fabricated using PLD on STO (001) substrate with different O_2 partial pressures. Preferential nucleation and long range ordering of 71° domain walls was achieved by varying the plume density, indicating the importance of plasma plume dynamics for the evolution of domain structure in the films. The role of strain and electrostatic energies was also analyzed in conjunction. The thickness of BFO was varied to modulate the extent of strain, while the electrostatic conditions were tuned by the thickness of LSMO.

TT 55.8 Wed 11:45 EMH 225

Domain Engineering of the Bulk Photovoltaic Effect in Bismuth Ferrite — •David Knoche[1,2], Niranjan Ramakrishnegowda[1,2], Yeseul Yun[1,2], and Akash Bhatnagar[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany

The photovoltaic (PV) effect in multiferroic bismuth ferrite (BFO) can be largely attributed to the bulk photovoltaic (BPV) mechanism. The mechanism is associated to the absence of inversion symmetry in these materials. The principle of the BPV effect, that results in an above-bandgap open circuit voltage (V_{oc}), differs from the well-known photovoltaic effect observed in semiconductors like silicon, and still demands in-depth analysis. In this regard, the contribution of ferroic aspects,

such as orientation of domains, is crucial and can be potentially used as a tuning parameter.

Thin films of single crystalline $BiFeO_3$ were grown epitaxially via pulsed laser deposition. Planar electrodes with different in-between distances were deposited on top of the sample. The domain orientations within the measurement gap were manipulated by applying high electric fields across the electrodes. Gradual increment in the applied electric field was crucial in obtaining intermediate domain architectures, that were visualized with piezo force microscope (PFM). Photoelectrical response was measured in conjunction to evaluate the influence on Voc and short circuit current.

TT 55.9 Wed 12:00 EMH 225

Investigation of a-domain formation in Pb(Zr,Ti)O3 thin films — •Niranjan Ramakrishnegowda[1,2], Yeseul Yun[1,2], Daesung Park[1,2], and Akash Bhatnagar[1,2] — [1]Zentrum für Innovationskompetenz SiLi-nano, Halle (Saale), Germany — [2]Martin Luther Universität Halle-Wittenberg, Halle (Saale), Germany

Strain engineering of ferroelectric/ferroelastic domains is an active area of research nowadays, as it provides an exotic pathway to tune the resultant properties of ferroic materials. Since the domains can be also ferroelastic, the extent of strain, applied via the substrate-film lattice parameter mismatch, can be used to define the domain width, orientation and position. However, the persistence of the strain across the thickness of the film is largely affected by growth related process parameters.

In the case of $Pb(Zr,Ti)O_3$, one of the most widely investigated ferroelectric, recent studies involving asymmetric substrates allowed to fine tune the nucleation of a-domains, and the associated domain wall thickness. The proposed prerequisite condition of $a_{film} < a_{substrate} < c_{film}$ was satisfied. In this work we attempt to further analyze this condition by growing PZT films on symmetric $SrTiO_3$ substrates. The role of depolarization field was evaluated by the use of conductive oxide layers sandwiched between the film and the substrate. The usually neglected contribution of target density and purity will be also elaborated.

TT 55.10 Wed 12:15 EMH 225

Continuous control of morphotropic phases by strain doping — •Andreas Herklotz[1], Stefania Florina Rus[2], Er-Jia Guo[3], Kathrin Dörr[1], and Thomas Zac Ward[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania — [3]Oak Ridge National Laboratory, Oak Ridge, USA

The realization of a strain-driven morphotropic phase boundary in epitaxial $BiFeO_3$ (BFO) films has broadened this definition to single-phase materials and opened up great potential for advanced applications. However, a greater success of morphotropic systems in thin film technologies would require a *ex situ* control of the thin film's composition or strain state that is practically impossible with standard epitaxy approaches. Here we demonstrate that *ex situ* strain doping via low-energy helium implantation induces a complete phase transition from epitaxial rhombohedral-like to supertetragonal BFO films. This control over morphotropic phases is highly tunable and fully reversible via a high temperature anneal. We argue that strain doping of morphotropic films creates a new phase space based on internal and external lattice stress that can be seen as an analogue to temperature-composition phase diagrams of classical morphotropic ferroelectric systems.

This effort was wholly supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), Materials Sciences and Engineering Division, with user projects supported at ORNLs Center for Nanophase Materials Research (CNMS).

TT 55.11 Wed 12:30 EMH 225

Mechanical reading of ferroelectric polarity — •Gustau Catalan[1], Kumara Cordero[2], and Neus Domingo[2] — [1]ICREA-Institucio Catalana de Recerca i Estudis Avançats, Barcelona, Catalunya — [2]ICN2-Institut Catala de Nanociencia i Nanotecnologia, Barcelona, Catalunya

Flexoelectricity is polarization induced by strain gradient. It is closely related to piezoelectricity (polarization induced by strain), a phenomenon for which it was originally viewed as potential substitute. More recently, however, it has become apparent that very exciting new functionalities can be achieved when we combine both flexoelectricity and piezoelectricity in ferroelectrics.

One such functionality, reported in 2012, was the seminal discovery that strain gradients induced by the tip of an atomic force microscope (AFM) could mechanically *write* ferroelectric domains without applying any voltage. Here, we would like to report the complementary effect: the combination of flexoelectricity and piezoelectricity allows *reading* the polar sign of ferroelectric domains from pure (voltage-free) mechanical response.

TT 56: Focus Session: Quantum Nanophotonics in Solid State Systems II (joint session HL/TT)

Organizers: Alexander Szameit(U Rostock), Ruth Oulton (U Bristol), and Stephan Reitzenstein (TU Berlin)

Time: Wednesday 9:30–13:15 Location: EW 201

Invited Talk TT 56.1 Wed 9:30 EW 201

The quantum knitting machine: a quantum dot as device for deterministic production of cluster states of many entangled photons — •David Gershoni — The Physics Department and The Solid State Institute, Technion, Haifa, 32000, Israel

Photonic cluster states are a resource for quantum computation based solely on single-photon measurements [1]. We use semiconductor quantum dots to deterministically generate long strings of polarization-entangled photons in a cluster state by periodic timed excitation of a precessing matter qubit [1-2]. In each period, an entangled photon is added to the cluster state formed by the matter qubit and the previously emitted photons. In our prototype device, the qubit is the confined dark exciton [3,4], and it produces strings of hundreds of photons in which the entanglement persists over five sequential photons [5]

[1] H. J. Briegel, "Versatile cluster entangled light", Science 354, 416 (2016)

[2] N. H. Lindner and T. Rudolph, "Proposal for pulsed on-demand sources of photonic cluster state strings", Phys. Rev. Lett. 103, 113602 (2009)

[3] E.Poem, et al, "Accessing the dark exciton with light", Nature Physics 6, 993, (2010)

[4] I. Schwartz, et al, "Deterministic writing and control of the dark exciton spin using short single optical pulses", Phys. Rev. X 5, 011009 (2015)

[5] I. Schwartz, et al, "Deterministic generation of a cluster state of entangled photons", Science 354, 434, (2016)

TT 56.2 Wed 10:00 EW 201

Time reordering of paired photons through two-photon strong coupling and generation of maximally entangled states in quantum dots — •Samir Bounouar[1], Christoph De La Haye[1], Max Strauss[1], Peter Schnauber[1], Alexander Thoma[1], Manuel Gschrey[1], Jan-Hindrik Schulze[1], Andre Strittmatter[2], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Abteilung für Halbleiterepitaxie, Otto-von-Guericke, Universität, 39106 Magdeburg, Germany

We show that strong coupling of a continuous laser field to the exciton-biexciton radiative cascade of a semiconductor quantum dot (QD) allows for the observation of the dressed states and the manipulation of the paired photons time ordering [1]. Moreover, two-photon Rabi oscillations of the dressed states population, due to the non-linear coherent driving of the radiative cascade, confirm the coherent nature of the two-photon driving. We also show that maximally entangled states can be efficiently generated from microlens-QD with non-zero

fine structure splitting and that their fidelity to the Bell states remains unaffected by the decoherence over the full wave-packet [2].

[1] S. Bounouar et al., Phys. Rev. Lett. 118, 233601 (2017). [2] S. Bounouar et al., (in preparation).

TT 56.3 Wed 10:15 EW 201

Quantum-optical spectroscopy of a two-level system using an electrically driven micropillar laser as resonant excitation source — •Sören Kreinberg[1], Tomislav Grbešic[1], Max Strauss[1], Alexander Carmele[2], Monika Emmerling[3], Christian Schneider[3], Sven Höfling[3], Xavier Porte[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [3]Technische Physik, Julius-Maximilians-Universität Würzburg, Germany

Two-level emitters constitute the core elements of photonic quantum systems and exploring their physics is at the heart of quantum optics. Of special interest is the strict-resonant optical excitation of such emitters to generate quantum light with close to ideal properties. Up till now related experiments have been performed exclusively using bulky lasers. This hinders the application of resonantly driven two-level emitters in quantum technology, which relies on the availability of compact sources of indistinguishable photons. Here we propose and demonstrate quantum-optical spectroscopy of a single QD embedded in a planar microcavity resonantly excited by an electrically driven high-β quantum dot micropillar laser. We obtain single photons with strong multi-photon suppression $g^{(2)}(0)$=0.02 and high photon indistinguishably V=0.57(9) under pulsed excitation with a repetition rate of 156 MHz. Our results demonstrate the exquisite potential of high-β microlasers as coherent excitation sources in quantum nanophotonics and pave the way to compact, resonantly driven quantum light sources.

TT 56.4 Wed 10:30 EW 201

Ultrafast electric phase control of a quantum dot exciton — •Alex Widhalm[1], Amlan Mukherjee[1,2], Sebastian Krehs[1], Björn Jonas[1], Nandlal Sharma[1], Peter Kölling[1,2], Andreas Thiede[2], Jens Förstner[1,2], Dirk Reuter[1], and Artur Zrenner[1] — [1]Physics Department, University of Paderborn — [2]Department of Electrical Engineering, University of Paderborn, Paderborn 33098, Germany

The coherent control of QD excitons can be performed in Ramsey type experiments, where the QD is excited with two phase locked optical $\frac{\pi}{2}$ pulses seperated by a time delay. Here we present an experiment, where the first pulse defines the phase of the exciton, which is subsequently manipulated by ultrafast Stark tuning of the exciton energy. The resulting phase shift is measured by quantum interference using the second $\frac{\pi}{2}$ pulse. We have already shown, that the coherent phase of a QD exciton can be manipulated electrically by phase-locked RF signals[1]. Here we have designed SiGe:C BiCMOS chips for the generation of ultrafast electric pulses (rise times <20 ps @ cryogenic operationality) and ultrafast photodiodes with embedded high quality InGaAs QDs. Electric connections have been established by short distance wire bonding. This hybrid approach enables us to perform electric control synchroneous to double pulse ps laser excitation. We are able to demonstrate electrically controlled phase manipulations with magnitudes up to 3π and the electric control of the QD occupancy on time scales below the dephasing time of QD exciton.

Ref: [1] S. de Vasconcellos et al., Nature Photonics 4, 545 (2010).

TT 56.5 Wed 10:45 EW 201

Telecom-wavelength GaAs-based quantum dots for practical single-photon sources — •A Musiał[1], Ł Dusanowski[1,2], P Holewa[1], P Mrowiński[1], A Maryński[1], K Gawarecki[1], N Srocka[3], T Heuser[3], D Quandt[3], A Strittmatter[3,4], S Rodt[3], S Reitzenstein[3], and G Sek[1] — [1]Faculty of Fundamental Problems of Technology, Wrocław Uni of Science and Technology, Wrocław, Poland — [2]Technical Physics, Uni of Würzburg, Würzburg, Germany — [3]Institute of Solid State Physics, Technical Uni of Berlin, Berlin, Germany — [4]Institute of Experimental Physics, Otto von Guericke Uni Magdeburg, Magdeburg, Germany

Quantum communication applications require stand-alone, high-purity on-demand single-photon sources (SPS) operating at telecom wavelengths, preferably fiber-coupled for easy integration with existing optical networks. In this regard, we evaluated the potential of GaAs-based quantum dots (QDs) grown by high-throughput and mature MOCVD technology. The emission wavelength was shifted to telecom wavelengths utilizing an InGaAs strain reducing layer. The electronic structure of the QDs was optimized for well-separated ground state exciton emission to allow for high single-photon purity and good thermal stability. Single QDs have been placed deterministically in nanophotonic structures for increased light extraction. The influence of temperature and excitation energy on single-photon generation was studied resulting in triggered high-purity single-photon emission under p-shell resonant excitation at 30K suitable for commercializing fiber-coupled single-photon sources based on cryogenic-free Stirling cryocoolers.

TT 56.6 Wed 11:00 EW 201

Quantum emitter coupled to photonic modes: superradiant to subradiant phasetransition generates a dark state cascade — Michael Gegg, Alexander Carmele, Andreas Knorr, and •Marten Richter — Institut für Theoretische Physik, Technische Universität Berlin, Germany

If an ensemble of quantum emitter like quantum dots, NV centers or atom are coupled to photonic or plasmonic modes, collective effects can lead to collective super- or subradiance. Here, we discuss a type of phase transition, that describes the transition from predominantly superradiant states to subradiant states with applications to quantum information storage. The simulation for a large number of two level systems is made possible by a method exploiting the permutation symmetry for identical system [1,2] available through the library PsiQuaSP [3]. In the described situation the important quantity for the generation of the subradiant states is the cavity decay and not the individual quantum emitter decay. Experimental signatures as well as entanglement properties are discussed.

[1] Phys. Rev. B 91, 035306 (2015)
[2] New J. Phys. 18, 043037 (2016)
[3] Sci. Rep. 7, 16304 (2017)
[4] New J. Phys. (in press), (2017), https://doi.org/10.1088/1367-2630/aa9cdd, arXiv:1705.02889

15 min. break.

Invited Talk TT 56.7 Wed 11:30 EW 201

Exploiting the Bright and the Dark Side of Deterministic Solid-State Quantum-Light Sources — •Tobias Heindel — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Quantum-light sources are key building blocks for future photonic technologies with applications in the fields of quantum communication, quantum computation and quantum metrology.

Here, we will review recent experiments exploiting quantum-light sources based on photonic microlenses deterministically fabricated above pre-selected semiconductor quantum dots (QDs). The first part of the talk will focus on experiments demonstrating the efficient, triggered generation of photon twins - a light state comprised of two temporally correlated photons degenerate in energy and polarization [1]. For this purpose, we select QDs whose exciton finestructure splitting equals the biexciton binding energy $\Delta E_{\mathrm{FSS}}=|E_{\mathrm{bin}}^{\mathrm{XX}}|$. In the second part, we demonstrate that we can exploit photonic QD microlenses to all-optically access the dark exciton (DE) state [2]. By clearly observing the quantum beats of the DE spin-eigenstates $|\uparrow\Uparrow \pm \downarrow\Downarrow\rangle$, we provide evidence for the robustness of the DE as a long-lived coherent spin-qubit and pave the way towards its wider application. Finally, we briefly discuss prospects of QD-based quantum-light sources for the realization of quantum-secured communication networks.

[1] T. Heindel et al., Nature Communications 8, 14870 (2017)
[2] T. Heindel et al., APL Photonics 2, 121303 (2017)

TT 56.8 Wed 12:00 EW 201

Two-photon interference with remote quantum dots at 1550 nm after quantum frequency conversion — •J. H. Weber[1], B. Kambs[2], J. Kettler[1], S. Kern[1], H. Vural[1], J. Maisch[1], S. L. Portalupi[1], M. Jetter[1], C. Becher[2], and P. Michler[1] — [1]IHFG, IQ$^{\mathrm{ST}}$ Center and SCoPE, Universität Stuttgart — [2]Fachrichtung Physik, Universität des Saarlandes

Two-photon interference (TPI) with telecom photons from remote quantum emitters is of key importance for future long-distance quantum networking. Here, quantum frequency conversion (QFC) is exploited to transfer single near-infrared photons from semiconductor quantum dots to the telecom C-band. We demonstrate that the presented technology opens the path for on-demand generation of highly bright single-photon emission at 1550 nm without the need for special sample design or intrinsic tuning mechanisms. Standing prove for

the feasibility of this hybrid technology, we report on TPI with remote quantum dots, being only limited to spectral wandering due to the charge environment of the bulk material. The feasibility of this technology is further strengthened by unprecedented overlap of measured TPI contrast and theoretical prediction which is only possible due to the convenient and highly stable tuning mechanism delivered by QFC. With this respect, the theoretical derivations consider both off-resonant TPI as well as inhomogeneous broadening and blinking of the emitters. Finally, we simulate wave propagation in optical fibers to study the effect of dispersion and experimentally demonstrate that 2 km of fiber delay does not affect the remote TPI visibility.

TT 56.9 Wed 12:15 EW 201

Photon-Number-Resolving Transition Edge Sensors for the Metrology of Quantum-Light Sources — •Marco Schmidt[1,2], Martin von Helversen[1], Fabian Gericke[1], Elisabeth Schlottmann[1], Manuel Gschrey[1], Peter Schnauber[1], Jan-Hindrik Schulze[1], André Strittmatter[1], Jörn Beyer[2], Sven Rodt[1], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany

Photon-number-resolving detectors (PNR) allow for direct access to the photon number distribution of nanophotonic light sources and can thus be exploited to explore the photon statistics of semiconductor-based non-classical light sources. In this work, we report on the realization of a stand-alone measurement system with two fiber-coupled transiton edge sensors (TESs) integrated within a compact adiabatic demagnetization refrigerator. The performance of the detector system is analyzed in terms of its detection efficiency, which is determined to be larger than 87 % (850 - 950 nm). As an exemplary application in QD-metrology, we employ this detector to evaluate the photon number distribution of QD-based single- and twin- photon sources [1] based on deterministically fabricated QD microlenses.

[1] T. Heindel et al., Nat. Commun. 8, 14870, (2017)

TT 56.10 Wed 12:30 EW 201

Hong-Ou-Mandel Experiment using Single-Photon Fock-States and Photon-Number Resolving Detectors — •Martin von Helversen[1], Jonas Böhm[1], Marco Schmidt[1,2], Jan-Hindrik Schulze[1], André Strittmatter[1], Sven Rodt[1], Jörn Beyer[2], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-12, 10587 Berlin, Germany

Quantum light sources based on semiconductor quantum dots (QDs) are promising candidates for many applications in the research fields of quantum metrology and quantum communication. Important characteristics of such emitters, e.g. the degree of single-photon purity and photon indistinguishability, are typically assessed via time-correlated measurements using silicon-based click detectors in Hanbury-Brown and Twiss (HBT-) and Hong-Ou-Mandel (HOM-) type configuration. Here, we employ a state of the art photon-number-resolving detection system based on two transition edge sensors (TES) to analyze the emission of a deterministically fabricated QD-based single-photon source and quantitatively compare our results with experimental data obtained for standard click detectors. Our results demonstrate that photon-number resolving detectors are very attractive tools for the metrology of quantum light sources.

TT 56.11 Wed 12:45 EW 201

Effect of second order piezoelectricity on exciton dipole, fine-structure and binding energies of multi-excitons in strain-tuned InGaAs/GaAs quantum dots — •Petr Klenovský[1,2], Petr Steindl[1,2], Johannes Aberl[3], Eugenio Zallo[4,5], Thomas Fromherz[3], Armando Rastelli[3], and Rinaldo Trotta[3] — [1]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic — [2]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic — [3]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Altenbergerstraße 69, A-4040 Linz, Austria — [4]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstraße 20, D-01069 Dresden, Germany — [5]Paul-Drude-Institut für Festkörperelektronik, Hausvogteilplatz 5-7, 10117 Berlin, Germany

We study the effects of nonlinear piezoelectricity on the exciton electric dipole moment, fine-structure, and binding energies of multi-exciton complexes in strain-tuned InGaAs/GaAs quantum dots and investigate the influence of various elements of the expansion of electrical polarization in terms of applied elastic stress. We find that a presence of a large built-in stressor (like quantum dot) is necessary for the dipole inversion to occur. Furthermore, the analysis provides a simple relation to estimate the influence of applied stress on the electrical polarization in zincblende nanostructures.

TT 56.12 Wed 13:00 EW 201

Strain tuning of deterministically fabricated quantum dot microlenses for advanced quantum communication — •Sarah Fischbach, Marco Schmidt, Ronny Schmidt, Arsenty Kaganskiy, André Strittmatter, Tobias Heindel, Sven Rodt, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Germany

Long distance quantum communication requires networks of quantum repeaters, which are based on the generation of indistinguishable pairs of entangled photons. Quantum dots (QDs) can generate entangled photons from their exciton-biexciton cascade and methods of semiconductor nanofabrication allow one to realize efficienct sources emitting highly indistinguishable photons.
Due to the random nature of the self-assembled growth process, QDs vary over a wide range in their emission wavelength. Deterministic nanoprocessing needs to be applied to integrate QDs matching a target wavelength. Additionally, to enable entaglement distribution, two QD-based sources need to be tuned into resonance by spectral fine-tuning. Strain tuning is a very accurate tuning method which maintains the high optical quality of the QD emission.
We demonstrate a tunable single-photon source based on a deterministically fabricated QD microlens which is positioned on top of a piezoactuator by a flip-chip goldbonding technique. QD microlenses can act as efficient single-photon sources with low $g^{(2)}(0)$-values and a high photon indistinguishability, which are now equipped with the feature of strain tunability.

TT 57: Topological Semimetals III

Time: Wednesday 10:00–11:15 Location: A 053

TT 57.1 Wed 10:00 A 053

Anomalous Hall effect in topological magnetic materials — •Kaustuv Manna[1], Lukas Muechler[1,2], Ting Hui Kao[1], Rolf Stinshoff[1], Nitesh Kumar[1], Jürgen Kübler[1], Gerhard H. Fecher[1], Chandra Shekhar[1], Yan Sun[1], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ, USA

In recent years, topological semimetals have emerged as a new frontier in the condensed matter community. With the interplay between the structural asymmetry and spin-orbit interaction, and details of Berry phase, new topological states are being discovered. Though inversion symmetry breaking Weyl fermion is demonstrated in TaAs family of compounds, the time-reversal breaking examples remain elusive. Here we demonstrate the formation of magnetic nodal lines in a topological magnetic Heusler compound Co_2MnGa. Without spin-orbit coupling (SOC), we find three nodal lines due to the band crossing in majority spin channel. With SOC, nodal lines split up giving rise to the Weyl nodes, whose momentum space distributions depend on the magnetization direction. We observe giant anomalous Hall conductivity of 1600 $\Omega^{-1}cm^{-1}$ with room temperature anomalous Hall angle 12% in Co_2MnGa. In- fact, by suitable manipulations of the crystal symmetries and the band structures of the materials, one can selectively tuned the anomalous Hall conductivity from 0 to values up to 1600 $\Omega^{-1}cm^{-1}$ in various magnetic Heusler compounds for next-generation topo-spintronics applications.

TT 57.2 Wed 10:15 A 053

Evolution of the surface states of the Luttinger semimetal under compressive strain and broken inversion symmetry: relation to Dirac and Weyl semimetals — •Julian-Benedikt Mayer, Maxim Kharitonov, and Ewelina Hankiewicz — Institute for Theoretical Physics and Astrophysics, Würzburg, Germany

Luttinger semimetal, the quadratic-node semimetal for $j = 3/2$ electrons under full cubic symmetry, is the parent highest-symmetry minimal model for a variety of topological and/or strongly correlated materials, such as HgTe, α-Sn, and iridate compounds. Recently, Luttinger semimetal has been demonstrated [1] to exhibit surface states of topological origin that can be attributed to approximate chiral symmetry. In the present work, we theoretically study the effect of the symmetry-lowering perturbations on these surface states within an analytical model. Under compressive strain lowering rotational symmetry, Luttinger semimetal becomes a Dirac semimetal with a pair of double-degenerate linear nodes. Breaking further inversion symmetry, the system turns into a Weyl semimetal, with each Dirac node split into four Weyl nodes [2]. We analyze the corresponding evolution of the surface states, connecting the surface-state structures in the linear regime near the nodes and in the quadratic regime of the Luttinger semimetal away from the nodes. In particular, we demonstrate agreement of the Chern numbers with the chiralities of the surface states.

[1] M. Kharitonov, J.-B. Mayer, and E. M. Hankiewicz, Phys. Rev. Lett., in press; arXiv:1701.01553 (2017).
[2] J. Ruan, S.-K. Jian, Yao, H. Zhang, S.-C. Zhang, and D. Xing, Nature Comm. 7, 11136 (2016).

TT 57.3 Wed 10:30 A 053

Appearance of the universal value e^2/h of the zero-bias conductance in a Weyl semimetal-superconductor junction — Songbo Zhang[1], •Fabrizio Dolcini[2], Daniel Breunig[1], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Dipartimento di Scienza Applicata e Tecnologia del Politecnico di Torino, I-10129 Torino, Italy

We study the differential conductance of a time-reversal symmetric Weyl semimetal-superconductor (N-S) junction with an s-wave superconducting state. We find that there exists an accessible regime where the zero-bias differential conductance acquires the universal value e^2/h per unit channel, independent of the pairing and chemical potentials on each side of the junction, due to a perfect cancellation of Andreev and normal reflection contributions. This universal conductance can be attributed to the interplay of the unique spin/orbital-momentum locking and s-wave pairing that couples Weyl nodes of the same chirality. We expect that the universal conductance can serve as a robust and distinct signature for time-reversal symmetric Weyl fermions, and be observed in the recently discovered time-reversal symmetric Weyl semimetals.

TT 57.4 Wed 10:45 A 053

Exploring the Quantum Limit of Weyl semimetal candidates — •Tobias Förster[1], Johannes Klotz[1,2], Jochen Wosnitza[1,2], Chandra Shekhar[3], Binghai Yan[3], and Claudia Felser[3] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Max Planck Institute f. Chemical Physics of Solids, Germany

Non-centrosymmetric transition-metal mono-pnictides such as NbAs, NbP and TaAs attracted a lot of attention because their bandstructures show linear non-degenerate band crossings, dubbed Weyl nodes [1,2]. Additionally, for certain magnetic-field orientations, the highest de Haas-van Alphen frequencies observed are smaller than 50 T. For that reason, all bands are expected to be in the quantum limit at fields easily reachable by pulsed magnetic fields. Thus, these semimetals constitute an ideal playground to study the quantum limit by electric transport and magnetic-torque measurements. Our first results for NbP show an unexpected linear increase in magnetic-torque measurements. In our contribution we show the results of our magnetic-torque measurements on NbP, NbAs, TaP and TaAs in pulsed fields up to 70 T.

[1] J. Klotz *et al.*, Phys. Rev. B. **93** 121105 (2016).
[2] C. Shekhar *et al.*, Nat. Phys. **11** 645 (2015).

TT 57.5 Wed 11:00 A 053

Anomaly transport in graphene and Weyl semimetals normally explained — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Based on the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in Graphene and Weyl-systems realized as the infinite-mass limit of electrons with quadratic dispersion and a proper spin-orbit coupling. Correspondingly the currents possess no quasiparticle part but only anomalous parts. The intraband and interband conductivities are discussed. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents.

[1] Phys. Rev. B 94 (2016) 165415,
[2] Phys. Rev. B 92 (2015) 245425
[3] errata: Phys. Rev. B93 (2016) 239904(E)
[4] Phys. Rev. B 92 (2015) 245426

TT 58: Frontiers of Electronic-Structure Theory: Correlated Electron Materials IV (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 10:30–13:00 Location: HL 001

Invited Talk TT 58.1 Wed 10:30 HL 001

Correlating electrons via adiabatic connection approach: a general formalism, approximations, and applications — •Katarzyna Pernal — Institute of Physics, Lodz University of Technology, Poland

Electronic systems are usually described by assuming a model Hamiltonian, which only partially recovers electron correlation effects. To assure a quantitative description one faces a problem of recovering the missing part of the correlation. Over years different methods have been developed, most of them originating from the perturbation theory.

In my talk I will present another, fairly general, approach based on the adiabatic connection formalism. The idea itself is not novel although it has not been considered as a way of adding electron correlation for multireference models. Until recently it has not been realized that by combining the adiabatic connection (AC) with the extended random phase approximation one obtains a general tool capable of accounting for dynamical electron correlation for a broad class of multireference wavefunctions, applicable even to systems including strongly correlated electrons. It will be shown that the AC-based approximation yields excellent results when applied to multireference models, exceeding in accuracy second-order perturbation-theory-based methods.

TT 58.2 Wed 11:00 HL 001

Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: case study of LiF — •Chen Li[1], Ryan Requist[1], and Eberhard. K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem, Israel

We demonstrate that beyond Born-Oppenheimer (BO) effects can be accurately and seamlessly incorporated within a density functional framework. In alkali halides like LiF, there is an abrupt change in the ground state electronic distribution due to an electron transfer at a critical bond length $R = R_c$. We find that nonadiabatic electron-nuclear coupling produces a sizable elongation of the critical R_c by 0.5 Bohr, an effect which is very accurately captured by a simple and rigorously-derived nuclear mass-dependent correction to the exchange-correlation potential in density functional theory. Since this nonadiabatic term depends on gradients of the nuclear wave function and conditional electronic density, $\nabla_R \chi(R)$ and $\nabla_R n(r, R)$, it couples the Kohn-Sham equations at neighboring R points. Motivated by an observed localization of nonadiabatic effects in nuclear configuration space, we propose an approximation that reduces the search for nonadiabatic density functionals to the search for a single function. This work is a step towards bringing density functional theory beyond the limitations of the BO approximation.

TT 58.3 Wed 11:15 HL 001

Ground-State Quantum-Electrodynamical Density-Functional Theory — •Michael Ruggenthaler — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

In this talk I present a density-functional reformulation of correlated matter-photon problems subject to general external electromagnetic fields and charge currents [1]. I first show that for static minimally-coupled matter-photon systems an external electromagnetic field is equivalent to an external charge current. I employ this to show that scalar external potentials and transversal external charge currents are in a one-to-one correspondence to the expectation values of the charge density and the vector-potential of the correlated matter-photon ground state. This allows to establish a Maxwell-Kohn-Sham approach, where in conjunction with the usual single-particle Kohn-Sham equations a classical Maxwell equation has to be solved in order to capture the correlation induced by the transversal photon field. In the magnetic mean-field limit this reduces to a current-density-functional theory that does not suffer from non-uniqueness problems and if furthermore the magnetic field is zero recovers standard density-functional theory.

[1] "Ground-State Quantum-Electrodynamical Density-Functional Theory", M. Ruggenthaler, arXiv:1509.01417 (2017).

TT 58.4 Wed 11:30 HL 001

Design of auxiliary systems for observables: the dynamic structure factor and the electron addition and removal spectra — Marco Vanzini, Martin Panholzer, Lucia Reining, and •Matteo Gatti — LSI, CNRS, Ecole Polytechnique, Palaiseau, France

Density functional theory tells us that the external potential, and therefore all observables, are functionals of the ground state density. The exact functionals, however, are not known, and one has to find approximations. To obtain the density, Kohn and Sham have proposed the idea to use an "auxiliary system". Much research effort goes into finding better and better Kohn Sham potentials for the density and the total ground state energy. In order to access also observables other than the density, we have proposed to generalize the Kohn-Sham idea of an auxiliary system [1], and to design a "connector" that allows us to profit from calculations done in a model system [2,3]. We have recently shown that this is a successful strategy for the dynamic structure factor [2] and for the one-body spectral function of simple metals, semiconductors and insulators [3]. [1] M. Gatti, V. Olevano, L. Reining, and I. V. Tokatly, Phys. Rev. Lett. 99, 057401 (2007) [2] M. Panholzer, M. Gatti, and L. Reining, arXiv:1708.02992 [3] M. Vanzini, L. Reining, and M. Gatti, arXiv:1708.02450

TT 58.5 Wed 11:45 HL 001

Exact exchange energy of the ferromagnetic electron gas with dipolar interactions — •Camilla Pellegrini, Tristan Mueller, Kay Dewhurst, Sangeeta Sharma, and Eberhard K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We propose a density functional treatment of the magnetic dipole-dipole interaction as a spin-spin correction to the Coulomb force in the Breit-Pauli Hamiltonian. Within this microscopic approach, the Hartree-like term for the dipolar coupling corresponds to the classical magnetostatic energy currently implemented in micromagnetic calculations. In addition, we have derived quantum corrections by evaluating analytically the exact exchange energy (Fock term) for the homogeneous electron gas, within the linear response to a noncollinear magnetic field. We expect our functional to open the path towards a full ab initio description of inhomogeneous magnetic structures at the nanoscale, with applications to domain-wall operated spintronic devices.

TT 58.6 Wed 12:00 HL 001

Precise total-energy calculations at a significantly reduced cost — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In density-functional calculations, the total-energy functional is stationary with respect to the density, the Kohn-Sham orbitals and the Kohn-Sham effective potential. This means that approximations for these quantities only lead to total-energy errors of second order provided that the total-energy functional is evaluated accurately without further uncontrolled approximations.

Unfortunately, usually the Kohn-Sham orbitals and thus the kinetic part of the total energy are evaluated by using a projection of the potential into a finite subspace of basis functions. This approximation damages the stationarity of the total energy as a functional of the potential.

A technique will be discussed which can relieve this deficiency so that a considerably smaller subspace of basis functions can be used for a precise evaluation of the kinetic part of the total energy. The advantage will be illustrated for the particular example of angular projection potentials as they are used in the full-potential Korringa-Kohn-Rostoker Green function method.

TT 58.7 Wed 12:15 HL 001

Approach to Orbital-free DFT with Englert-Schwinger model — •Jouko Lehtomäki and Olga Lopez-Acevedo — COMP Centre of Excellence, Department of Applied Physics, Aalto University, Finland

We briefly present the Englert and Schwinger (ES) model in comparison with other approaches to orbital-free DFT. Essential failure of many kinetic energy density functionals is that they can not describe the most tightly bound core electrons in a satisfactory manner. Englert-Schwinger model allows treating these problematic electrons with more accurate single-particle wavefunctions while still obtaining the self-consistent orbital-free solution to the electronic problem.

Specifically, we detail how the ES model compares to the more known Thomas-Fermi-Dirac-Weizsäcker model self-consistently in atoms. We look at the total energy and few geometric properties. We show qualitative improvement in Pauli potential, which shows unphysical singularities near nucleus when the most tightly bound electrons are not treated correctly. We present how augmentation of the model with Kohn-Sham orbitals allows us to explore all-electron solution to the OFDFT problem and how this paves way for an orbital-free DFT method which does not need pseudopotentials.

TT 58.8 Wed 12:30 HL 001

The Kerker Preconditioner for FLAPW Methods with Charge Density Mixing — •Miriam Hinzen, Edoardo Di Napoli, Daniel Wortmann, and Stefan Blügel — Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In metallic systems of larger size the self-consistent field convergence of electronic structure calculations is often slowed down substantially due to charge sloshing: close to the Fermi level, little change in energy can cause large fluctuations in charge density. Mathematically speaking, the problem is ill-conditioned. For plane-wave methods the Kerker preconditioner effectively solved this problem, but for many other electronic structure methods, in particular all-electron methods as the FLAPW or KKR methods, a real-space formulation would be needed. We developed a formulation of the Kerker preconditioner for FLAPW methods with charge density mixing, implemented in `FLEUR` [1]. Numerical experiments show an enormous reduction of the number of iterations needed for convergence; even more importantly, the SCF convergence has become independent of the system size.
[1] www.flapw.de

TT 58.9 Wed 12:45 HL 001

Effect of spin on the generalized Pauli constraints in Reduced Density Matrix Functional Theory — •Nicole Helbig[1], Iris Theophilou[2], and Nektarios N. Lathiotakis[3] — [1]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum

Jülich, D-52425 Jülich, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Vass. Constantinou 48, GR-11635 Athens, Greece

Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. Enforcing the generalized Pauli constraints during the energy minimization ensures that the 1RDM corresponds to a fermionic pure state. We demonstrate that these constraints are modified for open-shell systems if the spin degrees of freedom are taken into account. From the generalized Pauli constraints we also derive properties of the exact occupation numbers and natural orbitals which ensure that the 1RDM corresponds to an eigenstate of the total spin.

TT 59: Topological Insulators I (joint session TT/MA)

Time: Wednesday 11:45–13:00 Location: A 053

TT 59.1 Wed 11:45 A 053

Towards universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk, Juan Diego Urbina, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The quantum-classical transition of the transmission probability for two fermions propagating through a quantum point contact is a known manifestation of the celebrated Hong-Ou-Mandel (HOM) effect [1] in electron quantum optics [2]. As shown in [3], universal HOM correlations are expected by substituting the quantum point contact by a chaotic cavity in a mesoscopic regime [3], where universality appears due to universal correlations of the scattering matrix entries at different energies. Here we present an analytical and numerical study of these correlations and propose electron quantum optics with cavities as complex beam splitters and edge states as waveguides as a candidate to observe universal HOM correlations in topological insulators.

[1] C. K. Hong, Z. Y. Ou, L. Mandel, PRL **59**, 2044 (1987)
[2] E. Bocquillon et al., Annalen der Physik **526**, 1 (2014)
[3] J. D. Urbina et al., Phys. Rev. Lett. **116**, 100401 (2016)

TT 59.2 Wed 12:00 A 053

Effects of local approximations on topological phases — •Thomas Mertz, Karim Zantout, and Roser Valenti — ITP, Goethe University, Frankfurt am Main

We investigate the self-energy dispersion of topological models and its effect on the topological classification in terms of invariants computed in the framework of the so-called topological Hamiltonian, an auxiliary Fermi-liquid like theory. The concept of topology in physics has matured as a non-interacting theory, most of its properties deeply intertwined with the conventional band theory of solids. Recently, a lot of interest has shifted towards interacting systems, which have not been studied extensively from a topological point of view. Since the topological Hamiltonian is determined by the zero-frequency value of the self-energy only, which has been studied using local theories, we focus on the explicit momentum-dependence captured by methods such as TPSC and CPT.

TT 59.3 Wed 12:15 A 053

Spin-phonon scattering in edge states of two-dimensional topological insulators — •Solofo Groenendijk, Giacomo Dolcetto, and Thomas Schmidt — Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

We study theoretically the effect of electron-phonon scattering in 2D topological insulator (2DTI) edge states. Due to the spin-momentum locking in helical edge states, dynamical deformations of the edge modify the spin texture of the electronic edge states. In our work, we show that the resulting spin-phonon coupling ultimately leads to backscattering.

For a short channel, we compute the temperature-dependent conductance in the linear regime ($\beta eV < k_B T$) using the Kubo formula, and find $\delta G \propto T^5$ for the backscattering conductance. In the limit of a long edge channel, transport becomes diffusive and we compute the resistivity ρ using the semi-classical Boltzmann equation. In particular we find a metallic Bloch-Grüneisen behaviour for chemical potentials near the Dirac point.

Since this spin-phonon coupling arises even in ideal samples and since further imperfections (e.g. Rashba impurities, charge puddles, electron-electron interactions etc.) can only increase backscattering, our results impose a fundamental upper limit on the conductivity of 2D TI edge states.

TT 59.4 Wed 12:30 A 053

Topological invariants for Floquet-Bloch systems with chiral, time-reversal, or particle-hole symmetry — •Bastian Höckendorf, Andreas Alvermann, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, Greifswald, Germany

We introduce $\mathbb{Z}_2$-valued bulk invariants for symmetry-protected topological phases in $2+1$ dimensional driven quantum systems. These invariants adapt the W_3-invariant, expressed as a sum over degeneracy points of the propagator, to the respective symmetry class of the Floquet-Bloch Hamiltonian. The bulk-boundary correspondence that holds for each invariant relates a non-zero value of the bulk invariant to the existence of symmetry-protected topological boundary states. To demonstrate this correspondence we apply our invariants to a chiral Harper, time-reversal Kane-Mele, and particle-hole symmetric graphene model with periodic driving, where they successfully predict the appearance of boundary states that exist despite the trivial topological character of the Floquet bands. Especially for particle-hole symmetry, combination of the W_3 and the $\mathbb{Z}_2$-invariants allows us to distinguish between weak and strong topological phases.

[1] B. Höckendorf, A. Alvermann, and H. Fehske, J. Phys. A 50, 295301 (2017).
[2] B. Höckendorf, A. Alvermann, and H. Fehske, preprint, arXiv:1708.07420 (2017).

TT 59.5 Wed 12:45 A 053

Reduced many-body formulas for the macroscopic polarization and topological charge pumping — •Ryan Requist[1] and Eberhard K. U. Gross[1,2] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Fritz Haber Center for Molecular Dynamics, Jerusalem, Israel

In ab initio materials research, topological invariants and the macroscopic polarization are usually calculated in terms of an effective single-particle Kohn-Sham band structure, an approach which may give incorrect results even if the exact exchange-correlation potential is used. We propose a simple natural orbital geometric phase formula for the macroscopic polarization and verify that it accurately reproduces the polarization in the Rice-Mele-Hubbard model in strongly and weakly correlated regimes. An analogous formula based on a one-body reduced Berry curvature very accurately predicts the critical Hubbard interaction at which Thouless charge pumping is quenched. We discuss strategies for ab initio calculations of natural orbital geometric phases and the possibility of extending the approach to other topological invariants in correlated materials.

TT 60: Focus Session: Topological Defects in Superconductors and Magnets (joint session TT/MA)

Vortices in superconductors and skyrmions in magnets are two examples of topological objects that can form a lattice and have particle-like properties. Their orientation and symmetry is determined by the magnetic field and the interaction within the material. The scientific and methodological approaches are similar*both can be studied using transport and magnetization and both can be observed using neutron scattering and scanning microscopies. Nanofabrication, often with the help of hybrid structures, allows controlling and manipulating them. The latter is believed to play a key role in applications involving current carrying and magnetic memory devices. The aim of the colloquium is to present most recent advances with a particular focus on the cross-fertilization of research on topological defects in superconductivity and magnetism.

Organization: Sebastian Mühlbauer, TU München; Hermann Suderow, Universidad Autonoma de Madrid; Javier Villegas, Thales, Paris; Markus Garst, TU Dresden

Time: Wednesday 15:00–17:45 Location: H 0104

Invited Talk TT 60.1 Wed 15:00 H 0104

Stability and Emergent Electrodynamics of Skyrmions — •Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

Skyrmions and related topological spin textures in chiral magnets attract great interest as a possible route towards novel spintronics devices. A series of studies is reported on the topological stability of skyrmions in chiral magnets for different temperature versus field histories. The character of magnetic textures, notably as observed in bulk compounds, at surfaces and in thin epitaxial films will be addressed. Further, the response of the different magnetic phases in chiral magnets to electric currents and the associated spin currents across the magnetic phase diagram of selected systems has been measured. Based on the combination of electrical resistivity, Hall effect, planar Hall effect, ac susceptibility and kinetic small angle neutron scattering the interplay of spin transfer torques with defects for the different magnetic phases and phase boundaries will be discussed.

Invited Talk TT 60.2 Wed 15:30 H 0104

Optical Manipulation of Single Flux Quanta — •Philippe Tamarat — LP2N, Université de Bordeaux, Institut d'Optique Graduate School and CNRS, France

The semiconductor electronics scaling road map will probably reach its physical fundamental limits within the next decade. Alternative technologies such as superconducting electronics are appealing due to higher operating frequencies together with fundamentally lower switching energies. In this context, a promising method requires the manipulation of individual flux quanta close to a Josephson junction. Yet, handling of individual vortices remains challenging and has been performed only with local probe scanning microscopies, slow techniques that are heavy to implement in a cryogenic environment.

We introduce the concept of laser manipulation of individual flux quanta, based on local heating of the superconductor with a focused laser beam to realize a fast, precise and non-invasive manipulation of an Abrikosov vortex, in the same way as with optical tweezers. This simple and far-field optical method provides a perfect basis for sculpting the magnetic flux profile in superconducting devices like a vortex lens or a vortex cleaner. Various regimes of vortex manipulation are achieved, from the precise and rapid positioning of individual vortices to the generation of tight vortex bunches. This method will fuel fundamental investigations of the vortex matter and open up new research directions in quantum computation based on Josephson junctions. I will also present our latest advances towards the creation of Abrikosov vortices with light.

Invited Talk TT 60.3 Wed 16:00 H 0104

Skyrmion Lattices in Random and Ordered Potential Landscapes — •Charles Reichhardt — Los Alamos National Laboratory, Los Alamos, USA

Since the initial discovery of skyrmion lattices in chiral magnets [1], there has been a tremendous growth in this field as an increasing number of compounds are found to have extended regions of stable skyrmion lattices [2] even close to room temperature [3]. These systems have significant promise for applications due to their size scale and the low currents or drives needed to move the skyrmions [4]. We examine the driven dynamics of skyrmions interacting with random and periodic substrate potentials using both continuum based modelling and particle based simulations. In clean systems we examine the range in which skyrmion motion can be explored as a function of the magnetic field and current and show that there can be a current-induced creation or destruction of skyrmions. In systems with random pinning we find that there is a finite depinning threshold and that the Hall angle shows a strong dependence on the disorder strength. We also show that features in the transport curves correlate with different types of skyrmion flow regimes including a skyrmion glass depinning/skyrmion plastic flow region as well as a transition to a dynamically reordered skyrmioncrystal at higher drives. We find that increasing the Magnus term produces a low depinning threshold which is due to a combination of skyrmions forming complex orbits within the pinning sites and skyrmion-skyrmion scattering effects.

15 min. break.

Invited Talk TT 60.4 Wed 16:45 H 0104

Hedgehog Spin-Vortex Crystal Magnetic Order in Superconducting CaK($Fe_{1-x}M_x$)$_4As_4$ (M=Co, Ni) — •Anna Böhmer — Ames Laboratory, Iowa, USA — IFP, Karlsruhe Institute of Technology, Germany

Iron-based superconductors can support a number of antiferromagnetic phases, of which stripe-type antiferromagnetism is most common. It is found that Ni- and Co-doping in $CaKFe_4As_4$ suppresses superconductivity and stabilizes a new antiferromagnetic phase. This phase is studied using thermodynamic, transport, x-ray and neutron diffraction, as well as local magnetic measurements. A non-collinear antiferromagnetic structure preserving tetragonal symmetry is revealed. It is characterized by a superposition of the propagation vectors of the common stripe-type antiferromagnetism. This antiferromagnetic structure with a "hedgehog-type" moment motif is stabilized by the reduced symmetry of the $CaKFe_4As_4$ structure.

This work was performed in collaboration with W. R. Meier, Q.-P. Ding, A. Kreyssig, M. Xu, S. L. Bud'ko, A. Sapkota, K. Kothapalli, J. M. Wilde, W. Tian, V. Borisov, R. Valentí, C. D. Batista, P. P. Orth, R. M. Fernandes, R. J. McQueeney, A. I. Goldman, Y. Furukawa and P. C. Canfield and supported by the Gordon and Betty Moore Foundation's EPiQS Initiative through Grant GBMF4411 and the US DOE, Basic Energy Sciences under Contract No. DE-AC02-07CH11358.

[1] W. R. Meier et al., arXiv:1706.01067 (2017).

Invited Talk TT 60.5 Wed 17:15 H 0104

Geometric Frustration and Ratchet Effect of Vortices in an Artificial-Spin/Superconductor Hybrid — •Zhi-Li Xiao[1,2], Yong-Lei Wang[1,3], Xiaoyu Ma[3], Jing Xu[1,2], Boldizsar Janko[3], and Wai-Kwong Kwok[1] — [1]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA — [2]Department of Physics, Northern Illinois University, DeKalb, Illinois 60115, USA — [3]Department of Physics, University of Notre Dame, Notre Dame, Indiana 46556, USA

Geometric frustration emerges when local interaction energies cannot be simultaneously minimized, resulting in numerous degenerate states. It exists in a large variety of material systems, such as water ice and pyrochlore crystals (spin ice), as well as various artificial systems including artificial spin ice, vortex ice, magnetic colloidal ice, and buckled

colloidal monolayers. However, it is difficult to achieve extensive degeneracy, especially in a two-dimensional (2D) system. Here, we report the realization of geometric frustration with massive degeneracy in a 2D system created in a superconducting thin film placed underneath an artificial-spin structure. The magnetic charges of the artificial-spins strongly interact with vortices in the superconductor, enabling the creation of controllable frustrated and crystallized vortex states by precise selection of the spin magnetic states. We reveal the various vortex states by molecular dynamic simulations and transport measurements. We demonstrate that a reprogrammable vortex ratchet effect can be achieved in this artificial-spin/superconductor heterostructure.

TT 61: Superconductivity: Superconducting Electronics II and Cryotechnique

Time: Wednesday 15:00–16:45 Location: H 2053

Invited Talk TT 61.1 Wed 15:00 H 2053

Quantum Thermodynamics on Superconducting Qubits — •Jukka Pekola[1], Bayan Karimi[1], Alberto Ronzani[1], Jorden Senior[1], Yu-Cheng Chang[1,2,3], ChiiDong Chen[1,3], and Joonas Peltonen[1] — [1]Aalto University School of Science, Helsinki, Finland — [2]National Taiwan University, Taipei, Taiwan, Republic of China — [3]Academia Sinica, Taipei, Taiwan, Republic of China

I present quantum refrigerators based on superconducting qubits. In the theoretical part I describe a four-stroke Otto refrigerator, and a model of it in different operation regimes. Experiments on a transmon type qubit coupled to two resonators demonstrate heat transport, where the quantum-classical border is determined by the relative strength of qubit-resonator and resonator-heat bath couplings, respectively.

TT 61.2 Wed 15:30 H 2053

Bi-stability in a Mesoscopic Josephson Junction Array resonator — •Phani Raja Muppalla[1,2], Oscar Gargiulo[1,2], Mathieu Juan[1,2], Lukas grunehaupt[3], Gerhard Kirchmair[1,2], and Ioan Pop[3] — [1]Insitute for quantum optics and quntum information, technikerstrasse 21 A, Innsbruck- Austria — [2]university of innsbruck, innsbruck, Austri — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

We present an experimental analysis of the Kerr effect of extended plasma resonances in a mesoscopic Josephson junction (JJ) chain resonator inside a rectangular waveguide. The Kerr effect manifests itself as a frequency shift that depends linearly on the number of photons in a resonant mode. We study the bi-stable behavior, using a pump probe scheme on two modes of the JJ array, exploiting the Cross-Kerr effect in our system. In order to understand the behavior of the bi-stability we perform continuous time measurements to observe the switching between the two metastable states. We observe a strong dependence of the switching rates on the photon number and the drive frequency.

TT 61.3 Wed 15:45 H 2053

An on-demand source of anti-bunched microwave photons — •Florian Blanchet[1], Romain Albert[1], Salha Jebari[1], Alexander Grimm[2], and Max Hofheinz[1] — [1]Univ. Grenoble Alpes & CEA, INAC-PHELIQS, Grenoble, France — [2]Departement of Applied Physics, Yale University, New Haven, USA

Most superconducting devices use the Josephson junction in the zero-voltage branch where the junction behaves as a nonlinear inductor. However, Cooper pairs can tunnel through the Josephson junction also at non-zero bias voltage if the energy of a tunneling Cooper pair can be dissipated, e.g. in the form of photons [1]. By coupling the junction to a transmission line, we can detect these photons associated to inelastic Cooper pair tunneling [2] and measure their statistics.

In most configurations, the emitted photons have the same Poisson statistics as the tunneling Cooper pairs, corresponding to independent tunneling events. However, by designing particular high-impedance microwave circuits, we can tune the photon statistics to also be non-classical[3]. I will show that the photons emitted by such a circuit can be strongly anti-bunched.

In addition, we have replaced the Josephson junction by a SQUID which allows us to modulate the effective Josephson energy by applying magnetic flux pulses. We use these pulses to generate anti-bunched photons on demand up to rates > 150 MHz.

[1] PRL 73, 3455 (1994)
[2] PRL 106, 217005 (2011)
[3] PRL 115, 027004 (2015)

TT 61.4 Wed 16:00 H 2053

Green's function approach to normal-metal quasiparticel traps — •Raphael Schmit and Frank Wilhelm-Mauch — Theoretical Physics Department, Saarland University, 66123, Saarbrücken, Germany

Decoherence mechanisms affect the storage of quantum information. Origin are e.g. usually unwanted interactions between the qubit and its environment. In the case of superconducting qubits, additional decoherence comes from the coupling between the qubit's degree of freedom and the non-equilibrium quasiparticle (QPs) excitations in the superconductor the qubit is made of. The underlying mechanism – mainly QP tunneling through a Josephson junction – is highly dependent on the location of the QPs: Those far away from junctions have much less contribution to decoherence than the ones close to it. While their generation is difficult to prevent, trapping them in less active regions of the device provide a practicable way to improve the device performance.

The performance of normal-metal QP traps simply consisting of a normal metal island which is in contact with the superconductor, can be investigated by a voltage biased NISN juntion. We are applying a Green's function formalism – the Keldysh technique in the dirty limit with a quasiclassical approximation – to investigate the properties of the non-equilibrium QPs in the junction. Physical quantities like the order parameter, the QP density of states or their density are accessible via the self-consistent solutions of the Usadel equations that are computed numerically.

TT 61.5 Wed 16:15 H 2053

Quantum information in heat engines — •Mohammad Ansari[1] and Yuli Nazarov[2] — [1]Forschungszentrum Juelich, Juelich, Germany — [2]Delft University of Technology, Delft, Netherlands

We present a universal relation between the flow of a Renyi entropy and the full counting statistics of energy transfers. We prove the exact relation for a flow to a system in thermal equilibrium that is weakly coupled to an arbitrary time-dependent and nonequilibrium system. The exact correspondence, given by this relation, provides a simple protocol to quantify the flows of Shannon and Renyi entropies from the measurements of energy transfer statistics. This finds interesting applications in superconducting quantum bits, photocells, photosynthesis, and other quantum heat engines.

[1] M. H. Ansari, Y. V. Nazarov, Phys. Rev. B 91, 104303, (2015).
[2] M. H. Ansari, Y. V. Nazarov, Phys. Rev. B 91, 174307, (2015).
[3] M. H. Ansari, Y. V. Nazarov, J. Exp. Theor. Phys. 122, 389, (2016).
[4] M. H. Ansari, Phys. Rev. B 95, 174302, (2017).

TT 61.6 Wed 16:30 H 2053

A small two-stage PTC operating at liquid Helium temperature with 1 kW input power — •Bernd Schmidt[1,2], Matthias Vorholzer[2], Marc Dietrich[1], Jens Falter[1], Günter Thummes[1,2], and André Schirmeisen[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Cryocoolers provide temperatures of less than 4 K without the need of liquid Helium. Additionally, the Pulse Tube Cryocooler (PTC) has has no moving parts in the cold part, which leads to lower disturbances.

Many developments of PTCs aim for higher cooling power at 4.2 K (> 1.5 W). However, some applications only need small cooling powers (< 100 mW), but suffer from the intrinsic disturbances of cryocoolers.

In this talk we present a new two-stage GM-type PTC, driven by a commercial Helium compressor with only 1 kW input power. The PTC reaches a minimum temperature of 2.36 K and provides a cooling power of 72 mW at 4.2 K. (1) It was initially designed to cool down SNSPDs and transition-edge bolometers. First measurements with low-noise Nb-SQUIDs were already made. Since the PTC can be easily driven by a portable generator, it is also suitable e.g. for in-field

measurements like geophysical studies.

Funding via the BMBF joint project "SUSY" (grant No 13N13444) is gratefully acknowledged.

[1] Cryogenics 88 (2017) 129

TT 62: Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)

Time: Wednesday 15:00–18:30 Location: H 3010

Invited Talk TT 62.1 Wed 15:00 H 3010

Efficient Simulation of Quantum Thermalization and Dynamics — •Frank Pollmann — Department of Physics, Technical University of Munich, 85748 Garching, Germany

The past decade has seen a great interest in the question about whether and how quantum many-body system locally thermalize. It has been driven by theoretical findings involving the long sought demonstration that many-body localization (MBL) exists as well as the derivation of exact bounds on chaos. In my talk, I will introduce matrix-product state (MPS) based methods that allow for an efficient numerical simulation of the quantum thermalization dynamics. Firstly, I will show that, contrary to the common belief that the rapid growth of entanglement restricts simulations to short times, the long time limit of local observables can be well captured using the MPS based time-dependent variational principle. Secondly, I will discuss how mixed states can be represented using dynamically disentangled purified states. These novel methods allow to extract transport coefficients, e.g. the energy diffusion constant, efficiently.

TT 62.2 Wed 15:30 H 3010

Prethermalization without canonical transformations — Marc Alexander and •Marcus Kollar — Theoretische Physik III, Universität Augsburg

Weakly quenched quantum systems often exhibit a prethermalization regime on short to intermediate time scales, which is usually derived using canonical transformations [1,2]. We show how to skip this step and directly obtain the transient behavior, the long-time average, and the dressed constants of motion for arbitrary time-dependent protocols. We apply these results to fermionic Hubbard models for a variety of time-dependent perturbations.

[1] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008)
[2] M. Kollar et al., Phys. Rev. B **84**, 054304 (2011)

TT 62.3 Wed 15:45 H 3010

Universal prethermal states in slowly driven many-body systems — •Tobias Gulden[1], Netanel Lindner[1], Erez Berg[2], and Mark Rudner[3] — [1]Technion - Israel Institute of Technology — [2]University of Chicago — [3]University of Copenhagen

A key challenge in the search for new non-equilibrium phases of matter is the tendency of closed many-body systems to indefinitely absorb energy from a driving field. Generically this leads to an infinite temperature state where any interesting quantum, and in particular topological, effects are washed out. Here we show that in fact heating can be used as a resource for establishing universal prethermal behavior which exhibits topological phenomena. The prethermalization regime which we consider occurs for low driving frequencies, and persists throughout a long time window. Recently such prethermal states were found in one dimensional topological pumps [Lindner, Berg, Rudner, PRX 2017]. We provide bounds on the lifetimes of states, study different manifestations of universal prethermal behavior in a variety of systems, and discuss probes for observing topological properties.

TT 62.4 Wed 16:00 H 3010

Non-Equilibrium Steady State Quantum Systems — •Michael Schuett and Markus Mueller — Condensed Matter Theory Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Recent experimental advances have sparked a growing interest in quantum systems out of equilibrium. Such systems can exhibit phenomena not found in equilibrium. A frequent price payed for this freedom is the intractability of the non-equilibrium system. Here we consider a tractable toy model, rich enough to exhibit interesting non-equilibrium properties in a driven steady state. Being a well characterized fixed point, the steady state selects a specific state from the vast set of out of equilibrium states. The scenario we consider are non-interacting Fermions driven around a mesoscopic scatterer. We construct the driven, current-carrying many-body state, based on non-interacting scattering states and determine the non-equilibrium Friedel oscillations. We show, based on non-interacting scattering states that experimentally detectable oscillatory magnetic field patterns arise from the emerging current pattern. Finally we generalize our construction of the steady states to include interactions and conclude with an outlook on interaction induced instabilities or chaoticity.

TT 62.5 Wed 16:15 H 3010

Non-equilibrium steady state of the ionic Hubbard model in strong electric fields — •Yusuf Mohammed[1] and Martin Eckstein[2] — [1]Universität Hambrug, Hamburg, Germany — [2]FAU, Erlangen, Germany

We investigate the transport properties and non-equilibrium steady state phases of the dissipative ionic Hubbard model driven by an electric field. In the ionic Hubbard model, metallic behavior is enhanced by a competition of band insulating and Mott insulating behavior. The system is analyzed by means of the inhomogeneous dynamical mean-field theory (DMFT), using the iterated perturbation theory as impurity solver. The steady states of this model are accessed directly through the Keldysh contour formalism. We found that with increasing electric field the sublattice polarization reduces, leading to a decrease in the screening of the gap and an increase in the electronic scattering rate. This results in a smaller current in the nonlinear regime of correlated ionic insulators compared the non interacting case. In addition, we observed a quasi-thermal distributions even in the negative differential resistance regime, due to electron-electron scattering.

15 min. break.

TT 62.6 Wed 16:45 H 3010

Irreversible dynamics in quantum many-body systems — •Markus Schmitt[1,2] and Stefan Kehrein[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Max-Planck-Institute for the Physics of Complex Systems, Dresden, Germany

Irreversibility, despite being a necessary condition for thermalization, still lacks a sound understanding in the context of quantum many-body systems. In our work [1] we approach this question by studying the behavior of generic many-body systems under imperfect effective time reversal, where the imperfection is introduced as a perturbation of the many-body state at the point of time reversal. Based on numerical simulations of the full quantum dynamics we demonstrate that observable echos occurring in this setting decay exponentially with a rate that is intrinsic to the system meaning that the dynamics is effectively irreversible.

[1] M. Schmitt and S. Kehrein, arXiv:1711.00015

TT 62.7 Wed 17:00 H 3010

Absence of dynamical localization in interacting driven systems — •David J. Luitz[1], Yevgeny Bar Lev[2,3], and Achilleas Lazarides[3] — [1]Physik Department T42, Technische Universität München, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

Using a numerically exact method we study the stability of dynamical localization to the addition of interactions in a periodically driven isolated quantum system which conserves only the total number of particles. We find that while even infinitesimally small interactions destroy dynamical localization, for weak interactions density transport is significantly suppressed and is asymptotically diffusive, with a diffusion coefficient proportional to the interaction strength. For systems tuned away from the dynamical localization point, even slightly, transport is dramatically enhanced and within the largest accessible systems sizes a diffusive regime is only pronounced for sufficiently small detunings.

[1] D. J. Luitz, Y. Bar Lev, A. Lazarides, *SciPost Phys.* **3**, 029 (2017)

TT 62.8 Wed 17:15 H 3010

Impurity induced quench dynamics in shallow Fermi seas: an analytic treatment — •Conor Jackson and Bernd Braunecker — University of St Andrews, St Andrews, United Kingdom

We investigate the Loschmidt echo for a system of free fermions after the introduction of a local quench impurity, taking account of the finite band depth. For a system with a large bandwidth, the sudden introduction of an impurity leads to the well-known Fermi-Edge Singularity and a characteristic power law decay in the Loschmidt echo in the long time limit. We examine analytically the effect of the finite band bottom at intermediate time scales, using a Riemann-Hilbert approach to evaluate the functional determinants induced by the fermionic statistics. On these time scales we find disruption of the entire Fermi sea, rather than simply the surface shakeup which leads to the standard result, and we can provide an analytic explanation of previous numerical results.

TT 62.9 Wed 17:30 H 3010

Anomalous Spin Precession under a Geometrical Torque — •Christopher Stahl[1,2] and Michael Potthoff[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Precession and relaxation predominantly characterize the real-time dynamics of a spin driven by a magnetic field and coupled to a large Fermi sea of conduction electrons. We demonstrate an anomalous precession with frequency higher than the Larmor frequency or with inverted orientation in the limit where the electronic motion adiabatically follows the spin dynamics. For a classical spin, an analytic expression which identifies the finite spin Berry curvature of the conduction electrons as the origin of the anomalous frequency is derived. Complementary studies for the minimal model of two coupled spins and calculations for the Kondo-impurity model verify that the anomalous precession is also present for a quantum spin and suggest that the derived formula for the frequency of the classical spin can be applied to the quantum case by replacing the classical spin components by the corresponding expectation values.

[1] C. Stahl and M. Potthoff, PRL 119, 227203 (2017)

TT 62.10 Wed 17:45 H 3010

The Lipkin-Meshkov-Glick model with Markovian dissipation — •João S. Ferreira and Pedro Ribeiro — CeFEMA, Instituto Superior Técnico, Universidade de Lisboa Av. Rovisco Pais, 1049-001 Lisboa, Portugal

Motivated by recent prototypes of enginereed atomic spin devices, we study a fully connected system of n spins 1/2, modeled by the Lipkin-Meshkov-Glick (LMG) model of a collective spin $s = n/2$, in the presence of Markovian dissipation processes. Employing semi-classical and variational methods and a systematic Holdstein-Primakov mapping, we determine the semi-classic equations of motion, the phase diagram and spectral properties of the Liouvillian by studying both the thermodynamic limit and $1/s$ corrections. Our approach reveals the existence of: dynamical phase transitions for finite s, tri-stable steady state regions and recurrent regions where the system fails to thermalize.

TT 62.11 Wed 18:00 H 3010

Tripartite information and scrambling in quantum lattice models — •Oskar Schnaack[1], Sebastian Paeckel[1], Thomas Köhler[1], Salvatore R. Manmana[1], Stefan Kehrein[1], and Markus Schmitt[1,2] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany

The tripartite information has been introduced as a quantitative observable-independent measure of scrambling by Hosur et al. [1]. We investigate its time-evolution for quantum lattice models with tunable integrability breaking and demonstrate that in contrast to integrable models generic systems scramble information irrespective of the chosen partitioning of the lattice. To compute the information measures of interest we introduce exact representations of permutation operators to obtain entanglement entropies of embedded subsystems using matrix product states.

[1] P. Hosur, X.-L. Qi, D. A. Roberts, B. Yoshida, JHEP02 (2016) 004

TT 62.12 Wed 18:15 H 3010

Real-time dual bosons: role of magnetic time scales. — •Sergey Brener — Universität Hamburg, Germany

We describe magnetic dynamics within the framework of dual bosons on keldysh contour. In particular the role of separating of electron and magnetic time-scales is considered.

TT 63: Topology: Quantum Hall Systems

Time: Wednesday 15:00–16:45 Location: A 053

TT 63.1 Wed 15:00 A 053

Strain-Induced Landau Levels in Arbitrary Dimensions with an Exact Spectrum — •Stephan Rachel[1], Ilja Goethel[2], Daniel P. Arovas[3], and Matthias Vojta[2] — [1]University of Melbourne, School of Physics — [2]TU Dresden, Institut für Theoretische Physik — [3]UC San Diego, Department of Physics

Certain nonuniform strain applied to graphene flakes has been shown to induce pseudo-Landau levels in the single-particle spectrum, which can be rationalized in terms of a pseudomagnetic field for electrons near the Dirac points. However, this Landau level structure is, in general, approximate and restricted to low energies. Here, we introduce a family of strained bipartite tight-binding models in arbitrary spatial dimension d and analytically prove that their entire spectrum consists of perfectly degenerate pseudo-Landau levels. This construction generalizes the case of triaxial strain on graphene's honeycomb lattice to arbitrary d; in $d = 3$, our model corresponds to tetraxial strain on the diamond lattice. We discuss general aspects of pseudo-Landau levels in arbitrary d.

TT 63.2 Wed 15:15 A 053

Properties of the one-particle density matrix in an interacting Chern insulator — Andrew Hayward[1], Marie Piraud[2], and •Fabian Heidrich-Meisner[2,3] — [1]LMU Munich, Germany — [2]TU Munich, Germany — [3]Georg-August-University Goettingen, Germany

The notion of a topological insulator is rooted in the physics of non-interacting particles but generalizes to interacting systems. Here we investigate how much of the topological properties of an interacting Chern insulator is encoded in the single–particle quantities derived from the one-particle density matrix (OPDM) computed in the many-body ground state. The diagonalization of the OPDM yields the occupation spectrum and its eigenfunctions. In a concrete example, we study how the occupations evolve as a function of interactions and how the eigenfunctions are deformed away from the non-interacting limit. After resolving potential ambiguities in defining OPDM eigenbands, we compute the Chern numbers for these emergent OPDM bands, which are necessarily quantized. The behavior of these quantities, occupations, OPDM eigenfunctions, and OPDM Chern numbers, across a transition into a topologically trivial phase is discussed.

This research is supported by DFG Research Unit FOR2414.

TT 63.3 Wed 15:30 A 053

Emergent Chern-Simons excitations due to electron-phonon interaction on hexagonal lattices — •Andreas Sinner and Klaus Ziegler — Institut für Physik, Theorie II Universität Augsburg Universitätsstr. 1 D-86159, Augsburg, Germany

We address the problem of Dirac fermions interacting with inplane optical phonons. A gap in the spectrum of fermions leads to the emergence of the Chern-Simons excitations in the spectrum of phonons. We study the effect of those excitations on observable quantities: the phonon dispersion, the phonon spectral density, and the Hall conductivity.

[1] A. Sinner, K. Ziegler, Phys. Rev. B 93, 125112 (2016).

TT 63.4 Wed 15:45 A 053

Protected pseudohelical edge states in Z_2-trivial proximitized graphene — •Tobias Frank, Petra Högl, Martin Gmitra, Denis Kochan, and Jaroslav Fabian — Universität Regensburg

We investigate topological properties of models that describe graphene on realistic substrates which induce proximity spin-orbit coupling in graphene [1]. A Z2 phase diagram is calculated for the parameter

space of (generally different) intrinsic spin-orbit coupling on the two graphene sublattices, in the presence of Rashba coupling. The most fascinating case is that of staggered intrinsic spin-orbit coupling which, despite being topologically trivial, Z_2=0, does exhibit edge states protected against time-reversal scattering for zigzag ribbons as wide as micrometers. We call these states pseudohelical as their helicity is locked to the sublattice. The spin character and robustness of the pseudohelical modes is best exhibited on a finite flake, which shows a finite spin current in the crossection of the flake, and exhibit spin-flip reflectionless tunneling at the armchair edges.

This work was supported by the DFG SFB Grant No. 689, 1277 (A09 and B07) and GRK Grant No. 1570, and the International Doctorate Program Topological Insulators of the Elite Network of Bavaria. We received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 696656. The authors gratefully acknowledge the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project.

[1] M. Gmitra, D. Kochan, P. Högl, J. Fabian, PRB 93 155104 (2016)

TT 63.5 Wed 16:00 A 053

Topological edge states in graphene from proximity effect — •Petra Högl, Tobias Frank, Denis Kochan, Martin Gmitra, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Placing graphene on transition-metal dichalcogenides can increase its spin-orbit coupling by orders of magnitude [1] and leads to the formation of edge states protected against time-reversal scattering in zigzag ribbons [2]. We investigate an effective model for such systems in the presence of proximity-induced exchange splitting [3], which breaks time reversal symmetry and allows for quantum anomalous Hall states. We show the chiral edge states for zigzag and armchair ribbons and prove their topological character by computing the Chern number. From the bulk gap closing and Chern number for a wide parameter space of staggered intrinsic spin-orbit coupling and uniform exchange splitting (and vice versa) we identify distinct topological phases with Chern number ± 2 (± 1). By adding proximity-induced s-wave superconductivity to the system we get particle-hole symmetric doubling of the number of edge states and topological superconducting phases with Chern number ± 4 (± 2). This work is supported by IDK Top. Ins. of ENB, DFG SFB 689, GRK 1570, and by the EU Seventh Framework Prog. under Grant Agreement No. 604391 Graphene Flagship.

[1] M. Gmitra, D. Kochan, P. Högl, J. Fabian, Phys. Rev. B 93, 155104 (2016)
[2] T. Frank, P. Högl, M. Gmitra, D. Kochan, J. Fabian, arXiv: 1707.02124
[3] K. Zollner, M. Gmitra, T. Frank, J. Fabian, Phys. Rev. B 94, 155441 (2016)

TT 63.6 Wed 16:15 A 053

Chiral Topological Phases from Artificial Neural Networks — Raphael Kaubruegger[1,3], •Lorenzo Pastori[1,2], and Jan Carl Budich[1,2] — [1]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden — [2]Institute of Theoretical Physics, Technische Universitaet Dresden, 01062 Dresden, Germany — [3]Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria

Motivated by recent progress in applying techniques from the field of artificial neural networks (ANNs) to quantum many-body physics, we investigate as to what extent the flexibility of ANNs can be used to efficiently study systems that host chiral topological phases such as fractional quantum Hall (FQH) phases. With benchmark examples, we demonstrate that training ANNs of restricted Boltzmann machine type in the framework of variational Monte Carlo can numerically solve FQH problems to good approximation. Furthermore, we show by explicit construction how n-body correlations can be kept at an exact level with ANN wave-functions exhibiting polynomial scaling with power n in system size. Using this construction, we analytically represent the paradigmatic Laughlin wave-function as an ANN state.

TT 63.7 Wed 16:30 A 053

Charge and energy fractionalization mechanism in one-dimensional channels — •Matteo Acciai[1,2,3], Alessio Calzona[1,2,4], Giacomo Dolcetto[4], Thomas L. Schmidt[4], and Maura Sassetti[1,2] — [1]Dipartimento di Fisica, Università di Genova, Via Dodecaneso 33, 16146 Genova, Italy — [2]SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy — [3]CNRS, CPT, Aix Marseille Université, Université de Toulon, Marseille, France — [4]Physics and Materials Science Research Unit, University of Luxembourg, L-1511, Luxembourg

We study the problem of injecting single electrons into interacting one-dimensional quantum systems, a fundamental building block for electron quantum optics. It is well known that such injection leads to charge and energy fractionalization. We elucidate this concept by calculating the nonequilibrium electron distribution function in the momentum and energy domains after the injection of an energy-resolved electron. Our results shed light on how fractionalization occurs via the creation of particle-hole pairs by the injected electron. In particular, we focus on systems with a pair of counterpropagating channels, and we fully analyze the properties of each chiral fractional excitation which is created by the injection. We suggest possible routes to access their energy and momentum distribution functions in topological quantum Hall or quantum spin-Hall edge states.

[1] Phys. Rev. B **94**, 035404 (2016)
[2] Phys. Rev. B **96**, 075144 (2017)

TT 64: Frustrated Magnets - α-$RuCl_3$ and Cu-based Materials

Time: Wednesday 15:00–18:15 Location: HFT-FT 101

TT 64.1 Wed 15:00 HFT-FT 101

Electronically highly cubic conditions for Ru in α-$RuCl_3$ — •Stefano Agrestini[1], Chang-Yang Kuo[1], Kyung-Tae Ko[1], Zhiwei Hu[1], Deepa Kasinathan[1], Hari Babu Vasili[2], Javier Herrero-Martin[2], Manuel Valvidares[2], Eric Pellegrin[2], Anne Henschel[1], Marcus Schmidt[1], Ling-Yun Jang[3], Arata Tanaka[4], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]NSRRC, Hsinchu, Taiwan — [4]Department of Quantum Matter, Hiroshima University, Higashi-Hiroshima, Japan

α-$RuCl_3$ is the most promising candidate for the long-sought materialization of the Kitaev model. Prerequisite for these expectations is that the non-cubic crystal field splitting is small compared to the spin-orbit coupling (SOC) and, hence, does not perturb in a significant way the description of the electronic ground state in terms of the $J_{eff} = 1/2$ state. In this context, contradictory reports are available in literature.

In this talk I present a study of the local Ru 4d electronic structure of $RuCl_3$ by means of polarization dependent x-ray absorption spectroscopy at the Ru-$L_{2,3}$ edges. The observed linear dichroism is vanishingly small indicating that electronically the Ru 4d local symmetry is highly cubic. Consistent with our magnetic circular dichroism measurements, the ratio of the orbital and spin moments is found to be 2.0, the value expected for a $J_{eff} = 1/2$ ground state. The data thus show that as far as the Ru 4d local properties are concerned, $RuCl_3$ is an ideal candidate for the realization of the Kitaev physics.

TT 64.2 Wed 15:15 HFT-FT 101

High pressure magnetization measurements in α-$RuCl_3$ — •Gaël Bastien[1], Randirley Beltrán Rodríguez[1], Paula Lampen Kelley[2], Steven Nagler[2], Ravi Yadav[3], Liviu Hozoi[3], Jeroen Van den Brink[3,4], Anja U B Wolter[1], and Bernd Büchner[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01171 Dresden, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [4]Department of Physics, Technical University Dresden, Helmholtzstrasse 10, 01069 Dresden, Germany.

α-$RuCl_3$ is a promising candidate for the realization of the Kitaev quantum spin liquid. Its structure consists of honeycomb layers of J_{eff}=1/2 Ruthenium atoms. However at ambient pressure, α-$RuCl_3$ shows an antiferromagnetic ground state below $T_N \approx$7K: the zig zag order. This order can be suppressed by the application of a magnetic field to induce the Kitaev quantum spin liquid ground state.

Another route to tune the magnetic properties of $\alpha-RuCl_3$ is the application of pressure. The magnetization under hydrostatic pressure was measured with a home built low background pressure cell

down to 2K and up to 2GPa. The antiferromagnetic ground state of α-$RuCl_3$ is indeed suppressed under pressure at $P_c \approx 0.2$GPa together with a collapse of the magnetic susceptibility for both field applied in and transverse to the basal plane. We discuss possible scenarios to explain the new pressure induced state and its origin and draw the pressure-temperature phase diagram.

TT 64.3 Wed 15:30 HFT-FT 101

Pressure induced structural phase transition and dimer formation in α-$RuCl_3$ — •Maximilian Kusch[1], Quirin Stahl[1], Theo Woike[1], Gaston Garbarino[2], Francisco Javier Martinez[2], Mohamed Mezouar[2], Lisa Leissner[3], Kwang-Yong Choi[4], and Jochen Geck[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, 01069 Dresden, Germany — [2]European Synchrotron Radiation Facility, BP 220, F-38043 Grenoble Cedex, France — [3]Institut für Anorganische Chemie, Technische Universität Bergakademie Freiberg, D-09596 Freiberg, Germany — [4]Department of Physics, Chung-Ang University, Seoul 156-756, Republic of Korea

Currently α-$RuCl_3$ is the most promising candidate for the long sought realization of the Kitaev model, which is believed to be very close to a gapless spin-liquid. Under ambient conditions, however, α-$RuCl_3$ exhibits antiferromagnetic ordering below 7K, but several experimental studies indicate the proximity to the Kitaev limit nonetheless. In accordance very recent magnetization measurements as a function of pressure revealed a significant decrease in the magnetization. We therefore performed single crystal XRD as a function of pressure in the range $<$ 2GPa at 4 - 300K to determine the structural changes related to the magnetic transition. Our study shows that the monoclinic phase under ambient conditions transforms into a metastabile hexagonal phase followed by a trigonal phase featuring strong Ru-Ru dimer bonds. Specifically the latter transition coincides with the observation of a significant decrease in the magnetization. One possible explanation for this effect is the formation of a S=0 singlet state on the Ru-Ru dimers.

TT 64.4 Wed 15:45 HFT-FT 101

Ultrafast relaxation dynamics in a Kitaev spin-liquid candidate α-$RuCl_3$ — •Steinn Ymir Agustsson[1], Vladimir Grigorev[1], Tao Dong[2], Nanlin Wang[2], and Jure Demsar[1] — [1]University of Mainz, Germany — [2]Peking University, China

α-$RuCl_3$, which forms an almost ideal 2D honeycomb lattice with weak interlayer coupling, has been proposed to be a prime candidate for the realization of Kitaev physics. While α-$RuCl_3$ is an antiferromagnet at temperatures below 7-14 K (depending on the stacking configuration), numerous experiments suggest spin liquid behavior at temperatures above the Néel transition. To probe the dynamics in α-$RuCl_3$, we performed systematic temperature and excitation density dependent measurements of reflectivity dynamics with femtosecond time resolution, following photoexcitation via inter-site Ru d-d excitations. The low temperature dynamics is found to span timescales from 0.1 to 100 ps, and is strongly temperature and excitation density dependent near and below the Néel temperature. While the phase transition is clearly resolved, the anomalously slow dynamics extends far above the transition temperature. Finally, a structural transition with clear hysteresis was observed around 100 K, wit yet minor effect on carrier/spin relaxation dynamics.

TT 64.5 Wed 16:00 HFT-FT 101

Microwave absorption studies on the Kitaev-Heisenberg material α-$RuCl_3$ — •Christoph Wellm[1,2], Julian Zeisner[1,2], Alexey Alfonsov[2], Anja Wolter[2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], Matthias Vojta[4], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper- und Materialphysik, TU Dresden, D-01062 — [3]Fachrichtung Chemie und Lebensmittelchemie, TU Dresden, D-01062 — [4]Institut für Theoretische Physik, TU Dresden, D-01062

Topologically ordered states of matter have recently gained much attention due to their novel physical properties, the signatures of which can be experimentally probed. A prime example is the spin liquid realized in the Kitaev honeycomb lattice compass model, where fractionalization of particles leads to broad continuum-like features in the magnetic response. We will present the high-field microwave absorption results on the Mott-Hubbard-insulating material α-$RuCl_3$ which is, due to its structure and strong spin-orbit coupling, a promising candidate for the realization of Kitaev physics. Measurements on a single-crystal were conducted over a frequency range of ν = 70-660 GHz at temperatures ranging from 3-30 K. Strikingly, in addition to previously observed conventional gapped magnon modes, we find a highly unusual broad continuum characteristic of fractionalization which extends to energies below the lowest sharp mode and to temperatures significantly higher than the ordering temperature.

TT 64.6 Wed 16:15 HFT-FT 101

Thermal Hall effect in α-$RuCl_3$ — •Richard Hentrich[1,2], Bernd Büchner[1,2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], and Christian Hess[1,2] — [1]IFW Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, Germany — [3]Department of Chemistry and Food Chemistry, TU Dresden, Germany

The Kitaev-Heisenberg model is source of a topological quantum spin liquid with Majorana fermions and gauge flux excitations as fractional quasiparticles. The material α-$RuCl_3$ is composed of weakly van der Waals bound honeycomb layers of edge sharing $RuCl_6$ octahedra which has recently emerged as a prime candidate for realising such physics. We studied α-$RuCl_3$ by means of thermal transport measurements, a valuable tool to probe elementary excitations of systems with low dimensional spin structure.
While the in-plane, longitudinal heat transport is governed by heat conduction of phonons that strongly scatter off the magnetic excitations present in the system, studying the thermal Hall effect (Rhighi-Leduc effect) opens up a new path towards detecting a direct contribution of unconventional magnetic excitations to entropy transport.
We have observed a sizeable transversal heat conductivity κ_{xy}, the agreement of which with the theoretical predictions for the pure Kitaev model being suggestive of heat transport by fractionalised quasiparticles in α-$RuCl_3$.

15 min. break.

TT 64.7 Wed 16:45 HFT-FT 101

Magnetic excitations and lattice dynamics in the $s = 1/2$ pseudo-kagome system $Cu_3Bi(SeO_3)_2O_2(Br,Cl)$ — Vladimir Gnezdilov[1], Dirk Wulferding[2,3], •Peter Lemmens[2,3], Vladimir Kurnosov[1], Yurii Pashkevich[4], Peter Berdonosov[5], and Alexander Vasiliev[5] — [1]ILTPE, NASU, Kharkov, Ukraine — [2]IPKM, TU-BS, Braunschweig, Germany — [3]LENA, TU-BS, Braunschweig, Germany — [4]DonFTI, NASU, Donetsk, Ukraine — [5]MSU, Moscow, Russia

The francisites $Cu_3Bi(SeO_3)_2O_2Br$ and $Cu_3Bi(SeO_3)_2O_2Cl$ form layered pseudo-kagome structures, resulting in a highly spin frustrated state [1]. Our temperature- and field-dependent study uncovers strong lattice dynamics in $Cu_3Bi(SeO_3)_2O_2Cl$, that are absent in the -Br system. The origin of a low-energy excitation emerging in the magnetically ordered phase is discussed with respect to its magnetic field response and selection rule.

Work supported by DFG Project LE967/16-1.

[1] Gnezdilov, et al., PRB 96, 115144 (2017).

TT 64.8 Wed 17:00 HFT-FT 101

High magnetic field study of the frustrated quantum magnet atacamite — •Stefan Süllow[1], Leonie Heinze[1], Marcelo Jaime[2], Xiaxin Ding[2], Vivian Zapf[2], Anja U.B. Wolter[3], and Kirrily C. Rule[4] — [1]TU Braunschweig, Braunschweig, Germany — [2]NHMFL, Los Alamos, USA — [3]IFW Dresden, Dresden, Germany — [4]The Bragg Institute, ANSTO, Australia

The mineral atacamite $Cu_2Cl(OH)_3$ has been proposed to represent a frustrated quantum magnet [1,2]. From a basic magnetic characterization in low magnetic fields, it can be inferred that long range magnetic order occurs below T_N = 9 K and $\sim$ 10 T (ordering vector q = [1/2 0 1/2]), while magnetic saturation is attained only for fields beyond 50 T. This difference in field scales likely reflects low dimensionality and/or geometric frustration of the magnetic system. Therefore, we have carried out a magnetostrictive high magnetic field study, this way establishing the essential features of the magnetic phase diagram for all crystallographic axes in fields up to 65 T. We find rich phase diagrams for all directions and discuss these in terms of possible magnetic models accounting for the properties of atacamite.

[1] X. G. Zheng, et al., Phys. Rev. B **71**, 174404 (2005).
[2] L. Heinze, et al., Physica B (2017), http://dx.doi.org/10.1016/j.physb.2017.09.073.

TT 64.9 Wed 17:15 HFT-FT 101

Neutron diffraction, muon spin rotation and Raman scattering investigation of the multiferroic antiferromagnetic quantum spin chain system $CuCrO_4$ — J. M. Law[1,5], V. Pomjakushin[2], G. Pascua[2], H. Luetkens[2], Th. Hansen[3], R. Glaum[4], A. Schulz[1], J. Wosnitza[5], and •R. K. Kremer[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland — [3]Institut Laue Langevin, F-38042 Grenoble, France — [4]Institut für Anorganische Chemie, Universität Bonn, Gerhard-Domagk-Strasse 1, D-53121 Bonn, Germany — [5]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, D-01314 Dresden, Germany

Long-range magnetic ordering in multiferroic spin-chain compound $CuCrO_4$ was investigated by powder neutron diffraction and muon spin rotation measurements. Consistently, both methods find incommensurate long- range antiferromagnetic ordering below 9.0(3) K. The magnetic structure was determined from neutron powder diffraction patterns based on the propagation vector τ=(1,0,0.546(1)). The magnetic moment at 2K was refined to 0.67(10) μ_B. Low-temperature high-magnetic-field measurements of the magnetization and the dielectric polarization show the multiferroic phase to extend up to $\approx$ 23 T, after which a new, yet unknown phase appears. Full saturation of the magnetic moment is expected to occur at fields $\gg$ 60 T. Raman scattering and low-temperature x-raypowder diffraction measurements are used to correlate magnetic, structural and dielectric properties.

TT 64.10 Wed 17:30 HFT-FT 101

Thermodynamic investigations of the anisotropic triangular Heisenberg antiferromagnet $Cs_2CuCl_{4-x}Br_x$ — •Ulrich Tutsch[1], Oleksandr Tsyplyatyev[2], Lars Postulka[1], Markus Kuhnt[1], Bernd Wolf[1], Natalija van Well[1], Franz Ritter[1], Cornelius Krellner[1], Burkhard Schmidt[3], Peter Kopietz[2], and Michael Lang[1] — [1]Physikalisches Institut and — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt, SFB/TR 49, 60438 Frankfurt (M), Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The system $Cs_2CuCl_{4-x}Br_x$ is known to be a good realization of the $S = 1/2$ 2D anisotropic triangular Heisenberg antiferromagnet. Its border compounds ($x = 0, 4$) have been intensively studied by neutron scattering experiments, ESR and thermodynamic methods, so that the ratio J'/J of the coupling constants of 0.34 ($x = 0$) and 0.41 ($x = 4$) is known with a high degree of accuracy. We will present specific heat results for the two intermediate compounds with $x = 1, 2$ which can be synthesized with a fully ordered halide sublattice when grown at relatively low temperatures from an aqueous solution. A $C \propto T$ behaviour is observed at low temperatures for both compounds although $Cs_2CuCl_2Br_2$ already shows a rather high value $J'/J \approx 0.7$. Our experimental results are in good agreement with our theoretical calculations, which demonstrate that a $C \propto T$ behaviour at low temperatures can be a result of strong quantum fluctuations in $S = 1/2$ 2D anisotropic triangular Heisenberg antiferromagnets, contrary to the general believe that it reflects quasi-1D behaviour.

TT 64.11 Wed 17:45 HFT-FT 101

Magnetic and magneto-elastic couplings in $Cs_2CuCl_{4-x}Br_x$ with x = 0, 1, 2. — •Bernd Wolf, Satya Krishna Thallapaka, Elena Gati, Lars Postulka, Franz Ritter, Cornelius Krellner, and Michael Lang — Physics Institute Goethe University, SFB/TR 49, 60438 Frankfurt, GermanyFrankfurt,

Like for the intensively investigated quasi-2D frustrated triangular quantum antiferromagnet Cs_2CuCl_4, the newly discovered stoichiometric compounds $Cs_2CuCl_{4-x}Br_x$ with x = 1, 2 exhibit a well-ordered local Cu environment due to a site-selective substitution of the halid atoms. We present $\chi(T, p)$ data from which the magnetic coupling constants are extracted based on a $J_1 - J_2$ model. We find that $Cs_2CuCl_3Br_1$ and $Cs_2CuCl_2Br_2$ exhibit a distinctly larger degree of geometric frustration of $J_1/J_2 = 0.47$ and 0.63, respectively, as compared to 0.29 for the pure Cl material. From the variation of the susceptibility under hydrostatic He-gas pressure up to 4 kbar for the different materials we extract the pressure dependence of J_1 and J_2 as well as the magneto-elastic coupling constants. Compared to other low-dimensional spin systems, the magneto-elastic couplings are at least two orders of magnitude smaller. We assign this behavior to structural peculiarities of this class of materials where structural rigid units, containing the magnetic centres, are embedded in a highly compressible matrix.

TT 64.12 Wed 18:00 HFT-FT 101

Anomalous Hall effect in frustrated antiferromagnet HoAgGe — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, University Augsburg

Geometric frustration in magnetic systems arises from competing magnetic interactions that cannot be satisfied simultaneously and leads to a variety of exotic ground states. Recent theoretical calculations show frustrated antiferromagnet Mn_3Ir will exhibit the anomalous hall effect (AHE), because of the three rotation symmetry of Mn kagome lattice. Then the AHE is observed in non collinear antiferromagnet Mn_3Sn at 300K due to the Berry curvature in momentum space.

HoAgGe, which crystallize in the hexagonal ZrNiAl-type structure, is an antiferromagnet below 11K. The Ho atoms form a distorted Kagome lattice. With high quality single crystal, we investigate the transport and magnetic property at 2K. Obvious hysteresis can be observed from hall resistance and magnetroresistance between 1T and 3T. However, there is no hysteresis from M(H) curve at the same field region, indication the hysteresis not coming from the magnetization. There are probably some non collinear antiferromagnetic structure under field, which has no contribution to magnetization, but will contribute to the anomalous hall effect (AHE), namely the hysteresis in hall resistance between increasing and decreasing field.

To investigate the origin of AHE in this system, we conduct single crystal neutron diffraction at 2K and under magnetic field. And the determination of the non collinear frustrated magnetic structure of HoAgGe is still in progress.

TT 65: Quantum-Critical Phenomena II

Time: Wednesday 15:00–18:30 Location: HFT-FT 131

TT 65.1 Wed 15:00 HFT-FT 131

Nematic phase transition of Dirac fermions — •Jonas Schwab[1], Kai Sun[2], Zi Yang Meng[3], Igor Herbut[4], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Physics Department, University of Michigan, Ann Arbor, MI 48109, USA — [3]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [4]Department of Physics, Simon Fraser University, Burnaby, British Columbia V5A 1S6, Canada

We consider Dirac fermions, as realized by a pi-flux tight binding model on a square lattice, coupled to an Ising model in a transverse field. The coupling is chosen such that the ordering of the Ising spins triggers a meandering of the Dirac fermions and thereby a nematic deformation of the "Fermi" surface. The model is amenable to sign-problem free quantum Monte Carlo simulations such that the nature of the transition for various couplings and flavor number of Dirac fermions can be analyzed in detail.

TT 65.2 Wed 15:15 HFT-FT 131

Investigation of magnetic fluctuations in the ferromagnet UGe_2 by means of Modulated Intensity by Zero Effort (MIEZE) — •Franz Haslbeck[1,2], Steffen Säubert[1,3], Christian Franz[3], Marc Janoschek[2,4], and Christian Pfleiderer[1] — [1]TU Munich, Germany — [2]Institute for Advanced Study, TU Munich, Germany — [3]MLZ, TU Munich, Germany — [4]LANL, USA

It is well known that the critical fluctuations associated with magnetic quantum critical points (QCP) are crucial for the emergence of novel states of matter such as unconventional superconductivity. However, their exact nature remains an outstanding question. Most notably, according to theory both the relaxation time and correlation length of the fluctuations are expected to diverge when the QCP is approached. However, to date this has not yet been observed, partially because this requires extreme energy and momentum transfer resolution. Here we show that for ferromagnetic QCPs this problem may be overcome using the newly developed longitudinal MIEZE (Modulated Intensity by

Zero Effort) option at the instrument RESEDA at MLZ (Garching). To showcase the feasibility of this approach we have investigated the magnetic fluctuations in the material UGe_2 at ambient pressure in a small angle scattering geometry. Our results demonstrate that this technique allows studying ferromagnetic critical fluctuations with an energy resolution that is almost two orders of magnitude higher than for classical triple axis spectroscopy while simultaneously providing access to small momentum transfers. In conclusion, this suggests that MIEZE may be used to obtain new insights in ferromagnetic QCPs.

TT 65.3 Wed 15:30 HFT-FT 131

Exact solution of the spin-1/2 XXX chain with off-diagonal boundary fields — •Andreas Klümper and Dennis Wagner — Wuppertal University

The spin-1/2 Heisenberg chain with periodic boundary conditions is a seminal model of integrable resp. exactly solvable systems. It is known that the Heisenberg chain with arbitrary boundary fields is still integrable, but so far defied an explicit solution for the case of off-diagonal fields which break the $U(1)$ symmetry. As the magnetization is no longer a good quantum number, the direct application of the Bethe ansatz fails.

Here we show how the problem can be solved by a set of non-linear integral equations (NLIEs). Instead of two NLIEs as in the case of the periodically closed chain, we find a set of three NLIEs from which the eigenvalues of the Hamiltonian can be obtained. Finally, we present results for the spectrum in the conformal limit.

TT 65.4 Wed 15:45 HFT-FT 131

Tricriticality in the spin-1 XXZ chain with explicit bond dimerization — •Satoshi Ejima[1], Tomoki Yamaguchi[2], Florian Lange[1], Yukinori Ohta[2], and Holger Fehske[1] — [1]Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany — [2]Department of Physics, Chiba University, Chiba 263-8522, Japan

Applying the matrix-product-state based density-matrix renormalization group technique to the spin-1 XXZ chain with bond dimerization, we explore the competition between two different symmetry-protected-topological phases, Peierls and Haldane states. The bond dimerization narrows the Haldane phase, and only dimerized and Néel state survive for large dimerization. The critical line between these two states exhibits the continuous Ising transition with central charge $c = 1/2$, which terminates at a tricritical point, belonging to the universality class of the dilute Ising model with central charge $c = 7/10$. Above this point, the quantum phase transition becomes first order. We provide compelling evidence for the (tricritical) Ising quantum phase transition, simulating corresponding critical exponents, $\beta = 1/8$ (1/24) and $\nu = 1$ (5/9).

TT 65.5 Wed 16:00 HFT-FT 131

Spin and valence bond dynamics across a deconfined quantum critical point in a fermionic SU(3) model — •Zhenjiu Wang[1], Hui Shao[2], and Fakher.f Assaad[1] — [1]Institut for Theoretische Physik und Astrophysik, University Wuerzburg, Am Hubland, D-97074 Wuerzburg, Germany — [2]Beijing Computational Science Research Center, Beijing 100193, China

We consider a model of SU(3) fermions coupled to a transverse Ising field that harbors deconfined phases and phase transitions between antiferromagnetic (AFM) and valence bond solid (VBS) states [1]. Here, we supplement the model with a flux term and use the auxiliary field quantum Monte Carlo algorithm to and map out the phase diagram in the transverse field and flux plane. Special emphasis is placed on the VBS and AFM dynamics across the phase transition. An improved stochastic analytic continuation method reveals a spinon-continuum in the proximity of the DQCP.

TT 65.6 Wed 16:15 HFT-FT 131

Dimensional Corssover in a Bosonic Quantum Gas — •Dominik Strassel[1,2], Denis Morath[1], Polina Matveeva[1], Imke Schneider[1], Axel Pelster[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, University Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Competence Center for High Performance Computing, Fraunhofer ITWM, 67663 Kaiserslautern, Germany

The emergence of new properties from low-dimensional building blocks is a universal theme in different areas in physics. Considering a $1D$–$3D$ transition, for instance, it is far from obvious if the power laws from the underlying $1D$ theory can predict the critical transition temperature, when it increases from zero as a function of inter-chain hopping [1]. Our model is represented by $1D$ tubes with hopping between them, which can be simulated in experiments with the help of optical lattices [2]. Combining large-scale Quantum Monte-Carlo simulations – using a canonical measurement – with analytical chain mean-field calculations and an effective potential approach to calculate the Landau potential, we show that the behavior of the critical ordering temperature as a function of the inter-chain hopping does not follow a universal power law of the known universality classes for fixed dimensions, but the exponents that we found can be interpreted as a novel type of scaling behavior.

[1] B. Irsigler and A. Pelster, Phys. Rev. A 95, 043610 (2017)
[2] A.Vogler, R. Labouvie, G. Barotini, S.Eggert, V. Guarrera, and H. Ott, Phys. Rev. Lett. 113, 215301 (2014)

15 min. break.

TT 65.7 Wed 16:45 HFT-FT 131

Microstructuring $YbRh_2Si_2$: Insights from low temperature resistance — •Alexander Steppke[1], Sandra Hamann[1], Markus König[1], Daniel Hafner[1], Andrew P. Mackenzie[1], Kristin Kliemt[2], Cornelius Krellner[2], and Manuel Brando[1] — [1]MPI for Chemical Physics of Solids, Noethnitzer Str. 40, 01187 Dresden — [2]Goethe-Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt am Main

In the prototypical Kondo lattice $YbRh_2Si_2$ signatures of quantum critical fluctuations, recently discovered superconductivity below 2 mK [1] and topological changes of the Fermi surface [2] are established from different experimental probes. Still absent are data of the resistive transition into the superconducting state and high-resolution magnetoresistance data to further investigate the topological transitions. Both face a similar challenge of measuring resistance with minimal dissipation at very low temperatures. We applied focused ion beam structuring to change the geometry and therefore increase the resistance, leading to both a higher resolution and reducing influences from contact resistances. First measurements exhibit an order of magnitude improvement in resolution, revealing quantum oscillations at high applied fields. Additionally the controlled geometry is a first step to explore in-plane strain to change the magnetic properties in the vicinity of the quantum critical point.

[1] E. Schuberth et al., Science 351, 485 (2016).
[2] H. Pfau et al., PRL 110, 25 (2013).

TT 65.8 Wed 17:00 HFT-FT 131

Superconductivity and Quantum Critical Behavior in the antiferromagnetically ordered Heavy Fermion Compound Ce_3PtIn_{11}. — Jan Prokleška, Marie Kratochvílová, Klára Uhlířová, Vladimír Sechovský, and •Jeroen Custers — Faculty of Mathematics and Physics, Charles University, DCMP, Ke Karlovu 5, 121 16 Praha 2, Czech Republic

Ce_3PtIn_{11} (tetragonal, space group $P4/mmm$). The material belongs to the $Ce_nT_mIn_{3n+2m}$ class of layered materials which comprises a numerous amount of compounds including $CeCoIn_5$ and $CeRhIn_5$. At ambient condition the material shows remarkable properties: in the absence of magnetic field, Ce_3PtIn_{11} undergoes two successive magnetic transitions at $T_1 = 2.2$ K and $T_N = 2.0$ K, respectively, and becomes superconducting (SC) below $T_c = 0.35$ K. Upon applying hydrostatic pressure (p) T_1 and T_N reduce and intersect with the SC state at $p \approx 1.1$ GPa. Extrapolation of $T_N \to 0$ reveals a critical pressure of $p_c = 1.3$ GPa, i. e., the quantum critical point (QCP). Here, T_c is maximum. This strongly suggests that critical fluctuations associated with the magnetic QCP are responsible for Cooper-pairing. A salient detail with respect to the interplay of magnetism and superconductivity is that Ce_3PtIn_{11} possesses two non-equivalent Ce-sites. Ce2 resides the Wyckoff $1a$ place (C_{4v} symmetry). The ion is experiences $CeIn_3$ environment ($CeIn_3$ is an AFM). The Ce1-site occupies the $2g$ position (D_{4h} symmetry). Its surrounding is identical to Ce-atoms in Ce_2PtIn_8 (superconductor).

TT 65.9 Wed 17:15 HFT-FT 131

$CeRh_2As_2$: a Ce-based Kondo-lattice system very close to a possible multipolar quantum critical point — •Seunghyun Khim[1], Jacintha Banda[1], Daniel Hafner[1], Dongjin Jang[1,2], Manuel Brando[1], and Christoph Geibel[1] — [1]Max Planck Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Max Planck-POSTECH/KOREA Center for Complex Phase Materials, Po-

hang, Republic of Korea

We have recently grown single crystals of the new compound $CeRh_2As_2$ and studied its physical properties. Resistivity, specific heat (C_p) and magnetic susceptibility results evidence a strong Kondo interaction with $T_K \sim 25$ K. At zero field, two transitions occur at $T_1 \sim 0.2$ K and $T_2 \sim 0.3$ K. T_1 and T_2 much smaller than T_K place this system very close to a hybridization induced quantum critical point (QCP). With magnetic fields T_1 is gradually suppressed, suggesting its magnetic origin. T_2, on the other hand, increases slowly with fields, similar to the quadrupolar order in CeB_6. The suggestive quadrupolar order at T_2 is compatible with high-T C_p data that imply an effective quasi-quartet ground state which provides a quadrupolar degree of freedom. Therefore our result indicate $CeRh_2As_2$ to be a unique Kondo-lattice system of strong potential relevance for the multipolar QCPs.

TT 65.10 Wed 17:30 HFT-FT 131

Highly anisotropic strain dependencies in $PrIr_2Zn_{20}$ — •Andreas Wörl[1], Takahiro Onimaru[2], Yoshifumi Tokiwa[1], Keisuke Matsumoto[2], Toshiro Takabatake[2], and Philipp Gegenwart[1] — [1]Experimentalphysics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Japan

Exotic Kondo physics, driven by the hybridization between electric quadrupole moments and conduction electrons, generates novel metallic phases. In $PrIr_2Zn_{20}$ the local T_d symmetry of the Pr-ions forms the non-Kramers ground-state doublet which is a key prerequisite to explore quadrupole driven states of matter. The material displays antiferroquadrupolar order at $T_Q = 0.11$ K, which is suppressed by magnetic fields $B \leq 5$ T applied along the [001] direction. Superconductivity sets in at $T_c = 0.05$ K. The significant enhancement of Seebeck coefficient as well as anomalies in specific heat and electrical resistivity at the critical magnetic field at $B = 5$ T prompted speculations about a quadrupolar quantum critical point. To clarify potential quadrupolar quantum criticicality, we investigated thermal expansion and magnetostriction parallel and perpendicular to magnetic fields $\boldsymbol{B} \parallel [001]$. Linear thermal expansion and magnetostriction display huge uniaxial anisotropy, whereby volume changes are vanishingly small. We conclude that magnetic field is not an effective parameter to tune the hybridization of localized $4f^2$ and conduction electrons in $PrIr_2Zn_{20}$ and exclude the formation of a quadrupolar quantum critical point at $B \approx 5$ T.

TT 65.11 Wed 17:45 HFT-FT 131

Critical phenomena in the honeycomb antiferromagnet $BaNi_2V_2O_8$ — •Ekaterina Klyushina[1,2], Bella Lake[1,2], Johannes Reuther[1,3], Nazmul Islam[1], Bastian Klemke[1], and Martin Mansson[4,5] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Festkörperphysik Technische Universität Berlin, Germany — [3]Freie Universität, Berlin, Germany — [4]Materials Physics, KTH Royal Institute of Technology, Stockholm Kista, Sweden — [5]Laboratory for Neutron Scattering & Imaging, Paul Scherrer Institute, Villigen, Switzerland

Here we investigate the critical phenomena in the quasi-two dimensional (2D) Heisenberg honeycomb antiferromagnet $BaNi_2V_2O_8$. Both the temperature regions below and above ordering temperature T_N were explored using the technique of neutron diffraction. The critical exponent of the order parameter and the thermal decay of the correlation length were measured and analysed by applying several theoretical approaches. The temperature dependence of the spontaneous magnetization is found to follow the power law predicted for a 2D XY magnetic system confirming the 2D planar character of $BaNi_2V_2O_8$ even below T_N. At the high temperatures, the thermal decay of the correlation length is fitted well by the 2D isotropic Heisenberg approach, however the agreement becomes worse when the temperature is close to T_N. Indeed, only the expression derived by Berezinskii, Kosterlitz and Thousless is found to be in a good agreement with the experimental data within the temperature range just above the T_N. This result suggests the presence of a free vortex phase close to T_N.

TT 65.12 Wed 18:00 HFT-FT 131

Coherent low energy resonant excitation of heavy-fermion systems — •Shovon Pal[1], Christoph Wetli[1], Johann Kroha[2], Cornelius Krellner[3], Kristin Kliemt[3], Oliver Stockert[4], Hilbert v. Loehneysen[5], and Manfred Fiebig[1] — [1]ETH Zurich — [2]Bonn University, Germany. — [3]Goethe University Frankfurt, Germany. — [4]MPI Dresden, Germany. — [5]KIT, Germany.

Quantum phase transitions (QPT) describe a change between two ground states of a many-body system resulting from quantum fluctuations. Rare-earth heavy-fermion systems such as $CeCu_{6-x}Au_x$ show a QPT between a fully Kondo-screened paramagnetic Fermi-liquid phase and an antiferromagnetically (AFM) ordered phase. When excited by THz pulses, the system disintegrates near the QPT and coherently recovers on timescales in the order of picoseconds, characteristic to the Kondo temperature. We use THz time-domain spectroscopy to probe Kondo quasi-particle spectral weight at such ultrafast timescales. Temperature-dependent examination of samples with different Au concentrations reveals that in the heavy fermion ($CeCu_6$) and the quantum critical ($CeCu_{5.9}Au_{0.1}$) samples, the Kondo weight first shows a logarithmic increase by lowering the temperature until 30 K, followed by a decrease as we enter the quantum critical regime below the Kondo temperature. While in $CeCu_{5.9}Au_{0.1}$ the Kondo weight is destroyed below 5 K, $CeCu_6$ shows a drop of about 40%. The $CeCu_5Au$ sample being deep in the AFM phase does not exhibit visible Kondo weight at any temperatures despite the fact that low-temperature specific heat measurements reveal a sizeable Fermi-liquid-like contribution.

TT 65.13 Wed 18:15 HFT-FT 131

Slow dynamics around the field-induced quantum critical points in the organic spin-dimer system $C_{28}H_{32}N_4O_2$ (BY310) — •Paul Eibisch[1], Lars Postulka[1], Bernd Wolf[1], Ulrich Tutsch[1], Yulia Borozdina[2], Martin Baumgarten[2], and Michael Lang[1] — [1]Physikalisches Institut Goethe-Universität — [2]Max Planck Institut für Polymerforschung

Interacting spin-dimer networks exhibit a vast diversity of exotic physical states in connection with a field-induced ordered phase between two quantum critical points. Examples include Bose-Einstein-condensates of magnetic excitations for 3D systems as well as Luttinger liquids in 1D or BKT topological order in 2D. Spin-dimer systems, based on organic radicals, represent suitable candidates to explore this physics due to their high degree of tunability in terms of interaction strengths and dimensionality. We present results of the specific heat, susceptibility and magnetic Grüneisen parameter of the organic spin-dimer system $C_{28}H_{32}N_4O_2$, consisting of tolane-bridged iminio nitroxide radicals. Measurements were performed in a field range up to 6 T and for temperatures down to 30 mK. A field-induced ordered phase was found at fields between 1.86 T and 4.3 T for temperatures $T \leq 540$ mK. Of particular interest is the observation made in AC susceptibility at $T < 1$ K which indicates very slow dynamics of the spin system in the vicinity of both quantum critical points.

TT 66: Spintronics (joint session MA/TT)

Time: Wednesday 15:00–17:00 Location: EB 202

TT 66.1 Wed 15:00 EB 202

Spin Hall Magnetoresistance in uniaxial antiferromagnet/Pt heterostructures — •Richard Schlitz[1,2], Tobias Kosub[3], Andy Thomas[4], Kornelius Nielsch[4,5], Denys Makarov[3], and Sebastian T.B. Goennenwein[1,2] — [1]Institut für Festkörper- und Materialphysik, TU Dresden, 01062 Dresden, Germany — [2]Center for Transport and Devices of Emergent Materials, TU Dresden, 01062 Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [4]Leibniz Institute for Solid State and Materials Research Dresden (IFW Dresden), Institute for Metallic Materials, 01069 Dresden, Germany — [5]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany

Antiferromagnets recently attracted a lot of interest as candidate materials for spintronic applications. In this study, we investigate the spin Hall magnetoresistance (SMR) in uniaxial antiferromagnet (AFM)/Pt bilayers. Our results suggest that experiments close to the Neel temperature of the AFM layer allow to study the magnetic phase diagram of the AFM. By rotating the magnetic field in three orthogonal rotation planes, we establish the 3D fingerprint of the SMR also in AFM/Pt heterostructures, giving further insights into the impact of anisotropy and domain pattern. Finally, we propose an extension of the monodomainization model put forward recently in conjunction with measurements on NiO/Pt heterostructures [1] which provides an alternative explanation on the origin of the negative SMR signature.

[1] J. Fischer *et al.*, arxiv:1709.04158 (2017)

TT 66.2 Wed 15:15 EB 202

Current induced Nèel vector manipulation in Mn_2Au and associated giant anisotropic magnetoresistance — •Bodnar Stanislav[1], Šmejkal Libor[1,2,3], Gomonay Olena[1], Sinova Jairo[1], Sapozhnik Alexey[1], Elmers Hans-Joachim[1], Kläui Mathias[1], Filianina Mariia[1], and Jourdan Martin[1] — [1]Mainz University, Staudinger Weg 7, 55128 Mainz, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 00 Praha 6, Czech Republic — [3]Faculty of Mathematics and Physics, Charles University, Department of Condensed Matter Physics, Ke Karlovu 5, 12116 Praha 2, Czech Republic

Antiferromagnetic materials could be used as active elements in spintronics. This requires the ability to switch and read-out the Néel vector state. In our work we demonstrate for Mn_2Au, a good conductor with a high ordering temperature suitable for applications, reproducible switching of the Nèel vector using current pulse generated bulk spin-orbit torques and read-out by magnetoresistance measurements. Reversible and consistent changes of the longitudinal resistance and planar Hall voltage of star-patterned epitaxial $Mn_2Au(001)$ thin films were generated by pulse current densities of 10^7 A/cm^2 . The symmetry of the torques agrees with theoretical predictions and a large read-out magnetoresistance effect of more than 6 % is reproduced by ab initio transport calculations.

TT 66.3 Wed 15:30 EB 202

Granularity Effects in Antiferromagnetic Spintronics Devices — •Tobias Kosub[1], Patrick Appel[2], Brendan Shields[2], Patrick Maletinsky[2], René Hübner[1], Jürgen Lindner[1], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]University of Basel, Basel, Switzerland

Antiferromagnetic thin film systems have recently become an important focus in spintronics as all-electrical writing and reading mechanisms were discovered [1-3]. The early device prototypes have clearly shown that the extrinsic effects of film strain, granularity and non-zero magnetization are decisive factors in actual performance. Such thin film effects do not merely bring about small alterations to the expected behavior, but can indeed make or break functionality.

In this context, we demonstrate two new complementary methods to study the impact of granularity on the magnetism of antiferromagnetic thin films. We show extremely sensitive Zero-Offset Hall measurements of the non-zero magnetization as well as Nitrogen Vacancy Magnetic Microscopy of the domain patterns for Cr_2O_3 thin films.

We can track the magnetic ordering in both real and statistical space and we derive important quantities such as pinning and the intergranular exchange.

[1] T. Kosub et al., *Nature Commun.* **8**, 13985 (2017).
[2] T. Kosub et al., *Phys. Rev. Lett.* **115**, 097201 (2015).
[3] P. Wadley et al., *Science* **351**, 587 (2016).

TT 66.4 Wed 15:45 EB 202

Defect induced magnetism — A framework for all-semiconductor spintronics — •Lukas Botsch[1], Israel Lorite[1], Yogesh Kumar[1], Pablo Esquinazi[1], Tom Michalsky[1], Joachim Zajadacz[2], and Klaus Zimmer[2] — [1]Felix-Bloch-Institute for Solid State Physics, Leipzig University, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V., Leipzig, Germany

Combining the so-called defect induced magnetism (DIM) phenomenon — inducing magnetic order in nominally non-magnetic materials through defects — with acceptor/donor doping in semiconducting materials opens a whole new degree of engineering freedom to design spintronic devices. The DIM phenomenon is known to exist in a variety of materials such as different oxides, nitrides and carbon based materials. We demonstrate the versatility of this framework by showing its application in an all-semiconductor spin-filter device, prepared at the surface of a ZnO microwire by low energy ion implantation. This device is based on a spin-blockade effect that arises at the interface between highly doped magnetic and lightly doped non-magnetic regions at the surface of the wire. The device can be tuned to operate in a large range of temperatures and shows strong spin filtering.

TT 66.5 Wed 16:00 EB 202

p-type co-doping effect in III-Mn-V dilute ferromagnetic semiconductors — •Chi Xu[1,2], Ye Yuan[1,2], Mao Wang[1,2], Roman Böttger[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

III-Mn-V based diluted magnetic semiconductors offer an opportunity to explore various aspects of carrier transport in the presence of cooperative phenomena. In this work, we demonstrate the efficiency of an alternative approach to control the carrier state through involving one magnetic impurity Mn and one electrically active dopant Zn. Mn-doped and Zn co-doped Ga-V films have been prepared by combining ion implantation and pulsed laser melting, followed by a systematic investigation on the magnetic and transport properties of (Ga,Mn)P by varying Mn concentration as well as by Zn co-doping. Changes of electrical, magnetic and magneto-transport behavior of the investigated Ga-Mn-V films were observed after co-doping with Zn. The changes are caused by interstitial Mn atoms which are transferred from substitutional sites or formation of Mn-Zn dimers.

TT 66.6 Wed 16:15 EB 202

Dynamics of Mn Local Moments in Metallic and Semiconducting Pnictides — M. A. Surmach[1], P. Y. Portnichenko[1], Z. Deng[2,3], C. Q. Lin[2,4,5], J. K. Glasbrenner[6], I. I. Mazin[6], D. L. Sun[7], Y. Liu[7], C. T. Lin[7], A. Ivanov[8], J. T. Park[9], J. A. Rodriguez-Rivera[10,11], and •D. S. Inosov[1] — [1]TU Dresden, Germany — [2]Inst. of Physics, Beijing — [3]Center for High Pressure Sci. & Technol., Beijing — [4]Univ. of Chinese Academy of Sciences, Beijing — [5]Collab. Innov. Center of Quantum Matter, Beijing — [6]Naval Research Lab., Washington, USA — [7]MPI-FKF, Stuttgart, Germany — [8]ILL, Grenoble, France — [9]MLZ, Garching, Germany — [10]Univ. of Maryland, USA — [11]NIST Center for Neutron Research, USA

We have investigated the effects of Mn doping in two materials isostructural to 122-type iron-based superconductors by neutron spectroscopy. First, we discuss the excitation spectrum of Mn-substituted $BaFe_2As_2$, where local magnetic clusters pinned to the impurity sites lead to an emergence of (π, π) magnetic excitations. We discuss their 3D character and the origin of the spin gap. The 2$^{\text{nd}}$ class of materials derives from the isostructural semiconductor $BaZn_2As_2$, giving rise to a dilute magnetic semiconductor upon Mn substitution. Hole doping by K provides an opportunity to tune the carrier concentration and the amount of magnetic moments independently. The resulting compound, $(Ba_{1-x}K_x)(Zn_{1-y}Mn_y)_2As_2$, is a ferromagnet with the maximal Curie

temperature of 230 K. It offers a versatility of chemically tailored properties, as the hole doping is decoupled from spin injection and occurs in a different crystallographic layer.

TT 66.7 Wed 16:30 EB 202

Quasiclassical theory of the Rashba-Edelstein magnetoresistance — •Sebastian Tölle[1], Michael Dzierzawa[1], Ulrich Eckern[1], and Cosimo Gorini[2] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Faculty of Physics, University of Regensburg, 93040 Regensburg, Germany

In a recent experiment, a magnetoresistance originating from Rashba spin-orbit coupling in a metallic heterostructure has been observed [1]. We consider a 3D Rashba metal with mass anisotropy [2] attached to a ferromagnetic insulator and employ the quasiclassical approach to derive a set of coupled spin-diffusion equations. Due to the spin transfer torque, the current-induced spin polarization (Edelstein effect) acquires a characteristic dependence on the polarization direction of the ferromagnet which manifests itself as a signature in the magnetoresistance. Our theoretical results reproduce several qualitative features of the experiments. In particular, the Elliott-Yafet spin relaxation plays a major role in explaining the temperature dependence of the observed signature.

[1] H. Nakayama et al., Phys. Rev. Lett. 117, 116602 (2016);
H. Nakayama et al., Appl. Phys. Lett. 110, 222406 (2017).
[2] V. Brosco and C. Grimaldi, Phys. Rev. B 95, 195164 (2017).

TT 66.8 Wed 16:45 EB 202

Geometric phase switching in spin interferometry — •Henri Saarikoski[1], Andres Reynoso[2], Diego Frustaglia[3], Jose-Pablo Baltanás[3], Makoto Kohda[4], and Junsaku Nitta[4] — [1]RIKEN Center for Emergent Matter Science, Wako, Saitama 351-0198, Japan — [2]Instituto Balseiro and Centro Atómico Bariloche, 8400 Bariloche, Argentina — [3]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [4]Department of Materials Science, Tohoku University, Sendai 980-8579, Japan

The geometric (Berry) phase acquired by an electron in a cyclic evolution depends on the topology of the driving fields. An oscillating field in the adiabatic limit does not result in a Berry phase in contrast to a rotating field that gives a Berry phase of π. We consider here theoretically topological geometric phase switching in quasi-two-dimensional mesoscopic ring systems where the geometric phase is of nonadiabatic (Aharonov-Anandan) type of geometric phase. The driving field results from interplay between Bychov-Rashba and Dresselhaus [001] spin-orbit fields and an in-plane magnetic field. We find that the geometric phase switching is imprinted both in the resistance as well as in anisotropy oscillations of the ring. We compare results with experiments in circular and polygonal ring systems.

TT 67: Skyrmions III (joint session MA/TT/KFM)

Time: Wednesday 15:00–18:30 Location: EB 301

TT 67.1 Wed 15:00 EB 301

Skyrmion drag effect: — •Adel Abbout[1], Joseph Weston[2], Xavier Waintal[2], and Aurelien Manchon[1] — [1]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [2]CEA Grenoble, France.

In this work, we study the motion of skyrmionic magnetic textures and analyze the current induced by this motion using time-dependent non-equilibrium Green's function formalism implemented on a real-space tight-binding model. We focus on the time dependent distribution of the nonequilibrium charge and spin densities and discuss the corresponding topological Hall effect. The perturbation induced by this motion applies a torque on the whole texture. The influence of the generated current on the whole texture is discussed and its signature is unveiled in the renormalization of the damping parameter. A cooperative effect due to the collective motion of skyrmions is proposed in order to enhance the skyrmion's velocity. The stationary regime is analyzed as a function of the different parameters of the system and explained using the formalism of electronic pumping. A simple formula for the current is proposed.

TT 67.2 Wed 15:15 EB 301

Theory of tunneling vector spin transport on a magnetic skyrmion — •Krisztián Palotás[1,2], Levente Rózsa[3], and László Szunyogh[4] — [1]Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia — [2]University of Szeged, Szeged, Hungary — [3]University of Hamburg, Hamburg, Germany — [4]Budapest University of Technology and Economics, Budapest, Hungary

Spin-polarized scanning tunneling microscopy (SP-STM) demonstrated the creation and annihilation of individual magnetic skyrmions [1] that is promising for future technological use. The detailed microscopic mechanisms for these processes are, however, unknown. In the present work the tunneling spin transport of a magnetic skyrmion is theoretically investigated in SP-STM. The spin-polarized charge current [2] and tunneling spin transport vector quantities, the longitudinal spin current and the spin transfer torque are calculated in high spatial resolution within a simple electron tunneling theory for the first time. Beside the vector spin transport characteristics, the connections between conventional charge current SP-STM images and the magnitudes of the spin transport quantities are analyzed.

[1] N. Romming et al., Science 341, 636 (2013).
[2] K. Palotás et al., Phys. Rev. B 96, 024410 (2017).

TT 67.3 Wed 15:30 EB 301

Quantum dynamics of skyrmions in chiral magnets — •Christina Psaroudaki — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

We study the quantum propagation of a skyrmion in chiral magnetic insulators by generalizing the micromagnetic equations of motion to a finite temperature path integral formalism, using field theoretic tools. Promoting the center of the skyrmion to a dynamic quantity, the fluctuations around the skyrmionic configuration give rise to a time-dependent damping of the skyrmion motion. From the frequency dependence of the damping kernel, we are able to identify the skyrmion mass, thus providing a microscopic description of the kinematic properties of skyrmions. When defects are present or a magnetic trap is applied, the skyrmion mass acquires a finite value proportional to the effective spin, even at vanishingly small temperature. We demonstrate that a skyrmion in a confined geometry provided by a magnetic trap behaves as a massive particle owing to its quasi-one dimensional confinement. An additional quantum mass term is predicted, independent of the effective spin, with an explicit temperature dependence which remains finite even at zero temperature.

TT 67.4 Wed 15:45 EB 301

Optimizing the size of long-lived magnetic skyrmions — Anastasiya Varentsova[1], Stephan v. Malottki[2], Stefan Heinze[2], and •Pavel F. Bessarab[1,3] — [1]ITMO University, St. Petersburg, Russia — [2]University of Kiel, Kiel, Germany — [3]University of Iceland, Reykjavik, Iceland

Available experimental data on magnetic skyrmions in various materials demonstrate inverse correlation between the skyrmion size and skyrmion stability: small skyrmions tend to be less stable compared to large ones [1,2]. The question arises how fundamental this trend is and whether it is possible to obtain long-lived magnetic skyrmions at ambient conditions while keeping their size at the nanoscale.

Here, we demonstrate by means of transition state theory [3] and minimum energy path calculations [4] that the skyrmion lifetime at a given temperature is not a unique function of the skyrmion size and that it is possible to systematically tune material parameters so as to minimize the size of skyrmions while keeping their stability at a desired level. Based on this analysis we identify the most promising materials for the use as storage media based on magnetic skyrmions.

[1] W. Jiang *et al.*, Science **349**, 283 (2015).
[2] N. Romming *et al.*, Science **341**, 636 (2013).
[3] P.F. Bessarab *et al.*, Phys. Rev. B **85**, 184409 (2012).
[4] P.F. Bessarab *et al.*, Comput. Phys. Commun. **196**, 335 (2015).

TT 67.5 Wed 16:00 EB 301

Critical Phenomena in Confined Skyrmion Systems — •Jonathon Waters[1], Timothy Sluckin[1], Denis Kramer[1], Hans Fangohr[2], and Ondrej Hovorka[1] — [1]University of Southampton,

Southampton, UK — [2]European XFEL, Germany

There have been extensive studies which establish the magnetic phases and quantify the thermal phase transition behaviour in bulk helimagnetic materials. However, many proposed device applications, which will utilise the skyrmion phase of these materials, are expected to assume operation in confined geometries and, therefore, it is critical to access the role of the confinement and finite size effects on the stability of skyrmion phases. So far, there have been few studies aimed at understanding the finite system size effects on the thermal phase transition behaviour in these systems. This presentation will discuss our recent developments of systematic analysis of these fundamental effects.

We present large-scale Monte-Carlo simulations of cubic nanoparticles, modelled by a general Heisenberg model with Dzyaloshinskii-Moriya interaction (DMI), and establish phase diagrams for different combinations of exchange and DMI strengths. We apply several different annealing protocols when generating the phase diagram in order to establish the role of metastability and hysteresis in the phase behaviour of these systems. Finally we discuss the results of a finite system size scaling analysis and establish the dependence of critical phase transition temperature on the particle size.

TT 67.6 Wed 16:15 EB 301

Magnetic skyrmion dynamics in thin cylindrical nanodots — •Konstantin Guslienko[1,2] and Zukhra Gareeva[3] — [1]Depto. Física de Materiales, Universidad del País Vasco, UPV/EHU, 20018 San Sebastián, Spain — [2]IKERBASQUE, the Basque Foundation for Science, 48013 Bilbao, Spain — [3]Institute of Molecule and Crystal Physics, Russian Academy of Sciences, 450075 Ufa, Russia

Magnetic skyrmions, robust particle-like nanosize objects, attracted considerable attention due to promising applications in spintronics and information technologies. Being a kind of magnetic topological solitons in 2D spin systems, skyrmions exhibit a wide variety of unusual properties related to their topology. In this talk we focus on the low and high frequency dynamics of magnetic skyrmions in the systems of restricted geometry: isolated cylindrical nanodots. We consider Bloch- and Neel skyrmions as the ground magnetic state of thin circular nanodots stabilized due to an interplay of the isotropic and Dzyaloshinskii-Moriya exchange interactions, perpendicular magnetic anisotropy and magnetostatic interaction. We calculate spectrum of spin excitations over the skyrmion background and classify the eigenmodes according to their spatial symmetry. We show that only one gyrotropic mode (rotation of the skyrmion center position with the frequency about of 1 GHz) exists for the skyrmion of definite polarity and the other low frequency modes that are observed in the skyrmion excitation spectra correspond to spin waves. We found an asymmetry between azimuthal spin waves propagating in the clockwise and counter-clockwise directions that is closely related to the skyrmion topology.

TT 67.7 Wed 16:30 EB 301

Internal structure and stability of skyrmions in ferromagnet/heavy-metal multilayers — •Ksenia Chichay[1], Joseph Barker[2], and Oleg Tretiakov[2,3] — [1]Center for Functionalized Magnetic Materials (FunMagMa), Immanuel Kant Baltic Federal University, Kaliningrad, Russia — [2]Institute for Materials Research, Tohoku University, Sendai, Japan — [3]School of Natural Sciences, Far Eastern Federal University, Vladivostok, Russia

Magnetic Skyrmions are one of the fascinating and promising objects because of their small size and stability to perturbations such as electric currents and magnetic fields. The major mechanism to stabilize small skyrmions in ferromagnet/heavy-metal bilayers is the presence of Dzyaloshinskii-Moriya interaction (DMI).

In this work we investigate the stability and internal structure of an isolated skyrmion in bilayer (ferromagnet/heavy metal) and trilayer (heavy metal 1/ferromagnet/heavy metal 2) nanodisks. We study the static properties of the skyrmions and obtain the phase diagrams of the skyrmion existence depending on the thickness of the ferromagnetic layer and the DMI strength. We demonstrate the importance of fully taking into account the dipolar interaction even for a few atomic layers thin nanodisk and that together with DMI it has the stabilizing effect and defines the Skyrmion configuration. For the trilayer structures with two heavy-metal interfaces, we show that the type and configuration of the skyrmion can be controlled by the thickness of ferromagnet. Furthermore, the interplay of two interfacial DMIs can lead to the formation of magnetic structures with higher winding number.

TT 67.8 Wed 16:45 EB 301

Skyrmion dynamics under the influence of defects from DFT to ASD — •Jonathan Chico, Imara Lima Fernandes, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Any potential skyrmionic application must be able to handle the impact of defects on the movement of skyrmions. Until now, most approaches focussed on large skyrmions and thus phenomenological schemes in the micromagnetic regime. In this work we discuss the technologically much more promising small skyrmions.

Using a combination of first-principles calculations and atomistic spin dynamics, the motion of small skyrmions in Pd/Fe/Ir(111) with $3d$ and $4d$ atomic defects is studied. In general, two types of defects are found, attractive and repulsive [1]. It can be observed that depending on the chemical nature of the defect the current threshold needed to overcome the energy barriers, resulting from the impurities, varies. The obtained dynamical behaviour is richer than what is expected from the Thiele equation. The complexity of the different motion regimes are revealed and compared with what is known for larger skyrmions. The present study also shines light on how one can engineer defects-based pathways for controlled skyrmion motion.

[1] I. L. Fernandes *et al.* submitted (2017).

Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

TT 67.9 Wed 17:00 EB 301

First-principles study of skyrmion formation at $3d/4d$ transition-metal interfaces — •Soumyajyoti Haldar[1], Stephan von Malottki[1], Pavel F. Bessarab[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel, 24098, Kiel, Germany — [2]School of Engineering and Natural Sciences, University of Iceland, 107, Reykjavik, Iceland

Typically, it is assumed that for the formation of skyrmions with a diameter of a few nanometers a $3d/5d$ transition metal (TM) interface is required due to the large spin-orbit coupling of heavy TMs which leads to large Dzyaloshinskii-Moriya interaction (DMI). Here, we use density functional theory (DFT) as implemented in the FLEUR code [1] to demonstrate that ultrasmall skyrmions can also emerge at $3d/4d$ TM interfaces. We have calculated the magnetic interactions in atomic bilayers of Pd/Fe on the Rh(111) surface – a system which is similar to Pd/Fe/Ir(111) [2, 3] since Rh and Ir are isoelectronic $4d$- and $5d$-TMs. From our DFT calculations we parametrize an atomistic spin model including exchange interactions, DMI and the magnetocrystalline anisotropy energy (MAE). We find that both DMI and MAE are reduced with respect to Pd/Fe/Ir(111) which still allows a spin spiral phase at zero magnetic field due to DMI. Using spin dynamics simulations we find that a skyrmion phase occurs for both fcc and hcp stacking of the Pd layer at small magnetic fields of ~ 1 T. Depending on the stacking the skyrmion diameters amount to 4 to 6 nm.

[1] http://www.flapw.de [2] N. Romming *et al.*, Science **341**, 6146 (2013) [3] B. Dupé *et al.*, Nature Comm. **5**, 4030 (2014).

TT 67.10 Wed 17:15 EB 301

Frustration of the Dzyaloshinskii-Moriya interaction in ultrathin Co films — •Sebastian Meyer[1], Stephan Von Malottki[1], Bertrand Dupé[2], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universität zu Kiel, Leibnizstrasse 15, 24098 Kiel — [2]Institute of Physics, Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz

Non-collinear spin structures such as chiral domain walls and skyrmions are being intensively studied since they are promising for spintronic applications [1, 2]. The Dzyaloshinskii-Moriya interaction (DMI) is crucial for stabilizing these non-trivial magnetic states favoring a unique rotational sense. Here, we show frustration of the DMI in ultrathin Co films using density functional theory (DFT) as implemented in the FLEUR code [3]. We study Co monolayers and Pt/Co bilayers on the Ir(111) surface and calculate the energy dispersion of homogeneous flat spin spirals including spin-orbit coupling. Clockwise rotating spin spirals are preferred for large periods close to the ferromagnetic state while below a certain spin spiral period an anticlockwise sense is obtained. This effect arises due to competing DMI interactions with different neighbors that are of opposite sign. With our results from DFT, we parametrize an atomistic spin model and simulate domain wall properties using spin-dynamics simulations.

[1] S. S. P. Parkin *et al.*, Science **320**, 190 (2008)
[2] A. Fert *et al.*, Nature Nano. **8**, 152 (2013)

[3] www.flapw.de

TT 67.11 Wed 17:30 EB 301

Isolated skyrmions with vanishing anisotropy in Co/Ru(0001) — •Marie Böttcher[1,2], Marie Hervé[3], Jairo Sinova[1,4], Wulf Wulfhekel[3], and Bertrand Dupé[1] — [1]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Mainz, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]Academy of Sciences of the Czech Republic, Praha, Czech Republic

Magnetic skyrmions are localized and topologically stabilized non-collinear spin structures. They offer attractive perspectives for future spintronics applications, because they can be manipulated at lower current densities than domain walls [1]. The stabilization of skyrmions is usually attributed to a large Dzyaloshinskii-Moriya interaction (DMI). Here, we show that a strong DMI is not a necessary condition to obtain skyrmions in ultra-thin films. Co/Ru(0001) possesses a spin spiral ground state, although the DMI is weak. We attribute the stability of this spin texture to the simultaneous vanishing of anisotropy [2]. We determine the B-T phase diagram for this system using Monte Carlo simulations and show the magnetic field dependence of isolated skyrmions at magnetic fields with a ferromagnetic ground state. [1] A. Fert, *et al.* Nature Nano. **8**, 152 (2013). [2] M. Hervé *et al.* arXiv:1707.08519 (2017)

TT 67.12 Wed 17:45 EB 301

Magnetic skyrmions in curvilinear films — •Volodymyr Kravchuk[1,2], Denis Sheka[3], Attila Kakay[4], Oleksii Volkov[4], Ulrich Roessler[1], Jeroen van den Brink[1], Denys Makarov[4], and Yuri Gaididei[2] — [1]Leibniz-Institut fuer Festkoerper- und Werkstoffforschung, D-01171 Dresden, Germany — [2]Bogolyubov Institute for Theoretical Physics of National Academy of Sciences of Ukraine, 03680 Kyiv, Ukraine — [3]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Topological magnetic solitons on curvilinear magnetic films acquire new properties if the curvature radius is comparable with the size of the soliton. Earlier we demonstrated [1] that ferromagnetic skyrmions can be stabilized due to the curvature effects only without intrinsic chiral magnetic interactions. However, the curvature induced skyrmion is an excitation of the ground state, as well as a skyrmion in a planar film. Here we show that the combined action of the curvature and the chiral interaction can make skyrmion the ground state of the system [2]. Moreover, ferromagnetic skyrmion pinned on a curvilinear defect demonstrates a discrete set of equilibrium states. Transitions between different states can be controlled by external magnetic field. Thus, the periodically arranged curvilinear defects can result in a reconfigurable skyrmion lattice. This opens new perspectives on processing and storing of the information.

[1] V. Kravchuk et al., BRB 94, 144402 (2016). [2] V. Kravchuk et al., arXiv 1706.05653 (2017).

TT 67.13 Wed 18:00 EB 301

Skyrmion-Lattice Collapse and Defect-Induced Melting in Chiral Magnetic Films — •Leonardo Pierobon[1], Christoforos Moutafis[2], Michalis Charilaou[1], and Jörg Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, Switzerland — [2]School of Computer Science, University of Manchester, Manchester, UK

Complex spin textures arise in nanostructured magnets due to competing interactions, primarily the Heisenberg exchange and the Dzyaloshinskii-Moriya interaction (DMI), which promote spin collinearity and canting, respectively. Upon rotational-symmetry breaking, particle-like objects with non-trivial spin configurations, i.e., skyrmions, can be created. The winding of skyrmions bestows a topological protection on the system, and the transition to the topologically trivial ferromagnetic state requires a phase transition. Here, we systematically compare isotropic and anisotropic DMI systems by means of high-resolution numerical simulations. We show that in perfect systems skyrmion lattices can be inverted in a field-induced first-order phase transition, whereas the existence of even a single defect replaces the inversion with a second-order phase transition following a defect-induced lattice melting process. This radical qualitative change signifies the importance of employing such an analysis for all realistic systems in order to correctly interpret experimental data. Our results shed light on fundamental processes behind magnetic phase transitions, and pave the way for their experimental realization in technologically relevant multilayer materials.

TT 67.14 Wed 18:15 EB 301

Reservoir Computing with Random Skyrmion Fabrics — •Daniele Pinna[1], George Bourianoff[2], and Karin Everschor-Sitte[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [2]Intel Labs, Intel Corp, Austin, TX

Thanks to their many nanoscale properties, skyrmions are promising in applications ranging from non-volatile memory[1] and spintronic logic devices[2], to enabling the implementation of unconventional computational standards[3, 4]. In this talk we will discuss how a random skyrmion "fabric" composed of skyrmion clusters embedded in a magnetic substrate can be effectively employed to implement a functional reservoir computer. This is achieved by leveraging the nonlinear resistive response of the individual skyrmions arising from their current dependent AMR[5]. Complex time-varying current signals injected via contacts into the magnetic substrate are shown to be modulated nonlinearly by the fabric's AMR due to the current distribution following paths of least resistance as it traverses the geometry. By tracking resistances across multiple input and output contacts, we show how the instantaneous current distribution, reminiscent of Atomic Switch Networks, effectively carries temporally correlated information about the injected signal. This in turn allows us to numerically demonstrate simple pattern recognition.

[1] A. Fert, et al., Nature Nanotech. 8, 152-156 (2013). [2] X. Zhang, et al., Sci. Rep. 5, 9400 (2015). [3] D. Pinna, et al., arXiv:1701.07750 (2017). [4] G. Bourianoff, et al., arXiv:1709.08911 (2017). [5] D. Prychynenko, et al., arXiv:1702.04298 (2017).

TT 68: Topological Insulators and Weyl Semimetals (joint session MA/TT)

Time: Wednesday 15:00–18:15 Location: EB 407

TT 68.1 Wed 15:00 EB 407

Topological Phase Transitions from Relativistic Many-Body Calculations — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

We discuss topological phase transitions (TPTs) on the basis of relativistic *GW* and quasiparticle self-consistent *GW* (QS*GW*) calculations where the spin-orbit coupling is incorporated directly into the self-energy. TPTs can be caused by the variation of the thickness of a sample, the spin-orbit strength, alloying, strain, etc. The well known underestimation of band gaps in standard DFT translates into an overestimation of the inverted band gaps that are responsible for the topological character of materials. This results in standard DFT being unable to provide correctly the critical points of TPTs. As practical examples, we concentrate on semimetals Bi and Sb. In addition to the TPT that bismuth undergoes under strain [1], we discuss that a thickness-mediated TPT can also occur. This sheds light on the discrepancies about the topological or trivial character of bulk-like samples of Bi. Finally, we simulate $Bi_{1-x}Sb_x$ alloys varying the Sb concentration in order to find the critical concentration for which the system becomes a topological insulator.

[1] I. Aguilera *et al.*, Phys. Rev. B **91**, 125129 (2015).

Financial support from the Virtual Institute for Topological Insulators of the Helmholtz Association.

TT 68.2 Wed 15:15 EB 407

High throughput screening of two dimensional topoloigical insulators — •Xinru Li[1], Zeying Zhang[1,2], and Hongbin Zhang[1] — [1]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany — [2]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Tech-

nology, Beijing 100081, China

Topological insulators (TIs), with insulating band gaps and nontrivial edge states, have been widely investigated not only for its fundamental importance but also owing to its potential technological applications. The two-dimensional (2D) TIs are particularly interesting, as they can get easily implemented into devices. There have been many 2D TIs predicted theoretically or synthesized experimentally. However previous efforts have relied mostly on time-consuming trial-and-error procedures. Here, starting from a 2D materials database with 826 slab systems predicted to be stable, we performed high-throughput screening over all materials at the first principles level. For nonmagnetic 2D materials with small (< 0.1 eV)band gaps, maximally localized Wannier functions are constructed in an automated way in order to characterize the topological character by examining the surface states. Combined with explicit evaluation of the topological invariants, we have successfully identified one novel 2D TI, whose topological properties will be discussed in detail.

TT 68.3 Wed 15:30 EB 407

Classification of topological antiferromagnets for spintronics — •Libor Šmejkal[1,2], Jairo Sinova[1,2], and Tomáš Jungwirth[2] — [1]INSPIRE group, Uni Mainz, Germany — [2]Institute of Physics, Czech Academy of Sciences, Prague, Czech Rep.

Our recent prediction of the interplay between topological Dirac quasiparticles and spin orbit torques in antiferromagnets has opened new possibilities of studying topological spintronics [1]. In this talk we will classify topological antiferromagnets based on minimal models, present new material candidates and novel magneto-transport effects, e.g. tunable topological anisotropic magnetoresistance or quantum anomalous Hall effect. The presence of topological quasiparticles can lead to a large signal/noise ratios and novel functionalities in read-out signals in spintronics devices [2]. For example, based on ab initio theory, we have predicted a large anisotropic magnetoresistance reaching 6% in Mn2Au antiferromagnet which was recently observed in current induced torques experiments [3]. We will also demonstrate that antiferromagnets are natural candidates for combining magnetic order with topological Dirac quasiparticles owing to their unique effective time-reversal symmetries, which are not present in ferromagnets [1,2].

[1] L. Šmejkal, J. Železný, J. Sinova, and T. Jungwirth, Phys. Rev. Lett. 118 , 106402 (2017) [2] L. Šmejkal, Y. Mokrousov, B. Yan, and A. H. MacDonald, arXiv:1706.00670 [3] S. Yu. Bodnar, L. Šmejkal, M. Jourdan, et al. arXiv:1706.02482

TT 68.4 Wed 15:45 EB 407

Edelstein effect in Weyl semimetals — •Annika Johansson[1,2], Jürgen Henk[2], and Ingrid Mertig[2,1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

Using semiclassical Boltzmann transport theory, we predict a current-induced spin polarization in Weyl semimetals, similar to the Edelstein effect of surface states in Rashba systems or in topological insulators [1]. The theory is applied to the Weyl semimetal TaAs simulated by an effective two-band model [2,3], for which we estimate the magnitude of the effect. The main contribution comes from the topological surface states, i. e. the Fermi arcs, which provide an enormous current-induced spin polarization.

[1] V. M. Edelstein, Solid State Commun., **73**, 233 (1990) [2] S. Murakami and S.-i. Kuga, Phys. Rev. B **78**, 165313 (2008) [3] R. Okugawa and S. Murakami, Phys. Rev. B **89**, 235315 (2014)

TT 68.5 Wed 16:00 EB 407

Ferro- and ferrimagnetic coupling in Cr/Bi_2Se_3(0001) — •Andrey Polyakov[1], Katayoon Mohseni[1], E. Daryl Crozier[2], Manuel Valvidares[3], Victor N. Antonov[1], Lev V. Bekenov[1], Arthur Ernst[4], Holger L. Meyerheim[1], and Evgueni V. Chulkov[5] — [1]MPI für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Department of Physics, SFU Burnaby, BC Canada, V5A 1S6 — [3]Alba Synchrotron, 08290 Cerdanyola del Valles Barcelona, Spain — [4]Institut für Theoretische Physik, Johannes Kepler Universität, A 4040 Linz, Austria — [5]DIPC, 20018 San Sebastian/Donostia, Basque Country, Spain

Using surface x-ray diffraction, x-ray absorption fine structure and x-ray magnetic circular dichroism experiments in combination with ab-initio calculations we have studied the atomic and magnetic structure of ultra-thin Cr films deposited in the 0.2 to 2.5 monolayer thickness regime on Bi_2Se_3(0001). We find a complex pattern of different adsorption sites (substitutional, van-der Waals gap, and surface double layer formation) involving ferro- and ferri-magnetic exchange. Magnetic moments are close to $4\mu_B$ related to Cr^{2+}. Our study sheds new light on the understanding of magnetic doped topological insulators. Acknowledgements: Supported by SPP 1666. Work at the APS is supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

TT 68.6 Wed 16:15 EB 407

Circular-polarized-light induced spin characterization of Dirac-cone surface state at W(110) — •Koji Miyamoto[1], Henry Wortelen[2], Taichi Okuda[1], Jürgen Henk[3], and Markus Donath[2] — [1]HSRC, Japan — [2]WWU Münster, Germany — [3]MLU, Germany

Recently, for the topological surface state (TSS) of Bi_2Se_3, several groups have observed an interesting phenomenon by spin- and angle-resolved photoemission (SARPE): the observed spin features of the photoelectrons are strongly dependent on the light polarization [1]. This effect is currently highly debated in the field of optospintronics. So far, the observations of the effect are limited to surfaces with C_{3v} symmetry.

The surface of W(110) shows a spin-polarized Dirac-cone-like state within a spin-orbit-induced gap, which is reminiscent of a TSS [2]. Here, in contrast to so-far studied topological insulators, the surface structure has C_{2v} symmetry.

We studied spin feature of the Dirac-cone-like surface state along $\overline{\Gamma H}$ at W(110) by using SARPE with left and right circular polarized light. It is found that the observed spin textures is caused by spin dependent matrix element influenced by C_{2v} symmetry. This finding opens a new way to manipulate the spin polarization of photoelectron in systems with C_{2v} symmetry.

*[1] C. Jozwiak *et al.*, Nat., Phys. **9**, 293 (2013).
*[2] K. Miyamoto *et al.*, Phys. Rev. Lett. **108**, 066808 (2012).

TT 68.7 Wed 16:30 EB 407

Magnetization-direction tunable nodal-line and Weyl phases — •Zeying Zhang[1,2], Qiang Gao[2], ChengCheng Liu[1], Yugui Yao[1], and Hongbin Zhang[2] — [1]Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics, Beijing Institute of Technology, Beijing 100081, China — [2]Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

Emergent phenomena in materials with nontrivial topological nature have attracted intensive attention recently, as observed in both 2D and 3D topological insulators. From the symmetry point of view, nodal-line and Weyl semimetals are of particular interest, and they host intriguing properties such as negative magneto-resistance. In this work, we investigate a symmetry based three-band tight-binding model, after consider spin-orbit coupling (SOC) and different magnetization-directions, it is confirmed that the number of Weyl points and nodal line can be tuned by the magnetization direction. It is observed that the mirror symmetry plays a crucial role in protecting the degeneracy of nodal-lines. We propose a new class of materials C_4CrX_3 (X=Ge and Si) which host such a nontrivial semi-metallic phase. The systems have neither spatial inversion nor time reversal symmetries, but surprisingly it is observed that both Weyl points and nodal-lines exist in the ferromagnetic ground state. The degeneracy of nodal-lines can be controlled by the magnetization direction after considering SOC, confirmed by first-principles calculations.

15 min. break.

TT 68.8 Wed 17:00 EB 407

Topological jumps in a finite-size Dzyaloshinskii-Moriya antiferromagnetic chain — •Jaroslav Chovan[1,2] and Dominik Legut[1] — [1]IT4Innovations National Supercomputing Center VSB - Technical University Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]Department of Physics, Matej Bel University, Banska Bystrica, Slovakia

Recently, experiments with thin films of chiral ferromagnets MnSi and $CrNbS_6$ observed sudden jumps in magnetoresistence and/or magnetization induced by a magnetic field applied perpendicularly to the chiral axis. Subsequent theory traced the origin of these jumps to a field-induced transitions between topological sectors with different number of magnetic solitons and established the importance of boundary conditions. Here, we explore the topic in the context of a two-sublattice antiferromagnet. We thus carry out a detailed calculation of magnetic properties of a finite Heisenberg antiferromagnetic chain with

Dzyaloshinskii-Moriya interactions in the presence of external magnetic field. By comparing the energies of magnetic solitons from different topological sectors, we calculate the ground state dependence on the chain size N and the field H. We construct a phase diagram and analyze the topological jumps between the individual sectors in detail and discuss ambiguity in counting the number of magnetic solitons for even-number spin chain. Our results may guide future experiments.

This work was supported by Czech Science Foundation grant No. 17-27790S, project No. CZ.02.1.01/0.0/0.0/16_013/0001791, and Slovak Grant VEGA No. 1/0269/17.

TT 68.9 Wed 17:15 EB 407

Impact of in-gap states on the magnetic stability/excitations of dopants in topological insulators — •Juba Bouaziz, Julen Ibanez-Azpiroz, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Doping topological insulators with magnetic impurities breaks time reversal symmetry, leading to the prediction of a gap opening at the Dirac point when the magnetic moments are along the *c*-axis [1]. This could potentially functionalize the topological surface states by enabling control of the quantum anomalous Hall effect and dissipationless transport. Several investigations obtained conflicting results, generating a lot of controversy on this point. Since the orientation of the magnetic moments depends on their magnetic anisotropy energy, we use first-principles calculations to investigate isolated $3d$ and $4d$ transition metal impurities on the surfaces and in the bulk of Bi_2Te_3 and Bi_2Se_3. We explore the impact of impurity-induced in-gap states on the orientation of the magnetic moments, their dynamical spin-excitations and on the zero-point spin-fluctuations affecting the magnetic stability [2]. We propose to use scanning tunneling spectroscopy in the inelastic mode or in the electron spin resonance mode to verify our predictions. – Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

[1] Y. L. Chen et *al.*, Science. **329**, 659 (2010).
[2] J. I. Azpiroz et *al.*, Nano Lett. **16**, 4305 (2016).

TT 68.10 Wed 17:30 EB 407

Prediction of a magnetic Weyl semimetal with strong anomalous Hall and Nernst effect in the Heusler compensated ferrimagnet Ti_2MnAl — •Jonathan Noky[1], Wujun Shi[1,2], Lukas Müchler[3], Kaustuv Manna[1], Yang Zhang[1,4], Klaus Köpernik[4], Roberto Car[3], Jeroen van den Brink[4], Claudia Felser[1], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China — [3]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA — [4]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

We predict the inverse Heusler compound Ti_2MnAl, which is a compensated ferrimagnet with a Curie temperature of over 650 K, to be a magnetic Weyl semimetal. Despite the vanishing net magnetic moment, we calculate a large intrinsic anomalous Hall (AHE) and anomalous Nernst (ANE) effect. These effects stem directly from the Berry curvature distribution of the Weyl points, which are only 14 meV away from the Fermi level and isolated from trivial bands. Since spin-rotation symmetry is broken by the magnetic structure, the Weyl points are stable also without spin-orbit coupling. Additionally, because Weyl points of opposite topological charge show a large spatial separation, this system exhibits huge Fermi arcs.

Ti_2MnAl and, to a lesser extend, also Ti_2MnGa and Ti_2MnIn are first examples of systems with Weyl points, large AHE, and large ANE in spite of a vanishing net magnetic moment.

TT 68.11 Wed 17:45 EB 407

Magnetic Weyl Semimetal in Quasi Two-dimensional Half Metallic $Co_3Sn_2S_2$ and $Co_3Sn_2Se_2$ — •Qiunan Xu[1], Enke Liu[1], Lukas Muechler[2], Claudia Felser[1], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden 01187 , Germany — [2]Department of Chemistry, Princeton University, Princeton, New Jersey 08544, USA

A Weyl semimetal can exist in a time reversal or inversion symmetry breaking system. Since the Berry curvature is odd under time reversal, the Berry curvature from Weyl points are expected to generate a large anomalous Hall effect in time reversal symmetry breaking Weyl semimetals. Since the Weyl points are far away from Fermi energy for most of the candidate magnetic Weyl semimetals, Weyl points related physics was observed in them so far. In this work, we find a Weyl semimetal phase in half metallic ferromagnet $Co_3Sn_2S_2$ with Weyl points only 60 meV away from the Fermi level, which derive from nodal lines that are gapped by spin-orbit coupling. Therefore, the Weyl-related physics should be easy to detected by both surface ARPES and bulk transport measurements. Due to the Berry curvature deriving from the gapped nodal lines and Weyl points, its anomalous Hall conductivity can reach up to 1200 S/cm. Substituting S by Se, $Co_3Sn_2Se_2$ shows very similar property. Moreover, since $Co_3Sn_2S_2$ and $Co_3Sn_2Se_2$ are both easily grown quasi two-dimensional compounds, they provide an ideal platform for the study of magnetic Weyl physics and its future application in topological material based spintronic devices.

TT 68.12 Wed 18:00 EB 407

Core-Shell Nanowires of 3D Topological Insulators — •Kevin Geishendorf, Tommi Tynell, Kornelius Nielsch, and Andy Thomas — Institute for Metallic Materials, IFW Dresden

Topological insulators (TI) are promising candidates for next generation electronic/spintronic devices. The gapless surface states (SS) in TI exhibit a very high mobility and strongly suppressed backscattering due to spin-momentum locking. However, to exploit those advantageous one has to decrease the finit bulk conductance present in most TI systems.

One approach to achieve this reduction is to utilize band bending which occurs at the interface between two materials with different Fermi levels. The band bending leads to a charge depletion/ or accumulation near the interface. It therefore provides a tool to shift the fermi energy closer to the Dirac point.

In this work we have grown core-shell nanowires using Vapor-Liquid-Solid (VLS) growth and Atomic Layer Deposition (ALD). As core material Bi_2Se_3 and as shell materials Al_2O_3 and Sb_2Te_3 were employed. The uniformity, crystallinity and composition of those core-shell nanowire was investigated using TEM, nanodiffraction and EDX. Furthermore, devices for transport experiments were built using optical lithography and lift-off techniques. With those devices cryogenic magneto transport measurements have been performed revealing quantum interference effects such as weak-antilocalization and universal conductance fluctuations.

TT 69: Multiferroic Oxide Thin Films and Heterostructures II (joint session KFM/TT/MA)

Organizers: César Magén - University of Zaragoza, Aragón (Spain); Kathrin Dörr - Martin-Luther-Universität Halle-Wittenberg - Halle

Time: Wednesday 15:00–18:15 Location: EMH 225

Invited Talk TT 69.1 Wed 15:00 EMH 225

Merging Nonlinear Optics and Multiferroic Heterostructure Design — •Manfred Fiebig — Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland

Despite the large variety of valuable tools that are at our disposals for characterizing oxide thin films, some of their functionalities remain invisible. Buried layers and their ordering and interactions are difficult to access. We show how optical second harmonic generation (SHG) allows us to detect such hidden properties. We show how the real-time dynamics of a domain patterns in multiferroic $BiFeO_3$ is tracked by SHG through a ferromagnetic metallic cover layer, thus identify the magnetoelectric domain coupling nondestructively during the poling process [1]. SHG furthermore resolves the domain-wall architecture in tetragonal ferroelectric thin films. In $PbZr_{0.2}Ti_{0.8}O_3$ films it quantifies the buried distribution of a- and c-domains and reveals that c-domain walls exhibit a mixed Ising-Néel-type transverse rotation of polarization across the wall [2]. Finally, by coupling a laser beam into the deposition chamber, SHG follows the evolution of the spontaneous polarization of complex multiferroic heterostructure in real time and with monolayer sensitivity throughout the entire deposition process. Such in-situ SHG allows us tailor heterostructures with an arbitrary sequence of ordered states which could become the key to whole new class of functional ferroelectric materials [3].

[1] M. Trassin *et al.*, Adv. Mater. **27**, 4871 (2015). **[2]** G. De Luca*et al.*, M. Trassin, Adv. Mater. **29**, 1605145 (2017). **[3]** G. De Luca*et al.*, Nature Comm. **8**, 1419 (2017)

TT 69.2 Wed 15:30 EMH 225

Real-time observation of polarization emergence in ultrathin ferroelectric heterostructures — •Gabriele De Luca[1], Nives Bonacic[1], Johanna Nordlander[1], Corinne Bouillet[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, 8093, Zurich, Switzerland — [2]Institut de Physique et Chimie des Matériaux de Strasbourg CNRS UMR 7504, 67034, Strasbourg, France

The integration of functional properties into oxide multilayer architectures demands for atomic precision. In-situ diagnostic tools guarantee high structural quality but are usually insensitive to the functionality targeted with the actual deposition. The conventional optimization process requires multiple samples and ex-situ analysis. Here, we take advantage of the non-invasive nature of optical probes and monitor the functionality during growth. Taking ferroelectricity as a representative case, we show that optical in-situ second harmonic generation (ISHG) analysis can be performed simultaneous to the pulsed-laser-deposition growth operation. We follow the evolution of the spontaneous polarization in real time and with monolayer resolution throughout the deposition process [1]. Such direct access allows validating the growth of oxide heterostructures with an arbitrary sequence of up- and down-polarized ferroelectric layers. This is only the first step in the implementation of ISHG as a growth diagnostic tool. The in-situ access to emerging properties enables an unprecedented degree of control that can promote the engineering of oxides functionalities to a completely new level.

[1] G. De Luca et al., Nat. Commun. 8, 1419 (2017)

TT 69.3 Wed 15:45 EMH 225

Controlling the effect of the depolarizing field in $BaTiO_3$-$SrTiO_3$ multilayers — •Nives Bonacic[1], Gabriele De Luca[1], Shovon Pal[1], Marco Campanini[2], Marta D. Rossell[2], Morgan Trassin[1], and Manfred Fiebig[1] — [1]ETH Zurich, Department of Materials — [2]EMPA, Switzerland

The demand for ever-smaller devices has been approaching the fundamental limits of ultrathin ferroelectric films. In the low-thickness regime, maintaining a large, stable and switchable ferroelectric polarization relies on the control of the strain state, thickness, interface termination and electrostatic conditions. Achieving a robust polarization or a controlled domain state remains, however, challenging. Imperfect charge screening at interfaces results in non-cancellation of internal fields that can in extreme case annihilate ferroelectricity. Taking ($BaTiO_3$-$SrRuO_3$) capacitor-like heterostructures as a model system, we directly access the polarization and the domain state during the film deposition using optical second harmonic generation [1]. We observe a previously elusive impact of the evolving electrostatic environment on the $BaTiO_3$ domain state simultaneously with the growth. The initial phase of the top-electrode deposition is accompanied by temporary enhancement of built-in fields in the ferroelectric layer resulting in 180° domain formation. We discuss ways to manipulate the depolarizing field and control the polarization during the growth as it presents a possible route towards a novel class of oxide-electronic devices. [1] G. De Luca et al., Nat. Commun. 1419 (2017).

TT 69.4 Wed 16:00 EMH 225

In-situ characterization of improper ferroelectricity in ultrathin multiferroic h-$YMnO_3$ films — •Johanna Nordlander[1], Marta D. Rossell[2], Rolf Erni[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH, Zürich, Switzerland — [2]EMPA, Dübendorf, Switzerland

Improper ferroelectrics are materials whose ferroelectricity is driven by another, primary, order parameter. This type of ferroelectricity can lead to exotic properties that do not exist in standard ferroelectrics. In the case of bulk hexagonal manganites, the structural trimerization results in a topologically protected vortex domain structure. Due to their potential for extending existing technological applications with complex functional properties, there has been a revival of interest in hexagonal manganite thin films. Here we demonstrate the growth of highly oriented, epitaxial hexagonal $YMnO_3$ thin films using pulsed laser deposition. We use in-situ optical second harmonic generation (SHG) to non-invasively probe, in real time during and after the deposition process, the ferroic state of the films in the ultrathin regime. With the complementary use of reflection high-energy electron diffraction (RHEED), the emerging polarization of $YMnO_3$ is resolved with monolayer precision. The characteristic improper ferroelectric domain pattern in the ultrathin $YMnO_3$ films is investigated using scanning transmission electron microscopy. This work provides new insights in the early stage of improper ferroelectricity and domain state in hexagonal $YMnO_3$ thin films - especially the drastic influence of epitaxial strain and reduced dimensions on the ferroelectric Curie temperature.

TT 69.5 Wed 16:15 EMH 225

Multiferroic and magnetoelectric nanocomposites for data processing — •Wolfgang Kleemann — Physics Department, University Duisburg-Esssen, 47048 Duisburg, Germany

Switching of magnetism with electric fields and magnetic control of electric polarization are challenging tasks for multiferroic and magnetoelectric materials. Various composite realizations appear most promising for data processing applications: (1) We propose 2-2 nanocomposites based on magnetoelectric (ME) chromia (111) films (Cr2O3), which allow electric switching of the magnetization of epitaxially grown ultrathin ferromagnetic Co/Pt/Co trilayers via interfacial exchange bias. Random access memory (MERAM) and logic cell MEXOR have been approved [1]. (2) Regular 2-1 composites of magnetostrictive cobalt ferrite (CoFe2O4) nanopillars are PLD-grown in a piezoelectric film of barium titanate (BaTiO3). In a transverse magnetic field they exert a staggered shear stress-induced surface polarization pattern in the BaTiO3 environment [2]. Possible data storage applications will be discussed. (3) Ceramic 0-3 composites of antiferromagnetic-ferroelectric Bi(Fe,Co)O3 nanoclusters embedded in K0.5Bi0.5TiO3 reveal giant linear magneto-electric response via bilinear piezo-magneto-electric coupling, M = αE with α = 10-5 s/m [3]. They are candidates for future electrically addressable nanodot mass memory devices. [1] US Pat. 7,719,883 B2 (2010). [2] Nature Comm. 4, 2051 (2013). [3] Adv. Funct. Mater. 26, 2111 (2016).

15 min. break

TT 69.6 Wed 17:00 EMH 225

Local observables in inhomogenous systems — •Raffaele Resta[1] and Antimo Marrazzo[2] — [1]IOM-CNR, Trieste, Italy —

[2]THEOS, EPF Lausanne, Switzerland

When addressing inhomogenous systems (e.g. heterostructures) a key issue is which physical properties do (or do not) admit a local expression. It is known since long time that spin magnetization is indeed local, and that the density of spin magnetization is well defined quantity. It is also known (since the early 1990s) that instead polarization density is an ill defined concept. Bulk electric polarization P is a Berry phase of the electronic wavefunction: as such it does not admit any local representation. In analogy with P, orbital magnetization is a geometrical property of the electronic ground state; but at variance with P, it also admits a local representation with a well defined density in coordinate space [1,2]. Here we address one further property: the insulating/metallic character of a region in an inhomogeneous system. A well known tool to investigate this property is the local density of states, but it is not a ground-state property. According to Kohn (1964) the insulating/metallic character of a material stems from a different organization of the electrons in their ground state. We define a local "marker" which probes such organization, and we validate it by means of computer simulations.

[1] R. Bianco and R. Resta, Phys. Rev. Lett. 110, 087202 (2013)
[2] A. Marrazzo and R. Resta, Phys. Rev. Lett. 116, 137201 (2016)

TT 69.7 Wed 17:15 EMH 225

Magnetoelectric coupling and multicaloric effects in $SrMnO_3$ — Alexander Edström and •Claude Ederer — Materials Theory, ETH Zürich, Switzerland

$SrMnO_3$ is a G-type antiferromagnet where ferroelectricity can be induced by epitaxial strain or Ba-substitution. Furthermore, a transition to ferromagnetic order has been predicted under large tensile strain [1], and the two ordering temperatures can in principle be tuned to coincide by varying both strain and composition. $SrMnO_3$ is thus a very rare example of a multiferroic with proper ferroelectric and magnetic order and similar ordering temperatures.

We use first principles electronic structure calculations in combination with first-principles-derived effective model Hamiltonians to obtain the temperature and strain-dependent ferroelectric/magnetic phase diagram of $SrMnO_3$. We then explore coupling effects between the polar and magnetic order. A particular focus thereby are possible multi-caloric effects, i.e., adiabatic temperature changes induced by applied electric and/or magnetic fields, that are very promising for future solid state cooling devices [2].

[1] J. H. Lee and K. M. Rabe, Phys. Rev. Lett. 104, 207204 (2010).
[2] X. Moya, S. Kar-Narayan, and N. D. Mathur, Nature Mater. 13, 439 (2014).

TT 69.8 Wed 17:30 EMH 225

Octahedral tilting, phonons and Goldstone modes in 111-strained perovskites — Magnus Moreau[1], Astrid Marthinsen[1], Sinead Majella Griffin[2], Tor Grande[1], Thomas Tybell[1], and •Sverre Magnus Selbach[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, California, USA

Epitaxial strain has been extensively explored to enhance existing and enable new functional properties in perovskites oxide thin films, with the majority of the work done on 001-oriented films. Recent advances in film growth has made other epitaxial orientations possible, and particularly 111-oriented films show interesting properties because of the different symmetry and chemical bonding at the terminating (111) facet. We use density functional theory (DFT) calculations to study the different response to 111- and 001-strain of the octahedral tilt system and the crystal field splitting of perovskite oxides. Unlike 001-strain, 111-strain is parallel to the edges of the oxygen octahedra, and tensile 111-strain can emulate negative hydrostatic pressure, which is not easily realised experimentally for bulk materials. General trends for how 111-strain affects polar and rotational modes are outlined based on calculations of twenty common perovskites. Furthermore, we show that in SrMnO3 compressive 111-strain give rise to Goldstone-like phonon modes with a Mexican hat-shaped energy surface, while large tensile strain can induce polar Goldstone modes. The chemical and structural requirements for engineering structural Goldstone modes in 111-strained perovskites are finally discussed.

TT 69.9 Wed 17:45 EMH 225

Voltage controlled magnetization dynamics in nanostructured multiferroic multilayer systems — •Alexander F. Schäffer and Jamal Berakdar — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle (Saale), Germany

We investigate the control of magnetization dynamics by applying localized voltages in the framework of nanostructured multiferroic heterostructures. Manipulations of the magnetic anisotropy are spatially controlled by nanostructuring. This combination is utilized as a toolbox to excite or manipulate magnetic systems in order to manipulate multiple magnetic phenomena, such as the magnon dispersion, local spin current sources, or local non-collinear magnetic textures. Full-fledged numerical calculations for realistic systems along with basic analytical models will be shown in order to point towards opportunities for further experimental investigations and applications.

TT 69.10 Wed 18:00 EMH 225

Electronic and magnetic properties of $BaFeO_3$-Pt(111) in a quasicrystalline approximant structure — •Waheed A. Adeagbo, Igor V. Maznichenko, Hichem Ben-Hamed, Ingrid Mertig, and Wolfram Hergert — Institute of Physics, Martin Luther University Halle-Wittenberg, Germany

The first reported formation of an oxidic quasicrystal (OQC) $BaTiO_3$ (BTO) on Pt(111) has led to finding of other quasicrystalline (QC) perovskites like $SrTiO_3$ on the same substrate. Since these are non-magnetic, it is interesting to investigate the properties of magnetic perovskites in corresponding approximant structures. $BaFeO_3$ (BFO) has a very good lattice match with Pt(111) and also a robust magnetic properties which could add new interesting features to the QC systems. In this work we have carried out first principles study on the periodic BFO bulk crystals properties in the cubic (c-BFO) and the hexagonal ($6h$-BFO) phases. The derived OQC thin film which exhibits strong similarities to the BTO-derived OQC with respect to the local tiling geometry of Kepler's approximant was also studied both in the free standing and in the supported phase on Pt(111) surface. Our results shows that the anti-ferromagnetic $6h$-BFO bulk phase is preferable ground state to c-BFO phase. Like in BTO-OQC approximant, the BFO also shows all four Fe atoms surrounded by three O atoms with the FeO_3 units separated by Barium atoms with the total stoichiometry $Ba_5Fe_4O_{10}$. Since the exact oxidation states of the Fe and the role of O vacancy in the stabilization is unknown for these systems, the results of these will be presented together with the magnetic contribution.

TT 70: Frontiers of Electronic-Structure Theory: Correlated Electron Materials V (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Wednesday 15:00–17:45 Location: HL 001

Invited Talk TT 70.1 Wed 15:00 HL 001

Computational Approach to the Electronic Structure of Strongly Correlated Materials: Towards Theoretical Spectroscopy and Theory Assisted Material Design — •Gabriel Kotliar — Serin Physics Laboratory Rutgers University — Brookhaven National Laboratories

We will introduce a project, to build algorithms and a suite of open source codes, to compute the electronic structure of correlated materials. It involves different methods, to provide different compromises between speed and accuracy, and to treat different types of correlation (static and dynamic). The suite includes methods ranging from vertex corrected GW, rotationally invariant slave bosons and LDA+DMFT, and we will illustrate some of these methods (and their failures) in d and f electron systems.

TT 70.2 Wed 15:30 HL 001

Spectral properties of Sr2IrO4 from first principles — •Cyril Martins[1], Benjamin Lenz[2], and Silke Biermann[2,3] — [1]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin-orbit system Sr2IrO4 has raised tremendous interest recently, due to intriguing similarities to the high-Tc superconducting copper oxides.

We study the evolution of the electronic structure of Sr2IrO4 using a combination of ab-initio density functional theory and many-body techniques. The effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions are included on a first-principles level. We calculate the momentum-resolved spectral function and compare to recent photoemission data, finding good agreement with experiment.

TT 70.3 Wed 15:45 HL 001

Role of non-local correlations in doped Sr_2IrO_4 — •Benjamin Lenz[1], Cyril Martins[2], and Silke Biermann[1,3] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire de Chimie et Physique Quantiques, UMR 5626, Université Paul Sabatier, 118 route de Narbonne, 31400 Toulouse, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

When doping the spin-orbit system Sr_2IrO_4 recent photoemission experiments found pseudogap behavior at low temperatures, which raises the question of its relation to the pseudogap found in high-Tc superconducting copper oxides.

Here, we study the evolution of the electronic structure of Sr_2IrO_4 upon electron- and hole-doping by combining ab-initio density functional theory and two quantum cluster techniques. Our treatment includes the effects of spin-orbit coupling, distortions of the oxygen octahedra and Hubbard interactions on a first-principles level. We show that short-range antiferromagnetic fluctuations are crucial to account for the electronic properties of the material even in the high-temperature paramagnetic phase. Furthermore, pseudogap features in the momentum-resolved spectral function of the emerging exotic metallic state are analyzed and found to be in good agreement with experiment.

TT 70.4 Wed 16:00 HL 001

Describing the coupled structural and metal-insulator transition in rare-earth nickelates with DFT+DMFT — •Alexander Hampel and Claude Ederer — Materials Theory, ETH Zürich, Switzerland

Perovskite rare-earth nickelates, $R\mathrm{NiO_3}$, display a rich phase diagram, where all compounds with R from Pr to Lu undergo a metal-insulator transition (MIT) that is accompanied by a structural distortion. This distortion breaks the symmetry between formerly equivalent Ni sites and is related to a charge disproportionation driven by correlation effects, resulting in an insulating state. Here, we employ density functional theory together with dynamical mean field theory (DFT+DMFT) to explore the interplay between lattice distortions and electronic correlation effects in these compounds. By utilizing a symmetry-based distortion mode analysis, we are able to isolate the specific lattice distortion occurring at the phase transition. Calculating total energies within DFT+DMFT then allows us to relax the structures with respect to this distortion. We find, that the resulting distortion amplitudes and its variation across the series are in good agreement with experimental results. Our work highlights the capabilities of the DFT+DMFT method to describe complex materials with coupled electronic and structural degrees of freedom.

TT 70.5 Wed 16:15 HL 001

Magnetocrystalline anisotropy of FePt: LDA+DMFT study — •saleem Ayaz Khan[1], Junqing Xu[2], johan Schott[3], Ondřej Šipr[1], and Jan Minár[1] — [1]University of West Bohemia, Pilsen, Czech Republic — [2]LMU Munich, Germany — [3]Uppsala University, Sweden

In our recent work (Phys. Rev B, 94, 144436, 2016) we employed ab initio methods (FLAPW and KKR) to get a reliable value for the magnetocrystalline anisotropy (MCA) energy of FePt. The theoretical MCA energy of FePt (3.0 meV) is significantly larger than the experimental value (1.3 meV), implying that the LDA cannot properly describe the MCA of FePt. Considering that the MCA essentially arises from spin orbit coupling it appears that to obtain reasonable agreement with experiments, it is necessary to include orbital correlations. To account realistically for both the electronic and geometric structure of materials, we use a combined density functional and dynamical mean field theory, LDA+DMFT. Our computation is based on the fluctuation exchange approximation and an analytic continuation method for the self-energy. Our results show that dynamical correlation effects are important for a correct treatment of the 3d-5d hybridization in FePt, which in turn plays a significant role for the magnetocrystalline anisotropy

TT 70.6 Wed 16:30 HL 001

Diagnostics for plasmon satellites and Hubbard bands in transition metal oxides — •Steffen Backes[1], Hong Jiang[2], and Silke Biermann[1] — [1]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France — [2]College of Chemistry and Molecular Engineering, Peking University, China

The generally accepted picture of $SrVO_3$ is that of a correlated electron metal where a renormalized quasi-particle peak at the Fermi level coexists with upper and lower Hubbard bands, separated by Coulomb interaction U. Recently, this picture has become blurred with the rise in interest in additional plasmonic satellites. Distinguishing plasmonic features from Hubbard bands is a non-trivial question. In this talk we employ combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") to discuss the processes that give rise to these different satellites and show how to identify their origin in realistic materials. We present an application of this scheme to different transition metal oxides, which we find to exhibit both Hubbard and plasmonic satellites at similar energetic positions.

TT 70.7 Wed 16:45 HL 001

Phase transitions of the 2D Hubbard-Holstein model — •Teresa E. Reinhard[1], Uliana Mordovina[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA — [3]Nano-bio Spectroscopy Group and ETSF, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, San Sebastian, Spain

In the 2d Hubbard-Holstein model at zero temperature, a quantum phase transition between Mott and Peierls insulator can be observed. Whether a metallic phase emerges in between remains an open question [1,2]. As the emergence of the Mott phase is a many body effect, a description beyond the mean field level is crucial. At the same time, a method that can cope with two dimensions is needed.

To address this open question, we have extended Density Matrix Embedding Theory (DMET) from the purely electronic case [3,4] to coupled fermion-boson systems. DMET is an embedding theory which benefits from the exponentially decaying correlation in most quantum systems thus allowing a description beyond mean field at low cost.

We show the phase diagram of the 2d Hubbard-Holstein model at zero temperature obtained for different cluster sizes. [1] G. Knizia, G. K.-L Chan, Phys. Rev. Lett 109, 186404, (2012) [2] S. Wouters, C. A. Jiménez-Hoyos, G. K.-L. Chan, arXiv:1605.05547 (2016) [3] R. T. Clay and R. P. Hardikar, Phys. Rev. Lett 95, 096401 (2005) [4] J. Bauer, EPL 90 27002 (2010)

TT 70.8 Wed 17:00 HL 001

A quantum embedding theory combining many-body perturbation theory with configuration interaction — •Marc Dvorak and Patrick Rinke — Department of Applied Physics, Aalto University School of Science, 00076-Aalto, Finland

We present a new quantum embedding theory called dynamical configuration interaction (DCI). It captures non-local and static correlation in an orbital active space with configuration interaction (CI) and high-energy, dynamic correlation in the complementary bath space with many-body perturbation theory (MBPT). The formulation is general, but we focus on molecular systems with an *ab-initio* Hamiltonian. The conceptual key to our approach is to replace the exact electronic Hamiltonian in the bath space with one of excitations defined over the correlated ground state. This transformation is naturally suited to the language and methodology of many-body Green's functions. Correlation in the bath is therefore described at the quasiparticle level with Green's functions instead of with the many-body wave function. Our approach avoids computational and conceptual difficulties associated with Green's function embedding and improves upon wave function methods by including dynamical correlation from the bath space. A major advantage to DCI is that it naturally treats ground and excited states on equal quantum mechanical levels. For ground state properties, we present dimer dissociation curves for H_2 and N_2 in excellent agreement with exact results. Excited states of N_2 give excellent agreement with experiment, and we demonstrate the scalability of our method by computing excited states of a free-base porphyrin molecule.

TT 70.9 Wed 17:15 HL 001

Real-Structure Effects and Correlation in Layered Sodium Cobaltates — Sophie Chauvin[1,2], Silke Biermann[1], Lucia Reining[2], and •Claudia Rödl[3] — [1]Centre de Physique Théorique, École polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France — [2]Laboratoire des Solides Irradiés, École polytechnique, CNRS, CEA, Université Paris-Saclay, 91128 Palaiseau, France — [3]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Na-doped layered cobaltates Na_xCoO_2 feature a rich phase diagram with a plethora of physical phenomena ranging from metal-insulator transitions over magnetism to charge ordering. These instabilities of the electronic structure are mostly attributed to correlation effects within the quasi-2D CoO_2 layers. Here, we focus on $Na_{2/3}CoO_2$, a doping for which the system is metallic and exhibits an experimentally established charge disproportionation on the Co atoms.

We study the electronic properties of the CoO_2 layers and investigate the impact of the intercalated Na atoms on the electronic structure in the ordered layered superstructure. The problem is tackled from an *ab-initio* point of view using density-functional theory (DFT) and many-body perturbation theory (MBPT). Moreover, we study the static charge-density response of the material to understand instabilities in the system. Our approach complements recent model calculations from extended dynamical mean-field theory (EDMFT). The calculated results are compared to experimental spectroscopic data.

TT 70.10 Wed 17:30 HL 001

Slave rotor approach to impurity models with correlated dp orbitals — •Jakob Steinbauer and Silke Biermann — École Polytechnique, Palaiseau, France

We propose a slave rotor method for the solution of many-orbital quantum impurity problems, which maps the original problem onto one with reduced degeneracy. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states with d-electrons are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and test the method in the atomic limit.

TT 71: Quantum Information Systems (joint session HL/TT)

Time: Wednesday 15:00–17:30 Location: EW 203

TT 71.1 Wed 15:00 EW 203

Input-output theory for spin-photon coupling in Si double quantum dots — •Mónica Benito[1], Xiao Mi[2], Jacob M. Taylor[3], Jason R. Petta[2], and Guido Burkard[1] — [1]University of Konstanz — [2]Princeton University — [3]Joint Quantum Institute/NIST

The interaction of qubits via microwave frequency photons enables long-distance qubit-qubit coupling and facilitates the realization of a large-scale quantum processor. However, qubits based on electron spins in semiconductor quantum dots have proven challenging to couple to microwave photons. In this theoretical work [1] we show that a sizable coupling for a single electron spin is possible via spin-charge hybridization using a magnetic field gradient in a silicon double quantum dot. Based on parameters already shown in recent experiments, we predict optimal working points to achieve a coherent spin-photon coupling. Our predictions are in good agreement with recent measurements [2] which demonstrate strong coupling with spin-photon coupling rates of more than 10 MHz. These results open a direct path towards entangling single spins using microwave frequency photons. Furthermore, we employ input-output theory to identify observable signatures of spin-photon coupling in the cavity output field, which can provide guidance to the experimental search for strong coupling in such spin-photon systems and opens the way to cavity-based readout of the spin qubit.

[1] M. Benito, X. Mi, J. M. Taylor, J. R. Petta, and G. Burkard. arXiv:1710.02508.

[2] X. Mi, M. Benito, S. Putz, D. M. Zajac, J. M. Taylor, G. Burkard, and J. R. Petta. arXiv:1710.03265.

TT 71.2 Wed 15:15 EW 203

Synchronized high-fidelity quantum gates in Si/SiGe double quantum dots — •Maximilian Russ[1], D. M. Zajac[2], A. J. Sigillito[2], F. Borjans[2], J. M. Taylor[3], J. R. Petta[2], and Guido Burkard[1] — [1]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, Princeton University, Princeton, NJ 08544, USA — [3]JQI and QuICS, NIST and University of Maryland, College Park, MD 20742, USA

Motivated by recent experiments [1], we theoretically describe a high-fidelity controlled-NOT (CNOT) gate using the exchange interaction between the spins in neighboring quantum dots subject to a magnetic field gradient from a micromagnet. We use a combination of analytical calculations and numerical simulations to provide the optimal pulse sequences and parameter settings for the gate operation [2]. We present a synchronization method which avoids detrimental spin flips when the state of the control qubit is $|0\rangle$, and provide details about phase mismatches accumulated during the two-qubit gate. By synchronizing the resonant and off-resonant transitions and compensating these phase mismatches by phase control the overall gate fidelity can be increased significantly. Numerical simulations demonstrate a high tolerance towards charge noise coupled to the two spins due to a partial intrinsic refocussing mechanism.

[1] D. M. Zajac, A. J. Sigillito, M. Russ, F. Borjans, J. M. Taylor, G. Burkard, and J. R. Petta, arXiv:1708.03530 (2017)

[2] M. Russ, D. M. Zajac, A. J. Sigillito, F. Borjans, J. M. Taylor, J. R. Petta, and G. Burkard, arXiv:1711.00754 (2017)

TT 71.3 Wed 15:30 EW 203

Engineering of Coherent Defects in Silicon Carbide with Varying Irradiation Methods — •Christian Kasper[1], Victor Soltamov[1], Dmitrij Simin[1], Takeshi Ohshima[2], Vladimir Dyakonov[1,3], and Georgy Astakhov[1] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]National Institutes for Quantum and Radiological Science and Technology, Takasaki, Japan — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Out of the many possible material systems, quantum centers in silicon carbide (SiC) have proven themselves to be promising candidates for qubits [1]. Whereas a wide availability and easy handling are crucial for a functioning device, long-preserving spin coherence is also essential for such systems [2]. By using the pulsed-ODMR technique we compare the coherence properties of silicon vacancies created with two common methods: Neutron and electron irradiation. Particularly, the spin-lattice relaxation time (T1) and spin coherence time (T2) are measured in a broad range of the silicon vacancy density for each of the two irradiation methods. Additionally, Ramsey-fringes were measured while selecting a coherent spin package by applying a second microwave frequency.

[1] D. Riedel et al., Phys. Rev. Lett. 109, 226402 (2012)
[2] Simin et al., Phys. Rev. B 95, 161201(R) (2017)

TT 71.4 Wed 15:45 EW 203

Simulating high-fidelity two-qubit gates with singlet-triplet qubits generated by capacitive coupling and interqubit exchange interaction — •Michael Wolfe[1], Pascal Cerfontaine[1], Fernando Calderon-Vargas[2], Jason Kestner[3], and Hendrik Bluhm[1] — [1]JARA-Institute for Quantum Information, RWTH Aachen University, D-52074 Aachen, Germany — [2]Department of Physics, Virginia Tech, Blacksburg, VA 24061, USA — [3]Department of Physics, University of Maryland Baltimore County, Baltimore, MD 21250, USA

Two-qubit gates in singlet-triplet qubits can be generated via capacitive coupling or interqubit exchange interaction. Both methods suffer considerably from charge noise and nearly all approaches to mitigate this effect rely on the fact that the noise is slow compared to the gate time. We show that in the strictly capacitive case where gate times are much slower, maximally entangling gates with fidelities above 99% are achievable by operating the qubit in a sweet spot regime that is predicted by a Hund-Mulliken model [1]. In addition, we find comparable fidelities when both interqubit exchange and capacitive interactions are simultaneously used to generate entanglement. We compare these theoretical results with gates that are found using an optimization technique that numerically searches for high-fidelity two-qubit gates using a full-noise and control error model [2]. [1] Wolfe et al., arXiv:1709.09165 (2017) [2] Cerfontaine et al., PRL 113, 150501 (2014)

TT 71.5 Wed 16:00 EW 203

Microwave saturation spectroscopy of silicon vacancies in SiC — •Victor Soltamov[1], Christian Kasper[1], Georgy V. Astakhov[1], Sergej A. Tarasenko[2], Alexander V. Poshakinskiy[2], Andrey N. Anisimov[2], Pavel G. Baranov[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Ioffe Institute, 194021 St.Petersburg, Russia — [3]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg

Negatively charged silicon vacancy (V_{Si}) center in Silicon Carbide (SiC) has been attracting growing attention due to their use in quantum sensing with optical pumping [1]. The core of the sensing methods is to precise measurement of the optically detected magnetic resonance (ODMR) signal frequency shift, induced by the external fields. A sensitivity of the measurement improves when the V_{Si} ground-state microwave transitions are narrow. That is why, understanding of the mechanisms responsible for inhomogeneous broadening of the ODMR line is of great importance. To establish the mechanisms we provided the study of the V_{Si} ODMR linewidth by means of microwave saturation spectroscopy. We revealed the presence of two types of broadening namely induced by randomly distributed strain fields and by randomly distributed local magnetic fields. The results allowed deeper understanding of the V_{Si} ground spin state properties and to propose new measurement protocols for quantum sensing with the V_{Si} centers.

[1] H. Kraus et al., Sci. Rep. 4, 5303 (2014).

15 min. break.

TT 71.6 Wed 16:30 EW 203

Fabrication and Characterization of a Quantum Bus Prototype in Si/SiGe — •Inga Seidler[1], Arne Hollmann[1], Veit Langrock[1], Stefan Trellenkamp[2], Christian Neumann[3], Dominique Bougeard[3], Hendrik Bluhm[1], and Lars R. Schreiber[1] — [1]JARA-FIT Institute for Quantum Information, RWTH Aachen University, Germany — [2]Helmholtz Nano Facility, Forschungszentrum Jülich GmbH, Germany — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

Silicon based spin qubits in electrostatically defined quantum dots are well established and 1-qubit and 2-qubit gates are shown with high fidelities [1,2]. The missing link for building a large scale quantum computer is a long range coherent coupling mechanism. A candidate for a coupling mechanism is a 10 micron long quantum bus (QuBus), which transfers a single electron spin qubit along a 1D channel. We will present the concept of a QuBus that consists of a dense metal gate array required to appropriately shape the electrostatic potential within the channel. We optimized the fabrication yield of the three-layer metal gate pattern of the 320 nm long Si QuBus prototype. In addition, 10 mK transport measurements of a single electron transistor which operates as the charge sensor at the ends of a QuBus are shown.

[1] J. Yoneda ea., arXiv:1708.01454 [2] D. M. Zajac ea., arXiv:1708.03530

TT 71.7 Wed 16:45 EW 203

Towards atomic vapor based memories for quantum dot single photons - A variable EIT delay in Cesium — •Tim Kroh[1], Esteban Gomez Lopez[1], Janik Wolters[2], Alexander Thoma[3], Stephan Reitzenstein[3], Joahnnes S. Wildmann[4], Rinaldo Trotta[4], Eugenio Zallo[5], Armando Rastelli[4], Oliver G. Schmidt[6], and Oliver Benson[1] — [1]Humboldt-Universität zu Berlin — [2]Universität Basel — [3]Technische Universität Berlin — [4]Johannes Kepler Universität Linz — [5]Paul-Drude-Institut für Festkörperelektronik, Berlin — [6]IFW Dresden

Quantum memories will play a central part in synchronizing operational events in quantum networks, e.g. joint measurements between photons from different sources in order to implement entanglement swapping in quantum repeater protocols [1].

Here, we interface quantum light sources with an electromagnetically induced transparency (EIT) system, in principle suitable for quantum memory. First, we demonstrate precise strain-tuning of InGaAs quantum dot emission between the two 1.2 GHz hyperfine-split levels in the Cesium D1 transitions. Proceeding from this we explore the potential of EIT for variable delays for single photons [2]. In addition to application in synchronization of heralded single photon sources, these experiments lay the ground for atomic vapor-based quantum memories in hybrid quantum networks [3].

[1] Kimble, Nature 453, 1023 (2008)
[2] D. Höckel et al., Phys. Rev. Lett. 105, 153605 (2010)
[3] J. Wolters et al., Phys. Rev. Lett. 119, 060502 (2017)

TT 71.8 Wed 17:00 EW 203

Theory of long-range coherent electron shuttling devices in Silicon/Silicon-Germanium quantum wells — •Veit Langrock, Arne Hollmann, Inga Seidler, Lars R. Schreiber, and David P. DiVincenzo — JARA-FIT Institute for Quantum Information, RWTH Aachen University, Germany

Silicon quantum computing is at a stage where single qubits confined in electrostatically formed quantum dots with very long coherence times can be manufactured. To make the transition to large scale quantum computing, long range on chip coupling (over micrometer distances) is a building block that is currently still missing. A concept currently pursued experimentally is the coherent shuttling of electrons via moving electrostatic quantum dot configurations, with information encoded in the electron's spin state. In this talk, we present theoretical considerations and simulations regarding moving electrostatically formed quantum dots through a Silicon/Silicon-Germanium (Si/SiGe) quantum well. Emphasis will be put on the effects that interface disorder in the form of miscut steps along the Si/SiGe quantum well interfaces will have on the moving electron's spin environment, with the valley dependence in silicon playing a crucial role.

TT 71.9 Wed 17:15 EW 203

Spin-orbit interaction isotropy for holes in rectangular Si nanowires — •Marko J. Rancic, Christoph Kloeffel, and Daniel Loss — Department of physics, University of Basel

In this study we develop a model describing holes in rectangular nanowires in silicon (Si). In similarity with cylindrical nanowires, an electric field of intermediate strength can induce a sizable direct Rashba spin-orbit interaction (DRSOI). Our findings suggest that the magnitude of DRSOI is isotropic in case of germanium (Ge) due to the high degree of symmetry which Ge has. In contrast to that DRSOI is highly anisotropic in Si, dependant on the growth direction of the Si nanowire with respect to the main crystallographic axes. Still the DRSOI in si can be made significant ($\sim$ 0.5 meV) when the growth direction of the nanowire is chosen optimally, different to recent experimental studies.

TT 72: Poster Session: Correlated Electrons

Time: Wednesday 15:00–19:00 Location: Poster B

TT 72.1 Wed 15:00 Poster B

Fermi Surface determination of $CeAl_2$ via de Haas-van Alphen oscillations — •Michael Petrov, Chris Franz, Schorsch Sauther, Andreas Bauer, Mark Wilde, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

In this work, we revisit the Fermi surface properties of $CeAl_2$, a prototypical heavy-fermion compound that has attracted interest [1,2] because it promises tractable conditions for investigating the emergence of the heavy electron state in an f-electron system and its evolution across metamagnetic phase transitions [3]. In particular, the aim of the current research is a comprehensive picture of the Fermi surface properties, both, above and below the metamagnetic transitions. Torque magnetometry is used as a measurement technique for the de Haas-van Alphen (dHvA) effect that is complementary to the previously employed modulation technique. First results regarding both dHvA oscillations and the magnetic state via the non-oscillatory torque components are presented. The dHvA orbits are compared to the results of density functional theory calculations.

[1] Reinders *et al.*, JMMM **79**, 295 (1989)
[2] Pricopi *et al.*, Physica B: Condensed Matter **294**, 276 (2001)
[3] Schefzyk *et al.*, Solid State Communications **54**, 525 (1985)

TT 72.2 Wed 15:00 Poster B

Low-temperature properties of the non-centrosymmetric heavy-fermion compound $CeTAl_3$ (T = Cu, Ag, Au, Pd, Pt) — Christian Franz[3], Stefan Weber[1], •Jan Spallek[1], Alexander Regnat[1], Petr Cermak[2], Astrid Schneidewind[2], Andreas Bauer[1], Anatoly Senyshyn[2], and Christian Pfleiderer[1] — [1]Physik Departement, Technische Universität München, Garching, Deutschland — [2]JCNS-MLZ PANDA, Forschungszentrum Jülich, Garching, Deutschland — [3]Forschungsreaktor München 2, Garching, Deutschland

We report a comprehensive study of the series of non-centrosymmetric heavy-fermion compounds $CeTAl_3$ (T = Cu, Ag, Au, Pd, and Pt). Large single crystals have been prepared by means of optical floatzoning. The single-crystal ingots were characterized using Laue x-ray scattering, powder x-ray diffraction, and energy dispersive x-ray spectroscopy. For T = Cu, Au, Pd, and Pt the system crystallizes in the non-centrosymmetric I4mm crystal structure, while we observe a slight orthorombic distortion for T = Ag. Subsequently, the magnetization, specific heat, and electrical resistivity were investigated down to temperatures of 200 mK and in magnetic fields of up to 14 T revealing typical heavy-fermion behavior. At low temperatures, $CeCuAl_3$ and $CeAuAl_3$ order antiferromagnetically, whereas $CeAgAl_3$ is a ferromagnet. Indications of magnetic order are observed in $CePdAl_3$. Inelastic neutron scattering studies indicate the presence of so-called vibron modes, i.e., coupled modes of phonons and crystal electric field excitations.

TT 72.3 Wed 15:00 Poster B

Pressure and field dependent entropy of the heavy-fermion system CePdAl — •Kai Grube[1], Sebastian Kuntz[1], Chien-Lung Huang[2], Veronika Fritsch[3], and Hilbert von Löhneysen[1,4] — [1]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [2]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, United States — [3]Experimentalphysik VI, Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86159 Augsburg, Germany — [4]Physikalisches Institut, Karlsruher Institut für Technologie, 76049 Karlsruhe, Germany

In the heavy-fermion metal CePdAl long-range antiferromagnetic order coexists with geometric frustration of one third of the Ce moments. At low temperatures the Kondo effect tends to screen the frustrated moments. We used magnetic fields B to suppress the Kondo screening and studied the magnetic phase diagram and the evolution of the entropy with B and pressure employing thermodynamic probes. We estimated the frustration by introducing a definition of the frustration parameter based on the enhanced entropy, a fundamental feature of frustrated systems. In the field range where the Kondo screening is suppressed the liberated moments tend to destabilize the magnetic order and strongly enhance the frustration.

TT 72.4 Wed 15:00 Poster B

Evolution of magnetic order in $HoIn_{1-x}Cd_xCu_4$ — Christina Baumeister[1], Oliver Stockert[2], and •Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$HoInCu_4$ is a partially frustrated metal, crystallizing in the cubic $AuBe_5$ structure. The Ho ions carrying the magnetic moment form a fcc lattice, with alternating antiferromagnetic planes along [100], which are separated by frustrated planes as shown by neutron scattering experiments [1]. The partial frustration is manifested in magnetization and specific heat data, leading to a frustration parameter $f = 14.3$ [2]. In contrast, no signatures of magnetic frustration are found in isotructural $HoCdCu_4$ [3]. Here, Neutron scattering experiments point to a magnetic structure of ferromagnetic planes, which are stacked antiferromagnetically along the [111] direction [4]. We will present detailed measurements of magnetization and specific heat on the alloying series $HoIn_{1-x}Cd_xCu_4$ tracking the evolution of the magnetic order and the magnetic frustration as function of Cd content.

[1] O. Stockert *et al.*, Experimental Report, HMI B 612 (2006).
[2] V. Fritsch *et al.*, Phys. Rev. B, **71**, 132401 (2005).
[3] V. Fritsch *et al.*, Phys. Rev. B, **73**, 094413 (2006).
[4] O. Stockert *et al.*, Experimental Report, MLZ Garching (2017).

TT 72.5 Wed 15:00 Poster B

Crystal structure and magnetic properties of $CeMg_{3-x}Ag_x$ — •Alexander Engel[1], Georg Eickerling[2], Ernst-Wilhelm Scheidt[2], Philipp Gegenwart[1], and Veronika Fritsch[1] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Chemical Physics and Materials Science, Augsburg University, Germany

$CeMg_3$ crystallizes in a BiF_3 cubic heusler-phase type structure and is a heavy-fermion antiferromagnet with $T_N = 3.4$ K. Gradually substituting Mg with Ag makes it possible to tune the exchange interaction and hereby the antiferromagnetic order. Furthermore a structural phase transition accompanied by a charge density wave occurs for $x \geq 1.5$. This structural phase transition was confirmed by temperature dependent single crystal x-ray diffraction. Moreover we show measurements of electrical resistivity and heat capacity on polycrystals tracking the magnetic order and structural phase transition in the alloy-series of $CeMg_{3-x}Ag_x$ and discuss a possible structural quantum critical point.

TT 72.6 Wed 15:00 Poster B

3D topological Kondo insulators: effects of strong correlations onthe stability of topological phases — •Paul Züge[1], Soroush Arabi[1], Francisco Meirinhos[1], and Johann Kroha[1,2] — [1]Physikalisches Institut and Bethe Center for TheoreticalPhysics, Universität Bonn, Germany — [2]Center for Correlated Matter, Zhejiang University, Hangzhou, China

Topological Kondo insulators (TKI) are heavy-fermion (HF) materials where strong correlations generate a HF band with a hybridization gap around the Fermi level and the strong spin-orbit coupling in the 4f orbitals on the rare-earth sites, hybridizing with the light conduction

electron band, induces non-trivial topology with conserved topological invariants in these bands. Since in all relevant energy scales, the HF band width, the gap and quasiparticle decay rates are of comparable size, the Kondo temperature T_K, TKIs are ideal systems to study the stability of topological phases in the presence of interactions. However, most theoretical studies have been on the effective single-particle (mean-field) level up to now. We use the slave boson (SB) representation for the HF band and systematically expand around the SBMF saddle point, taking the Gaussian fluctuations of the SB field into account. Feeding the resulting self-energies back into the boson and fermion propagators, this leads to self-consistent saddle-point equations, which imply a finite spectral width for the HF states. We solve these equations self-consistently for the bulk of three-dimensional TKIs. We compute the HF and conduction electron spectral functions and analyse the stability of the topological hybridization gap.

TT 72.7 Wed 15:00 Poster B

Slave Boson Mean Field - revisited — •Jannis Seufert, David Riegler, Michael Klett, and Ronny Thomale — Institute for Theoretical Physics, University of Würzburg, Germany

Considering correlated electron systems where interactions constitute the dominant energy scale is a challenging problem in solid state physics. The Slave-boson mean field method provides an exact mapping of fermionic Hamiltonians into a description, where the interaction terms become bilinear in bosonic auxiliary fields, whereas terms which are bilinear in the original Hamiltonian transform to a mix of auxiliary bosonic and fermionic fields. A consecutive mean field treatment is therefore especially suitable to incorporate the impact of strong interactions, and yields a non-interacting effective band structure. Experimentally relevant quantities such as heat capacity or effective mass can be derived from the mean field variables, while dynamic quantities such as susceptibilities can be obtained from fluctuations around the saddle point. Evaluating susceptibilities allows to obtain phase diagrams, especially talking incommensurate magnetism by means of a magnetic, momentum dependent mean field into account. We provide a fresh look on the method of spin rotation invariant Slave-boson mean field with fluctuations around the saddle point, and its applications to investigate incommensurate magnetism and heavy fermion systems.

TT 72.8 Wed 15:00 Poster B

Towards the crystal growth of nuclear spin tuned $YbRh_2Si_2$ — •Thanh Duc Nguyen, Doan-My Tran, Sebastian Witt, and Cornelius Krellner — Physikalisches Insitut, Goethe-Universität Frankfurt am Main, D-60438 Frankfurt

The investigation of the heavy fermion compound $YbRh_2Si_2$ allows new insights concerning the interplay of quantum phase transitions and superconductivity. The compound shows at 70mK antiferromagnetic order which can be further suppressed to a quantum critical point. Recently, at 2mK a superconducting state was discovered [1]. Due to the ordering of the nuclear spin of ^{171}Yb and ^{173}Yb before the superconducting state emerges it is a matter of particular interest to investigate the evolution of the superconductivity in single crystals with pure zero and non-zero nuclear spins of the Yb-isotopes. To this end, we first need to optimize the metallothermic reduction of the rare earth element as the isotopes are only available as oxides. Furthermore, we present the optimization of down-scaling in mass the single crystal growth and we report two ways to regaining ytterbium from foreign phase $YbRhIn_5$.

[1] E. Schuberth et al., Science 351, 485 (2016).

TT 72.9 Wed 15:00 Poster B

High-Pressure studies on the quasi-one-dimensional heavy fermion metal $YbNi_4P_2$ — •Takaki Muramatsu[1], Kristin Kliemt[2], Cornelius Krellner[2], and Sven Friedemann[1] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is very unique system among correlated electron compounds due to the quasi-one-dimensional nature. The crystal structure is tetragonal $ZrFe_4Si_2$ type structure ($P4_2/mnm$) in which Yb chains along c-axis are separated by chains of edge-shared Ni tetrahedra. Below 0.17K, $YbNi_4P_2$ orders ferromagnetically (FM) with small ordered magnetic moment of $0.05\mu_B$ [1]. $YbNi_4P_2$ is a rare expample where a ferromagnetic quantum critical point can be accessed [2]. Here, we present high-pressure studies of $YbNi_4P_2$ using a diamond-anvil pressure cell. Application of pressure on strongly correlated electron system plays an important role to discuss the quantum criticality and to study the detailed properties of the system. In this work, temperature dependence of the electrical resistivity of $YbNi_4P_2$ was measured under high pressure to understand the basics of competing nature among 4f valence of Yb ion, long range magnetic order and Kondo effect.

[1] C. Krellner et al., New J. Phys, **13**, 103014 (2011).
[2] A. Steppke et al., Science, **339**, 933 (2013).

TT 72.10 Wed 15:00 Poster B

Crystal Growth with Flux Method and Characterization of $CeRu_2P_2$ — •Fabian Feldmann, Kristin Kliemt, and Cornelius Krellner — Physikalisches Inst., Goethe Univ., DE

$CeRu_2P_2$ is a rare-earth ternary phosphide with the tetragonal $ThCr_2Si_2$ type crystal structure. The electrical resistivity in [100] direction of $CeRu_2P_2$ shows a broad maximum at T = 180 K and metallic behavior for lower temperatures [1], indicative of a slightly intermediate valent system, which was confirmed recently in RIXS measurements [2]. Here, we report a crystal growth method for $CeRu_2P_2$. The single crystals have been grown in Sn-flux with temperatures up to 1500 °C. We have characterized the grown crystals with EDX and powder x-ray diffraction measurements. Furthermore, we present measurements of electrical resistivity, specific heat and magnetic susceptibility.

[1] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[2] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)

TT 72.11 Wed 15:00 Poster B

Characterization of Hf and Sc substituted $YbNi_4P_2$ single crystals — •Paul Denck, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe-University Frankfurt, D-60438 Frankfurt, Germany

The low lying Curie temperature, $T_C = 0.17$ K, of the heavy-fermion compound $YbNi_4P_2$ can be further suppressed by substituting P by As. The rare case of a ferromagnetic quantum critical point occurs in the substitution series $YbNi_4(P_{1-x}As_x)_2$ at $x \approx 0.1$ [1,2]. Single crystals $Yb_{1-x}Hf$, $Sc_xNi_4P_2$, with various hafnium and scandium concentrations were grown by the Czochralski method [3,4]. We characterized the room temperature crystal structure by powder x-ray diffraction and determined the change in the lattice constants for increasing content of the subtituent. Furthermore, these crystals were characterized by electrical transport, heat capacity, and magnetization measurements to investigate the effect of the substitution on the ferromagnetic order.

[1] C. Krellner et al., New J. Phys. **13**, 103014 (2011)
[2] A. Steppke et al., Science **339**, 933 (2013)
[3] K. Kliemt, C. Krellner, J. Cryst. Growth **449**, 129 (2016)
[4] K. Kliemt, C. Krellner, J. Phys.: Conf. Series **807**, 032005 (2017)

TT 72.12 Wed 15:00 Poster B

Hydrostatic-pressure tuning of the magnetic states in the frustrated itinerant system YFe_4Si_2 — •C. Thurn[1], B. Wolf[1], C. Krellner[1], N. Mufti[2], C. Geibel[2], and M. Lang[1] — [1]Physikalisches Institut, Goethe Uni, Frankfurt/M., SFB/TR49, Germany — [2]MPI CPfS, Dresden, Germany

Magnetic frustration can enhance quantum fluctuations which are supposed to be the key in creating exotic states. Whereas frustration is often found in insulators, frustrated magnetic metals are rare. The family of intermetallic AFe_4X_2 with A=Y, Lu, Zr and X=Ge, Si represents such frustrated itinerant systems in which the Fe ions are arranged on slightly distorted, edge-linked tetrahedra which promote the frustration. The properties of these compounds cover a wide range, including frustrated antiferromagnetic order and potentially paramagnetic states close to quantum-critical points. The substitution on the A and X sites here modifies the unit-cell parameters, suggesting a significant influence of chemical pressure on the ground-state properties. In order to mimic and fine-tune the effect of chemical pressure, we present a study of the magnetic properties of YFe_4Si_2 under hydrostatic pressures up to 4 kbar. This compound shows two consecutive magnetic phase transitions at ambient pressure which are strongly coupled to structural degrees of freedom. Our results indicate moderate pressure dependences of the two phase transitions. In order to investigate the interplay of the structure with magnetic frustration in more detail, we also discuss pressure tuning of the distinctly more frustrated system $ZrFe_4Si_2$ which might be located close to a quantum-critical point.

TT 72.13 Wed 15:00 Poster B

Higher order transport mechanisms using matrix product — •Simon Kothe, Lars-Hendrik Frahm, and Daniela Pfannkuche — 1. Institut für Theoretische Physik, Universität Hamburg

We investigate different methods to approach the Kondo regime of an

atom that is coupled to two reservoirs. In our model the atom is simplified as a spin, that is biased by a magne- tocrystalline anisotropy field and the exchange interaction to electrons in the reservoirs. As our first approach we use a perturbation ansatz to obtain equations of motion for the reduced density matrix of the spin. This allows us to calculate dynamics of the atom as well as trans- port properties. In our second approach we use matrix product states (MPS) to describe the state of the system and apply the density matrix renormalization group (DMRG) algorithm. The resulting transport properties show the importance of higher order coupling mechanisms.

TT 72.14 Wed 15:00 Poster B

Effective interactions between rotating impurities immersed in a bosonic bath — •Xiang Li and Mikhail Lemeshko — IST, Klosterneuburg, Austria

As first reported in [1], an impurity exchanging angular momentum with the environment can be described as a new quasiparticle, the angulon. The outcome of the angulon theory has been shown to be in good agreement with experiments on molecules rotating in quantum solvents [2]. Here, we study the direct and bath -mediated interactions between two rotating molecular impurities in a bosonic bath. A theory of bi-angulon quasiparticle is proposed.

[1] R. Schmidt and M. Lemeshko, Phys. Rev. Lett. 114, 203001 (2015)
[2] M. Lemeshko, Phys. Rev. Lett. 118, 095301 (2017)

TT 72.15 Wed 15:00 Poster B

Emergence of non-abelian magnetic monopoles in a quantum impurity problem — •Enderalp Yakaboylu, Andreas Deuchert, and Mikhail Lemeshko — IST Austria (Institute of Science and Technology Austria), Am Campus 1, 3400 Klosterneuburg, Austria

Recently it was shown that molecules rotating in superfluid helium can be described in terms of the angulon quasiparticles [1]. Here we demonstrate that in the experimentally realized regime the angulon can be seen as a point charge on a 2-sphere interacting with a gauge field of a non-abelian magnetic monopole. Unlike in several other settings, the gauge fields of the angulon problem emerge in the real coordinate space, as opposed to the momentum space or some effective parameter space. Furthermore, we find a topological transition associated with making the monopole abelian, which takes place in the vicinity of the previously reported angulon instabilities. These results pave the way for studying topological phenomena in experiments on molecules trapped in superfluid helium nanodroplets, as well as on other realizations of orbital impurity problems [2].

[1] M. Lemeshko, Phys. Rev. Lett. 118, 95301 (2017).
[2] E. Yakaboylu, A. Deuchert, and M. Lemeshko, arXiv:1705.05162.

TT 72.16 Wed 15:00 Poster B

Thomas Fermi regime of neutrons stars at finite temperature — •Kouidri smail — Departmet of Physics University of Saida Algeria

We present our numerical calculations to study the behavior of a neutron stars at finite temperature and in Thomas Fermi limit. This system of BEC is described by the famous Gross- Pitaevskii equation, which can be solved numerically using several method [1]. The term which contains the gravitational contribution is described by Poisson equation, that can be solved by iterative processus. Our work combines these two methods to study the time evolution of a self-gravitating.

TT 72.17 Wed 15:00 Poster B

Evolution of the order parameter close to the CDW quantum critical point in $Lu(Pt_{1-x}Pd_x)_2In$ — •Stefan Lucas[1], Thomas Gruner[1], Andreas Hoser[2], Manfred Reehuis[2], Karin Schmalzl[3], Michael Marek Koza[3], Christoph Geibel[1], and Oliver Stockert[1] — [1]Max Planck Institute for Chemichal Physics of Solids, Dresden, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]Institut Laue-Langevin, Grenoble, France

In contrast to magnetic quantum phase transitions being studied for many years, those driven by an instability of the crystal structure are hardly investigated so far. The intermetallic alloying series $Lu(Pt_{1-x}Pd_x)_2In$ represents a model system to study a Charge-Density-Wave (CDW) quantum critical point (QCP) occurring at $x \approx 0.58$ [1]. A strong and well defined maximum of the superconducting transition temperature right in the vicinity of the QCP indicates a close connection between the low-energy order parameter fluctuations and superconductivity. The important role of the structural fluctuations is already suggested in specific heat and resistivity measurements and was now investigated by neutron diffraction. We present the evolution of the superstructure (i.e. the order parameter) for different concentrations of $Lu(Pt_{1-x}Pd_x)_2In$ and discuss the role of critical fluctuations in this system.

[1] T. Gruner *et al.*, *Nat. Phys.* **13**, 967 (2017)

TT 72.18 Wed 15:00 Poster B

Crystal growth and soft phonon mode of the quantum critical CDW system $Lu(Pt_{1-x}Pd_x)_2In$ — •Thomas Gruner[1], Stefan Lucas[1], Satoshi Tsutsui[2], Koji Kaneko[3], Oliver Stockert[1], and Christoph Geibel[1] — [1]MPI CPfS, Dresden, Germany — [2]JASRI, SPring-8, Sayo, Hyogo, Japan — [3]JAEA Quantum Beam Science Center, Tokai, Ibaraki, Japan

The connection between a charge density wave (CDW) quantum critical point (QCP) and superconductivity (SC) is presently a hot topic. We recently reported the discovery of a CDW in $LuPt_2In$ at $T_{CDW} = 490\,K$, which can be continuously tuned to $T = 0$ by partially substituting Pd for Pt [1]. Moreover, $Lu(Pt_{1-x}Pd_x)_2In$ shows a sharp peak in the x dependence of the superconducting T_c just at the QCP, indicating a very unusual coupling between CDW and SC [1]. Here, we discuss the growth of large high-quality single crystals across the whole composition range. The challenge in growing them is the combination of high-melting elements with the low-melting In. We used these crystals for a series of momentum (Q) resolved inelastic x-ray scattering experiments. They provided a first insight into the Q, T and x dependence of the phonon softening connected with the CDW. In one phonon branch the phonon energy drops towards zero when T decreases towards $T_{CDW}(x)$ and Q approaches the CDW propagation vector. Our results provide an essential basis for analyzing the critical behaviour in this system. Furthermore, we present an improved structure model of the CDW state.

[1] T. Gruner et al., Nature Physics **13**, 967-972 (2017)

TT 72.19 Wed 15:00 Poster B

Ising tricriticality in the extended Hubbard model with bond dimerization — •Florian Lange, Satoshi Ejima, and Holger Fehske — Institut für Physik, Ernst-Moritz-Arndt Universität Greifswald, D-17489 Greifswald, Germany

We explore the quantum phase transition between symmetry protected topological and charge-density-wave insulating states in the one-dimensional, half-filled, extended Hubbard model with explicit bond dimerization. We show that the critical line of the continuous Ising transition terminates at a tricritical point, belonging to the universality class of the tricritical Ising model with central charge $c = 7/10$. Above this point, the quantum phase transition becomes first order. Employing a numerical matrix-product-state based (infinite) density-matrix renormalization group method we determine the ground-state phase diagram, the spin and two-particle charge excitations gaps, and the entanglement properties of the model with high precision. Performing a bosonization analysis we can derive a field description of the transition region in terms of a triple sine-Gordon model. This allows us to derive field theory predictions for the power-law (exponential) decay of the density-density (spin-spin) and bond-order-wave correlation functions, which are found to be in excellent agreement with our numerical results.

TT 72.20 Wed 15:00 Poster B

Fluctuation effects at the onset of $2k_F$ density wave order with one pair of hot spots in two dimensional metals — •Jachym Sykora[1], Tobias Holder[2], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Department of Condensed Matter Physics, Weizmann Institute of Science, Rehovot, Israel 76100

We analyze quantum fluctuation effects at the onset of charge or spin density wave order in two dimensional metals with an incommensurate $2k_F$ wave vector connecting a single pair of hot spots on the Fermi surface. We compute the momentum and frequency dependence of the fermion self-energy near the hot spots to leading order in a fluctuation expansion (one loop). Non-Fermi liquid behavior with anomalous frequency scaling, a vanishing quasi-particle weight, and a logarithmically divergent renormalization of the Fermi velocity are obtained. Going beyond the leading order calculation we find that the one-loop result is not self-consistent. Moreover, we show that any self-energy with a non-Fermi liquid frequency exponent wipes out the peak of the polarization function at the $2k_F$ wave vector, and thus destroys the mechanism favoring $2k_F$ density waves over those with generic wave

vectors.

TT 72.21 Wed 15:00 Poster B

Non-linear integral equations for the XXX-$\frac{1}{2}$-chain with off-diagonal boundary conditions — •Dennis Wagner and Andreas Klümper — Bergische Universität Wuppertal, Wuppertal, Germany

The off-diagonal Bethe-Ansatz is a method to solve integrable models that lack U(1)-symmetry and hence do not have a reference state for the application of the coordinate or algebraic Bethe ansatz. Within this work, it is tried to use an inhomogeneous T-Q relation for the XXX-$\frac{1}{2}$-chain with off-diagonal boundary conditions as well as the fusion hierarchy to derive non-linear integral equations. For concrete tests, the system size is reduced to $N = 4$, under the assumption, that the general procedure also holds for larger system sizes. To test the derivation of non-linear integral equations via this procedure, an inhomogeneous T-Q relation for the XXX-$\frac{1}{2}$-chain with periodic boundary conditions is investigated. Finally, for the chain with off-diagonal boundary fields a system of three non-linear integral equations is presented.

TT 72.22 Wed 15:00 Poster B

Quantum Monte Carlo simulations of quantum critical fermions — •Carsten Bauer[1], Yoni Schattner[2], Erez Berg[3], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Physics, Stanford University, Stanford, CA 94305, USA — [3]Department of Physics, University of Chicago, Chicago IL 60637, USA

While quantum critical phenomena in insulators are fairly well understood, their metallic counterparts pose a substantial theoretical challenge since the order parameter fluctuations can interact with gapless fermionic excitations on a Fermi surface. When driving the metal through a phase transition, this interplay can give rise to superconductivity and non-Fermi liquid behavior.

Fortunately, for certain classes of metallic quantum critical points this rich physics can be studied by determinant quantum Monte Carlo simulations, without suffering from the notorious fermion "sign problem". I will show numerically exact studies of different Fermi surfaces coupled to antiferromagnetic SU(2) order in two spatial dimensions. I will further demonstrate that Julia, a new dynamical programming language, is excellently suited for conducting such studies both with regards to speed and code complexity.

TT 72.23 Wed 15:00 Poster B

High-field ESR studies of the honeycomb-lattice material α-$RuCl_3$ — •Alexey N. Ponomaryov[1], E. Schulze[1,2], J. Wosnitza[1,2], P. Lampen-Kelley[3,4], A. Banerjee[3], J.Q. Yan[3], C.A. Bridges[3], D.G. Mandrus[3], S.E. Nagler[3], A.K. Kolezhuk[5], and S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Dresden, Germany — [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA — [4]University of Tennessee, Knoxville, TN, USA — [5]T. Shevchenko National University of Kyiv, Ukraine

We present high-field electron spin resonance (ESR) studies of the honeycomb-lattice material α-$RuCl_3$, a prime candidate to exhibit Kitaev physics. Two modes of antiferromagnetic resonance were detected in the zigzag ordered phase, with magnetic field applied in the *ab* plane. A very rich excitation spectrum was observed in the field-induced quantum paramagnetic phase. The obtained data are compared with results of recent numerical calculations, strongly suggesting a very unconventional multiparticle character of the spin dynamics in α-$RuCl_3$. The frequency-field diagram of the lowest-energy ESR mode is found consistent with the behavior of the field-induced energy gap, revealed by thermodynamic measurements.

This work was supported by DFG (project ZV 6/2-2).

TT 72.24 Wed 15:00 Poster B

RIXS on the j = 1/2 double perovskite Ba_2CeIrO_6 — •Chin Chyi Loo[1], Alessandro Revelli[1], Anna Efimenko[2], Marco Moretti Sala[2], Giulio Monaco[3], Thomas Koethe[1], Petra Becker[4], Ladislav Bohatý[4], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]II, Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, D-50937 Köln, Germany — [2]ESRF-The European Synchrotron, 71 Avenue des Martyrs, 38000 Grenoble, France — [3]Physics Department, University of Trento, Via Sommarive 14, 38123 Povo (TN), Italy — [4]Institute of Geology and Mineralogy, Section Crystallography, University of Cologne, Köln, Germany

Spin-orbit-entangled j=1/2 iridates were predicted to show novel quantum states of matter. However, real materials deviate from a pure j=1/2 state due to, e.g., a non-cubic crystal field. Resonant inelastic x-ray scattering (RIXS) at the Ir L edge is ideally suited to study the j = 1/2 character and to determine the non-cubic crystal field. In the double perovskite Ba_2CeIrO_6, the Ir ions form an fcc lattice and the local symmetry is close to cubic, with a monoclinic angle $\beta = 89{,}986°$ [1]. The RIXS spectra establish the local j =1/2 ground state as well as a crystal-field splitting of the excited j = 3/2 state of less than 100 meV, the smallest observed thus far in iridates.

[1] M. Wakeshima, D. Harada, Y. Hinatsu, *J. Mater. Chem.* **10** (2000) 419.

TT 72.25 Wed 15:00 Poster B

RIXS on $5d^5$ $Ba_3CeIr_2O_9$ and $Ba_3Ti_xIr_{3-x}O_9$ — •Alessandro Revelli[1], Marco Moretti Sala[2], Giulio Monaco[3], Petra Becker[4], Ladislav Bohatý[4], Thomas Koethe[1], Tobias Fröhlich[1], Maria Hermanns[5], Paul H.M. van Loosdrecht[1], Jeroen van den Brink[6], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]ESRF, Grenoble — [3]Dipart. di Fisica, Universita di Trento — [4]Abt. Kristallographie, Institut für Geologie & Mineralogie, Universität zu Köln — [5]Institut für Theoretische Physik, Universität zu Köln — [6]IFW, Dresden

Spin-orbit entangled $j = 1/2$ Mott insulators set the stage for fascinating novel quantum states of matter. In corner-sharing geometry of the IrO_6 octahedra, one finds strong Heisenberg exchange between $j = 1/2$ moments, while edge-sharing geometry features bond-directional Kitaev exchange. However, the case of face-sharing octahedra has hardly been explored. Using resonant inelastic x-ray scattering (RIXS), we study the $5d^5$ compound $Ba_3CeIr_2O_9$ with face-sharing octahedra forming triangular layers. Both hopping and spin-orbit coupling are large. The RIXS data reveal the first and exceptionally clean realization of the quasi-molecular-orbital scenario that was debated extensively (but refuted) for Na_2IrO_3. The ground state shows a total $j = 0$ singlet predominantly built from $j = 1/2$ moments with the corresponding triplet excitation lying at an extraordinarily large energy. For M=Ti, the compound $Ba_3Ti_xIr_{3-x}O_9$ exists for different values of x and shows Ti/Ir site disorder. In RIXS we observe a coexistence of $j = 1/2$ moments and quasi-molecular singlets.

TT 72.26 Wed 15:00 Poster B

Influence of the mixed-valence state of Ir on the structural properties of $Ba_3MIr_2O_9$ (M= In, Lu, Mg) — •Georg Bothmann[1], Tusharkanti Dey[1], Anatoliy Senyshyn[2], Philipp Gegenwart[1], and Alexander Tsirlin[1] — [1]Lehrstuhl für Experimentalphysik VI, Zentrum für Elektronische Korrelationen und Magnetismus, Univesität Augsburg, Deutschland — [2]FRM-II, Technische Universität München, Deutschland

Mixed-valence iridates are a new platform for frustrated magnetism as shown in [1]. It is suspected that the mixed-valence state may evolve with temperature. Here we used x-ray diffraction (using radiation from a synchrotron) and neutron powder diffraction in a broad temperature range to compare the mixed-valence In and Lu compounds of the $Ba_3MIr_2O_9$ family of hexagonal perovskites with the integer-valence Mg compound of the same family.

The temperature dependence of the structural parameters, including lattice constants and Ir-Ir distances, will be reported. Additionally the instability toward a monoclinic distortion will be discussed.

[1] T. Dey, Phys. Rev. **B 96** (2017) 174411

TT 72.27 Wed 15:00 Poster B

Honeycomb Kitaev iridate and rhodate thin films — •Maximilian Uhl[1], Sebastian Esser[1], Vladimir Roddatis[2], Vasily Moshnyaga[3], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany — [3]1. Physikalisches Institut, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Recently materials realizing the honeycomb Kitaev exchange attracted considerable attention (for a review see [1]). Li-based heavy transition metal oxides Li_2IrO_3 [2] and Li_2RhO_3 [3] are prototype systems in this class. For the latter material, up to now only polycrystals are available which display a spin-glassy ground state. Epitaxial thin films are thus of particular interest, as they could reveal the true ground state and its dependence on strain. We utilize the metal-organic aerosol deposition (MAD) technique [4] and report the successful growth of thin films of both materials, as well as their structural and magnetic character-

ization. This work is supported by the German Science Foundation through SPP 1666 and TRR 80.
[1] S.M. Winter *et al.*, J. Phys.: Condens. Matter **29** (2017) 493002.
[2] Y. Singh *et al.*, Phys. Rev. Lett. **108**, (2012) 127203.
[3] P. Khuntia *et al.*, Phys. Rev. B **96**, (2017) 094432.
[4] M. Jungbauer *et al.*, Appl. Phys. Lett. **105**, 251603 (2014)

TT 72.28 Wed 15:00 Poster B

Magnetization and specific heat of Cr-doped α-$RuCl_3$ — •Mohammad Hossein Haghighi[1,2], Gaël Bastien[1], Anja U. B. Wolter[1], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, 01069 Dresden, Germany — [3]Department of Chemistry and Food Chemistry, TU Dresden, 01069 Dresden, Germany

α-$RuCl_3$ crystallizes in a layered honeycomb structure and has been proposed as a candidate to realize a fractionalized Kitaev model with strongly frustrated, bond-dependent, anisotropic interactions between Ru^{3+} magnetic moments ($j = \frac{1}{2}$). By introducing Cr as dopant to this Mott insulator ($S = \frac{3}{2}$ at the Ru sites), one can investigate changes of the long-range order in the ground state of α-$RuCl_3$ as well as of the anisotropic Kitaev interactions and field-induced effects which appear upon doping. We report on susceptibility and specific heat measurements of $Ru_{1-x}Cr_xCl_3$, probing the effect of different doping levels on the magnetic and thermodynamic properties on single crystals for the full range $0 \leqslant x \leqslant 1$.

TT 72.29 Wed 15:00 Poster B

Influence of Negative Charge Carrier Doping in $Nd_2Ir_2O_7$ on Structure and Magnetic Behavior — •Sebastian Selter[1], Ameya Prabhune[1], Anja U. B. Wolter[1], Saicharan Aswartham[1], and Bernd Buechner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We present the influence of negative charge doping on the structure and magnetic behavior of rare earth iridate pyrochlore $(Nd_{1-x}Ca_x)_2Ir_2O_7$ and $Nd_2(Ir_{1-x}Ga_x)_2O_7$ with x = 0..0.2.

$Nd_2Ir_2O_7$ possesses a hyperkagome lattice of corner-shared IrO_6 and edge-shared NdO_8 units. This gives rise to magnetic frustration and an all-in-all-out (AIAO) ordering is observed at low temperatures. Further, this material undergoes a metal-to-insulator transition (MIT) at around 30 K. MIT is a phenomenon observed in all rare earth iridate pyrochlores, except for $Pr_2Ir_2O_7$ which is metallic down to lowest temperatures. However, $Nd_2Ir_2O_7$ shows the lowest MIT temperature compared to other rare earth iridate pyrochlores and therefore is nearest to a possible quantum MIT. Furthermore, band structure calculations suggest that a Weyl semimetallic state with broken time reversal symmetry may be stabilized by the AIAO order in $Nd_2Ir_2O_7$. Recently, a dependency of the magnetic behavior and the MIT on the oxygen position in the rare earth iridate pyrochlores was proposed from theoretical side. A strong coupling of the physical properties to the crystal structure in $Nd_2Ir_2O_7$ can be concluded.

TT 72.30 Wed 15:00 Poster B

Spin-orbital superexchange and spin-orbit coupling — •Pascal Strobel and Maria Daghofer — Universität Stuttgart Institut für funktionelle Materie und Quantentechnologie, 70569 Stuttgart, Deutschland

In recent years t_{2g} spin-orbital models on a honeycomb lattice have been studied with either strong or no spin-orbit coupling. In both cases the ground state was investigated in dependency of Hund's coupling as well as the ratio of superexchange and direct exchange. With nonexistent spin-orbit coupling one obtains exotic phases like dimer states, while in the case of strong SOC one can find a Kitaev spin liquid phase.

However the phase diagram for intermediate spin-orbit coupling is yet relatively unknown. While [1] proposed a phase diagramm for the superexchange limit, we still need to explore the direct exchange limit as well as the influence of crystal deformation.

In this work we investigate the influence of moderate SOC, Hund's coupling, as well as the ratio of superexchange and direct exchange on several ordered states, which might be candidates for a ground state at some point in the phase diagram. The analytical results of the superexchange limit can then be compared to the numerical ones of [1]. Of particular interest in this work is whether we can find exotic phases like a spin liquid even without strong spin orbit coupling.
[1] A. Koga, S. Nakauchi, J. Nasu, arXiv:1705.09659

TT 72.31 Wed 15:00 Poster B

Excitation spectra of hard-core bosons in strongly spin-orbit coupled Van Vleck-type d^4 Mott insulators — •Friedemann Aust and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

In spin-orbit coupled Mott insulators with a t_{2g}^4 electron configuration, the interplay of spin-orbit coupling, Hund's rule and Kugel-Khomskii superexchange can be mapped to an effective singlet-triplet model [1]. For honeycomb or triangular lattice geometries, as found in e.g. delafossite, interactions have a bond selective structure reminiscent of the Kitaev honeycomb model. However, the local degrees of freedom are not given by a spin but by a singlet ground state and low-lying triplet excitations, which can be seen as hard-core bosons.

We discuss this model in the presence of direct exchange in addition to inter-orbital superexchange. Going beyond analytic considerations, we use cluster perturbation theory (CPT) and the variational cluster approximation (VCA), where the hard-core constraint can be taken into account, to obtain magnetic excitation spectra in regimes dominated by Heisenberg, Kitaev, or less symmetric couplings.
[1] G. Khaliullin, Phys. Rev. Lett. 111, 197201 (2013).

TT 72.32 Wed 15:00 Poster B

Variational Cluster Approximation for d^4 systems — •Teresa Feldmaier and Maria Daghofer — Institut für funktionelle Materie und Quantentechnologien, Universität Stuttgart, Deutschland

We use the variational cluster approximation to investigate the phase diagram and one-particle spectral density of multi-band Hubbard models with strong spin-orbit coupling. The approach includes quantum fluctuations on a small cluster exactly, where frustration can be treated without additional complications, and long-range order on a mean-field level.
We will in particular investigate systems with four electrons per site, where a local singlet competes with itinerant triplet excitations that can condense into magnetic order. Further, the competition of Hund's rule and spin-orbit coupling with crystal-field splitting leads to various phases which are realized in some iridium and ruthenium compounds.

TT 72.33 Wed 15:00 Poster B

The Kitaev-Heisenberg bilayer: a series expansion analysis — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Braunschweig, Germany

We study two layers of a honeycomb Kitaev spin-model, coupled by additional interlayer Heisenberg exchange J to form a bilayer. Focusing on the limit of strong interlayer coupling, we present results of zero temperature series expansion calculations, based on the flow equation method. Allowing for anisotropic intralayer exchange $J_{x,y,z}$ and two types of layer stackings, we calculate the evolution of the ground state energy and the dispersion of the elementary triplon excitations in powers of $J_{x,y,z}$ up 9th order. The stability of the dimer phase with respect to triplon gap closure will be analyzed, based on Padé approximants. Additionally we will compare our results with bond-operator theory using the Holstein-Primakoff approximation.

TT 72.34 Wed 15:00 Poster B

Coexistence of phase transitions and hysteresis near the onset of Bose-Einstein condensation — Michael Maennel[4] and •Klaus Morawetz[1,2,3] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Informatik DV,Petersstr. 14,04109 Leipzig, Germany

Multiple phases occurring in a Bose gas with finite-range interaction are investigated [2]. In the vicinity of the onset of Bose-Einstein condensation (BEC), the chemical potential and the pressure show a van der Waals-like behavior indicating a first-order phase transition for weak interactions like Hartree-Fock or Popov approximation. However, for strong interactions there remains a multivalued region for the T-matrix approximation even after the Maxwell construction, which is interpreted as a density hysteresis [1]. This unified treatment of normal and condensed phases becomes possible due to the recently found scheme to eliminate self-interactions in the T-matrix approximation, which allows one to calculate properties below and above the critical temperature [3,4].
[1] Phys. Rev. A 87 (2013) 053617

[2] New J. Phys. 12 (2010) 033013
[3] J. Stat. Phys. 143 (2011) 482
[4] Phys. Rev. B 84 (2011) 094529

TT 72.35 Wed 15:00 Poster B

Quantum transport and response with spin-orbit coupling in magnetic fields — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Electronic transport in spin-polarized systems with impurity interactions and spin-dependent meanfields is discussed. The coupled quantum kinetic equations for the scalar and spin components for SU(2) are derived with special consideration of spin-orbit coupling and magnetic fields. Linearizing, the RPA spin and density dynamical responses to electric fields (polarized light) are presented for arbitrary magnetic fields, Several known effects are described: spin-Hall, anomalous Hall and optical Hall effect, spin-heat coupling. New transport coefficients occur due to the selfconsistent precession direction. Clarifying the relative importance of meanfield and scattering correlations, new modes due to magnetic fields and spin-orbit coupling are found and terahertz out-of plane resonances are predicted.
[1] Europhysics Letters, 104 (2013) 27005
[2] Phys. Rev. **B 92** (2015) 245425
[3] errata Phys. Rev. **B 93** (2016) 239904(E)
[4] Phys. Rev. **B 92** (2015) 245426
[5] Phys. Rev. **B 94** (2016) 165415

TT 72.36 Wed 15:00 Poster B

Magnetic ground state of the cubic perovskite $Ba_3NiNb_2O_9$ — •Sh. Yamamoto[1], G. Aslan Cansever[2], T. Gottschall[1], M. Uhlarz[1], C. G. F. Blum[2], A. Wolter-Giraud[2], S. Aswartham[2], S. Wurmehl[2], T. Herrmannsdörfer[1], S. Seiro[2], B. Büchner[2], and J. Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]IFW-Dresden, Germany

We investigated the magnetic spin-1 perovskite $Ba_3NiNb_2O_9$ by means of complex ac susceptibility measurements at extreme sample conditions. $Ba_3NiNb_2O_9$ with cubic perovskite structure (Pm-3m) has a random occupation of Nb(66 %)/Ni(33 %) at the center of the cubic perovskite unit cell. Different from the isostoichiometric sister compound, $Ba_3NiNb_2O_9$ with P-3m1 structure which shows both uud-spin configuration and multiferroicity, the magnetic properties of the investigated system have not been studied below 2 K yet. For our single crystals, we observe a spin freezing transition at around 0.7 K. Furthermore, the peak of χ' is suppressed by applying an external dc field of 200 mT and χ" shows a sudden onset near the freezing temperature.

TT 72.37 Wed 15:00 Poster B

Magnetism of the effective spin-1/2 chain compound $Cs_2CoCl_{4-x}Br_x$ — •Severin Kopatz[1], Oliver Breunig[1], Daniel Brüning[1], Ladislav Bohatý[2], Petra Becker[2], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Kristallographie, Universität zu Köln, Germany

Cs_2CoCl_4 contains $CoCl_4$ tetrahedra, which form one-dimensional chains along the crystallographic b axis. The orbital groundstate of Co^{2+} ($3d^7$, S=3/2) is split by a crystal field anisotropy D into two doublets and an easy-plane anisotropy of the magnetization is established and a description as an effective spin-1/2 XXZ chain arises. By considering thermal as well as virtual excitations of higher crystal field states, we find that the spin chain is in the XY-limit with an anisotropy $J_z/J_\perp \approx 0.12$ substantially smaller than previously believed [1]. Below 300 mK antiferromagnetic order evolves and several new phases are induced in magnetic fields [2]. Cs_2CoCl_4 is isostructual to $Cs_2CuCl_{4-x}Br_x$ where site-selective doping was used to characterize quasi 2D quantum antiferromagnets with different degrees of magnetic frustration [3]. Here, we present specific-heat studies on bromine doped $Cs_2CoCl_{4-x}Br_x$ for different x. Funded by the DFG via CRC 1238 Projects A02 and B01.
[1] O. Breunig *et al.*, Phys. Rev. Lett. **111**, 187202 (2013)
[2] O. Breunig *et al.*, Phys. Rev. B **91**, 024423 (2015)
[3] P. T. Cong *et al.*, Phys. Rev. B **83**, 064425(2011)

TT 72.38 Wed 15:00 Poster B

Persistent spin dynamics in $NaCaCo_2F_7$ as evidenced by μSR — •Sascha Albert Bräuninger[1], Rajib Sarkar[1], Jason W. Krizan[2], Philip Materne[1], Chris Baines[3], Hubertus Luetkens[3], Robert J. Cava[2], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ 08544, USA — [3]Laboratory for Muon-Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen, Switzerland

The fluoride pyrochlore $NaCaCo_2F_7$ is a newly discovered frustrated pyrochlore with a frustration index of $f = \frac{|\theta_{CW}|}{T_f} \approx 56$. While recent NMR experiments on $NaCaCo_2F_7$ suggested a spin frozen state below 3 K, neutron scattering experiments on the other hand proposed XY like antiferromagnetic spin clusters at low energies. We present μSR studies on $NaCaCo_2F_7$. Present results indicate the slowing down of the magnetic spin fluctuation upon cooling towards the NMR and neutron scattering spin frozen state transition temperature of $T_{sf} \approx 3.0$ K. The μSR relaxation rate increases slightly below this frozen state, and remains constant down to 20 mK. In the μSR window there is no indication of static magnetism in $NaCaCo_2F_7$. In longitudinal field (100-4000 G) the relaxation rate do not vary indicating that the spin fluctuations are dynamic, and this is persistent even at $T \approx 20$ mK. While persistent spin dynamics (PSD) appears to be a generic feature of frustrated magnetic systems, it is not clear so far for the present case whether this is associated with quantum fluctuations, spin-liquid physics, or some other effect.

TT 72.39 Wed 15:00 Poster B

Frustrated magnetism in the Eu-based intermetallic system $EuIr_2P_2$ — •Diego Gaspar Franco and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Deutschland

Frustration in magnetic systems is a topic of strong current interest, since it can result in unusual ground states. The majority of studies on frustration in magnetic systems have been performed on insulating spin systems, while frustrated metallic systems remain largely unexplored. Interesting effects may be expected for the later case from the interplay between itinerant electrons and frustrated magnetic degrees of freedom.

$EuIr_2P_2$ was in an early work proposed to order ferromagnetically based on the positive Curie-Weiss temperature, estimated from the high-temperature susceptibility [1]. However, our recent measurements conclusively show that it orders antiferromagnetically at $T_{N1} = 5$ K, in spite of the positive Curie-Weiss temperature. Besides there is a second magnetic transition at $T_{N2} = 3$ K. The size of the specific heat anomaly at TN1 is small compared to other S=7/2 systems. Furthermore we observe a large tail in the specific heat above T_{N1} indicative of strong magnetic fluctuations. These effects point to a magnetic structure with a significant degree of frustration due to different competing magnetic interactions.
[1] C. Lux, et al., J. Alloys and Comp. 200 (1993) 135

TT 72.40 Wed 15:00 Poster B

Magnetic properties of single crystalline clinoatacamite — •Jan Lennart Winter[1], Leonie Heinze[1], Dirk Menzel[1], Stefan Süllow[1], Pascal Puphal[2], Cornelius Krellner[2], Manfred Reehuis[3], and Ralf Feyerherm[3] — [1]Institute for Condensed matter pyshics, TU Braunschweig, Germany — [2]Physikalisches Institut, Goehte-Universität Frankfurt, Germany — [3]HZB Materialien und Energie, Berlin, Germany

In recent years, clinoatacamite $Cu_2Cl(OH)_3$ has been studied in the context of geometric magnetic frustration in a quantum spin system. Only, previous research has been performed on synthetic powder samples, raising questions about sample quality and (residual) magnetic anisotropy [1,2]. Here, for the first time, we report a detailed investigation on single crystalline clinoatacamite by presenting studies of the magnetic susceptibility/magnetization and by means of neutron scattering. Based on these measurements we derive the magnetic phase diagram, revealing a complex magnetic behavior with a multitude of different (field induced) phases. We discuss our results with respect to the role of magnetic frustration on the properties of clinoatacamite.
[1] Zheng X.G., Kawae T., Kashitani Y., Li C. S., Tateiwa N., Takeda K., Yamada H., Xu C. N., and Ren Y., Phys. Rev. B **71** 052409 (2005)
[2] H. Morodomi, K. Ienaga, Y. Inagaki, T. Kawae, M. Hagiwara, and X. G. Zheng, J. Phys.: Conf. Ser. **200**, 032047 (2010).

TT 72.41 Wed 15:00 Poster B

Crystal growth in aqueous solution of Cs_2CuCl_4 and $Cs_2ZnCl_{4-x}Br_x$ using the evaporation method — •Susanna

Rongstock, Nazia Kaya, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, D-60438 Frankfurt

In recent years, Cs_2CuCl_4 and Cs_2CuBr_4 have been extensively investigated both experimentally and theoretically, as they represent model systems for quasi-2D triangular-lattice quantum antiferromagnets. They attracted much attention due to their unconventional magnetic properties resulting from the interplay of strong quantum fluctuations in reduced dimensions, geometrical frustration and effects of spin-lattice interactions close to the field-induced quantum critical point (QCP). In triangular antiferromagnetis the heat capacity is a capable measurement technique to study the magnetism. To obtain the magnetic contribution, it is necessary to subtract the phononic contribution, by measuring the heat capacity of $Cs_2ZnCl_{4-x}Br_x$. Due to the high number of possible phases different preliminary phases are built during the crystal growth of the Cs_2CuCl_4-crystal. Hence to develop a solution which creates a preliminary phase free growing of the crystals is of interest. In this contribution we will present the preliminary phase development of the Cs_2CuCl_4-crystal at 30°C in dependence to the pH-value and the resulting modification of the solution as well as the heat capacity measurements of the Cs_2ZnCl_4-crystal. Additionally we will present the crystal growth method and the structural analysis of both systems.

TT 72.42 Wed 15:00 Poster B

Kagome systems - The search for new quantum spin liquid candidates — •Katharina M. Zoch, Pascal Puphal, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main

Kagome systems serve as the ideal candidates to obtain a realization of a quantum spin liquid (QSL), a class of matter where the spins do strongly fluctuate down to lowest temperatures thus preventing order. Two-dimensional Cu-based quantum spin systems are very promising to understand their physics. Hence high-quality single crystals with minimal amount of disorder are essential to investigate the intrinsic properties of QSLs. Two closely related systems realizing a kagome lattice are $YCu_3(OH)_6Cl_3$ and $Y_3Cu_9(OH)_{19}Cl_8$ which both show strong frustration. However, while having a similar structure the magnetic ground state is different [1]. This poster addresses the synthesis and properties of these and other kagome compounds analyzed with diffraction, VSM and specific heat.

[1] P.Puphal et al. J. Mater. Chem. C 5 (2017) 2629

TT 72.43 Wed 15:00 Poster B

Exploring the magnetic phase diagram of a metal-organic S = 1 triangular spin system. — •Sumanta Chattopadhyay[1], Thomas Herrmannsdörfer[1], Sudipta Kanungo[3], Sergei Zvyagin[1], Marc Uhlarz[1], Kaustuv Manna[4], Walter Schnelle[4], Jhuma Sannigrahi[5], Joachim Wosnitza[1], and Ranjan Patra[2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Panjab University, Chandigarh, India — [3]Department of Physics, IIEST, Howrah, India — [4]Max Planck Institute for Chemical Physics of Solids Dresden, Germany — [5]ISIS Facility, Rutherford Appleton Laboratory, Didcot, OX11 0QX, U.K.

We report on magnetic properties of a novel metal-organic S = 1 antiferromagnetic triangular spin compound with isolated Ni2+ triangles entitled as BHAP-Ni3. Specific heat measurements reflect an onset of magnetic correlation at low temperatures without any long-range order down to 300 mK, indicating the presence of an unusual magnetic ground state. ESR measurements performed at 1.5 K advocate this ground state to be a gapped one. Field-dependent magnetization measured on the single crystal shows anisotropic behavior with field applied parallel and perpendicular to the triangle plane. However, a clear plateau-like region is seen in both directions above 8 T which corresponds to half of the fully polarized value of Ni2+ moment. The presence of such half-magnetization plateau is quite unusual in the family of triangular magnets. High-field magnetization measurements using pulsed magnet show another field-induced plateau above 30 T corresponding to the fully polarized state of S = 1 triangles.

TT 72.44 Wed 15:00 Poster B

Magnetic and thermodynamic characterization of single crystals of $La_2MM'O_6$ (M = Mg, Zn, Co and M'=Ru, Ir) — •Randirley Beltrán[1], Gaël Bastien[1], Sebastian Gass[1], Anja U.B. Wolter[1], Ryan Morrow[1], Michael Vogl[1], Mihai Sturza[1], Sabine Wurmehl[1], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW-Dresden, Germany — [2]TU Dresden, Germany

In compounds with 4*d* and 5*d* transition metal oxides, among them the double perovskites $A_2MM'O_6$, strong magnetic frustration can be expected due to different origins: competing magnetic interactions and strong spin-orbit coupling. The arrangement of MO_6 and $M'O_6$ corner-sharing octahedra provide two (magnetic) sub-lattices that results in a variety of magnetic properties related with the competing exchange interactions. For nonmagnetic M ions, the fcc lattice structure of the magnetic M' ions has been theoretically proposed for hosting Kitaev interactions. In this work we probe the magnetic and thermodynamic properties of the double perovskite single crystals $La_2MM'O_6$ with M = Mg, Zn, Co and M' = Ir, Ru. We study the magnetic susceptibility and specific heat as function of different parameters, such as temperatue, magnetic field and orientation. Additionally, we use the application of hydrostatic pressure in the mixed 3*d*-5*d* compound La_2CoIrO_6 to tune the magnetic ground state of this system, because pressure leads to changes of the magnetic exchange couplings.

TT 72.45 Wed 15:00 Poster B

A SUSY-connection between classical spin spirals and free fermions — •Jan Attig[1], Krishanu Roy Chowdhury[2], Michael Lawler[2], and Simon Trebst[1] — [1]University of Cologne — [2]Binghamton University / Cornell University

The formation of coplanar spin spirals is a common motif in the magnetic ordering of many frustrated magnets. For classical antiferromagnets, geometric frustration can lead to a massively degenerate ground state manifold of spirals whose propagation vectors can be described, depending on the lattice geometry, by points (triangular), lines (fcc), surfaces (frustrated diamond) or completely flat bands (pyrochlore). Here we demonstrate an exact mathematical correspondence of these spiral manifolds of classical antiferromagnets with the Fermi surfaces of free-fermion band structures. We provide an explicit lattice construction relating the frustrated spin model to a corresponding free-fermion tight-binding model. We discuss implications of topological band structures in the fermionic system to the corresponding classical spin system and further expand this mapping by employing concepts from super symmetric quantum mechanics to extent the present work for quantum spin systems.

TT 72.46 Wed 15:00 Poster B

Frustrated magnetism in the Kondo lattice on a zig-zag ladder — •Lena Woelk, Matthias Peschke, and Michael Potthoff — I. Institut für Theoretische Physik

We study the magnetic phase diagram of the Kondo lattice model on the half-filled zig-zag chain as a function of the exchange coupling J and the hopping amplitudes t, t' in both the classical-spin and the quantum-spin case using a quantum-classical hybrid approach and the density matrix renormalization group (DMRG).

The competition between RKKY, superexchange, and the geometric frustration yields a complex phase diagram: We find multiple spiral phases, an antiferromagnetic phase as well as a small ferromagnetic region. In both the classical- and the quantum-spin case, we also find an extended region with a dimerized ground state, which consists of alternating ferro- and antiferromagnetic spin correlations along the rungs of the ladder. This alleviates the geometric frustration and is a precursor of quasi-long-range magnetic order.

The strong coupling limit $J \gg t$ can be described with perturbation theory. The spin correlations in both the classical- and the quantum-spin case are captured by an effective classical Heisenberg model. In the weak coupling limit one expects the spin correlations to be governed by RKKY theory, this is checked against our results.

TT 72.47 Wed 15:00 Poster B

Spin liquid behaviour in the disordered double perovskite $BaTi_{1/2}Mn_{1/2}O_3$ — M. R. Cantarino[3], •R. Sarkar[1], R.S. De Freitas[3], H. Luetkens[2], C. Baines[2], R. Lora-Serrano[4], R.P. Amaral[4], S. Brauninger[1], V. Grinenko[1], H.-H. Klauss[1], E. C. Andrade[5], and F. A. Garcia[3] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, PSI, 5232 Villigen PSI, Switzerland — [3]IFUSP, Univ. de São Paulo, 05508-090, São Paulo-SP, Brazil — [4]Univ. Fed. de Uberândia, Instituto de Física, 38400-902, Uberlrândia-MG, Brazil — [5]Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 369, São Carlos, SP, 13560-970, Brazil.

We present bulk susceptibility, heat- capacity and μSR experiments of the disordered double perovskite $BaTi_{1/2}Mn_{1/2}O_3$. Heat capacity

investigations down to $T = 0.1$ K and in magnetic fields up to 9 T exhibits a field dependent broad anomaly around $T = 3 - 7$ K, and no long range ordering. Macroscopic magnetic properties, measured down to $T = 0.5$ K, do not display as well any sign for phase transition. The zero field (ZF) and longitudinal field dependence μ^+ time spectra shows the absence of any static magnetism down to 20 mK. However, ZF μ^+ relaxation rate λ display a steep increase in the T interval $1.5 < T < 10$ K and levels up as a constant value indicating a correlated fluctuating ground state. Our experimental data and analysis suggests that $BaTi_{1/2}Mn_{1/2}O_3$ is a suitable candidate to host a spin liquid ground state.

TT 72.48 Wed 15:00 Poster B

Magnetisation of lithium nitridometalates and magnetite nanoparticles upon electrochemical cycling — •Elisa Thauer[1], Michael Richter[1], Manuel Fix[2], Anton Jesche[2], and Rüdiger Klingeler[1,3] — [1]Kirchhoff Institute for Physics,, Heidelberg University, 69120 Heidelberg, Germany — [2]EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany — [3]Center for Advanced Materials, 69120 Heidelberg University, Heidelberg, Germany

We report *in-situ* and *ex-situ* studies of the magnetic properties of lithium nitridometalates and magnetite nanoparticles upon electrochemical treatment. In $Li_2Li_{1-x}M_xN$ with M = Fe or Ni, the effect of delithiation, i.e. electrochemical change of the valence of the transition metal ions, on the magnetic properties was studied by means of *ex-situ* SQUID magnetometry. In case of $Li_{2.7}Fe_{0.3}N$ the initial hard magnetic ground state is suppressed by delithiation. In addition, a re-usable *in-situ* electrochemical cell was designed for operation in the SQUID magnetometer. Studies on Fe_3O_4 nanoparticles prove significant changes of the magnetisation upon electrochemical lithiation and delithiation.

TT 72.49 Wed 15:00 Poster B

Electron spin resonance studies on the frustrated tripod-Kagome material $Mg_2Gd_3Sb_3O_{14}$ — •Christoph Wellm[1,2], Julian Zeisner[1,2], Mihai Sturza[2], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper-und Materialphysik, TU Dresden, D-01062

As an example of a class of geometrically frustrated magnetic systems, the so-called tripod Kagome materials consisting of a modified pyrochlore lattice with nonmagnetic interlayers have been suggested as an interesting target of experimental investigation. Since the Kagome planes in these compounds are well separated from each other, two-dimensional magnetic behavior is expected. In our work we performed high-field electron spin resonance measurements on a powder sample of $Mg_2Gd_3Sb_3O_{14}$, a representative of a classical Heisenberg magnet, in which the magnetic Gd^{3+} centres are devoid of spin-orbit coupling. Measurements were conducted over a frequency range of 70-420 GHz and temperatures ranging from 3-50 K. The Gaussian shape of the spectra is consistent with a model where dipolar spin-spin interaction plays a dominant role, while the growing asymmetry of the lineshape upon decrease of temperature signifies an effective internal field building up, an indication of increasing short-range spin-spin-correlations. Furthermore, temperature dependent critical broadening of the linewidth and increase of the internal field strength provide insights into the dimensionality of the spin-spin correlations.

TT 72.50 Wed 15:00 Poster B

Probing the Kitaev-Heisenberg material α-$RuCl_3$ via field-dependent microwave absorption — •Christoph Wellm[1,2], Julian Zeisner[1,2], Alexey Alfonsov[2], Anja Wolter[2], Maria Roslova[3], Anna Isaeva[3], Thomas Doert[3], Matthias Vojta[4], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01171 — [2]Institut für Festkörper-und Materialphysik, TU Dresden, D-01062 — [3]Fachrichtung Chemie und Lebensmittelchemie, TU Dresden, D-01062 — [4]Institut für Theoretische Physik, TU Dresden, D-01062

Topologically ordered states of matter have recently gained much attention due to their novel physical properties, the signatures of which can be experimentally probed. A prime example is the spin liquid realized in the Kitaev honeycomb lattice compass model, where fractionalization of particles leads to broad continuum-like features in the magnetic response. We will present the high-field microwave absorption results on the Mott-Hubbard-insulating material α-$RuCl_3$ which is, due to its structure and strong spin-orbit coupling, a promising candidate for the realization of Kitaev physics. Measurements on a single-crystal were conducted over a frequency range of $\nu = 70$-660 GHz at temperatures ranging from 3-30 K. Strikingly, in addition to previously observed conventional gapped magnon modes, we find a highly unusual broad continuum characteristic of fractionalization which extends to energies below the lowest sharp mode and to temperatures significantly higher than the ordering temperature.

TT 72.51 Wed 15:00 Poster B

Interaction effects on surface flat bands in 3D Kitaev spin liquids — •Christoph Berke and Simon Trebst — Institut für theoretische Physik, Universität zu Köln

Frustrated quantum magnets can give rise to unconventional spin-liquid ground states. Paradigmatic examples are two- and three-dimensional Kitaev systems that exhibit gapless spin liquids which are best described as Majorana metals that, depending on the underlying lattice structure, exhibit Fermi surfaces, nodal lines or Weyl nodes. Here we will discuss the physics of nodal-line Kitaev spin liquids, which – in contrast to electronic nodal-line semimetals – are protected by the particle-hole symmetry inherent to Majorana fermions. Our interest is particularly on the flat-band surface states that accompany these bulk nodal lines. We explore the stability of these highly degenerate bands in the presence of additional interactions.

TT 72.52 Wed 15:00 Poster B

Thermodynamics of Kitaev magnets — •Bahareh Ghannad and Simon Trebst — University Of Cologne

Kitaev spin models are prototypical frustrated magnets that exhibit low-temperature spin liquid physics. This is true independent of whether the constituent spin degrees of freedom are classical O(3) Heisenberg spins or quantum SU(2) spin-1/2 spins. Here, we will discuss thermodynamic signatures of a variety of Kitaev spin models for different lattice geometries and contrast them for the classical and quantum case. Of particular interest are two-spin and four-spin correlation functions that reveal the nature of the spin liquid regime. We report results from both analytical approaches and large-scale numerical Monte Carlo simulations.

TT 72.53 Wed 15:00 Poster B

Majorana zero modes in the Kitaev honeycomb model — •Daniel Otten, Ananda Roy, and Fabian Hassler — JARA- Institute for Quantum Information, RWTH Aachen University, D- 52056 Aachen, Germany

Kitaev's honeycomb model is a quantum spin liquid that gives rise to an emergent static $\mathbb{Z}_2$ gauge field coupled to Majorana fermions. In presence of an applied external magnetic field, the system is, dependent on the choice of interaction strength, in a gapped, non-abelian phase. In this phase, the vortex excitations of the emergent $\mathbb{Z}_2$ gauge field have Majorana zero modes bound to them. We investigate the properties of these Majorana zero modes. Using Jordan-Wigner transformation, we map the effective Hamiltonian to that of a chiral p-wave superconductor. We analytically calculate the wave functions of the Majorana zero modes in the continuum limit and the energy splitting that arises when two vortices approach each other. Furthermore, to understand the implications of the zero modes in the original spin model, we calculate the spin-spin correlator and the dynamical structure factor in presence of these vortices. These results are relevant for possible experimental observations and characterizations of the Majorana zero modes in systems that are dominated by the interaction of the Kitaev honeycomb model.

TT 72.54 Wed 15:00 Poster B

Disorder and Correlations in 3D Kitaev Models — •Kevin O'Brien[1], Maria Hermanns[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden

Kitaev's honeycomb model is an example of an exactly solvable interacting spin-1/2 model with exchange frustration, providing theorists with the rare opportunity to study the physics of spin fractionalization in its quantum spin liquid groundstate with full analytical control. In their groundstate, the spin-1/2 moments fractionalize into a static, gapped Z2 gauge field as well as into fermionic excitations which may be gapped or gapless. The nature of the gapless phase depends both on the dimension of the underlying lattice and on the projective nature of certain discrete symmetries. The resulting nodal structure of the

fermionic excitations ranges from nodal lines to Dirac nodes in 2D and from full Fermi surfaces to nodal lines and even Dirac/Weyl nodes in 3D. While spin-spin correlations in the Kitaev model are short-ranged in general, there are certain long-ranged four-spin correlations which are sensitive to the nodal structure of the fermionic excitations. In this work we investigate the nature in which these correlation functions are determined by the gapless fermionic excitations. Additionally, we examine the role which disordering of the Z2 gauge field plays in altering these correlations. Finally, we explore the connection between the gauge-disordered Kitaev spin liquid and finite temperature calculations.

TT 72.55 Wed 15:00 Poster B

Thermodynamics of a gauge-frustrated Kitaev spin liquid — •Tim Eschmann[1], Petr A. Mishchenko[2], Yasuyuki Kato[2], Yukitoshi Motome[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Applied Physics, University of Tokyo

Kitaev spin models are prototypical frustrated magnets in which the spin degrees of freedom fractionalize and the emergent spin liquid ground state can be described in terms of Majorana fermions coupled to a $\mathbb{Z}_2$ gauge field. It is by now well known that varying the underlying lattice structure, these spin liquids can be described as Majorana metals with a topological band structure that includes the formation of Dirac or Weyl nodes, nodal lines, or entire Majorana Fermi surfaces. Here our focus will be on the physics of the concurrently forming $\mathbb{Z}_2$ gauge field. Typically, this (static) gauge field orders at low temperatures, with a finite-temperature (inverted Ising) transition occurring in three-dimensional settings. We will discuss an explicit example that goes beyond this paradigmatic situation where the gauge field is found to be subject to geometric frustration, the thermal ordering transition is suppressed, and a residual zero-temperature entropy arises. We discuss a variety of thermodynamic signatures of this physics obtained from large-scale, sign-free quantum Monte Carlo simulations of the underlying Kitaev model.

TT 72.56 Wed 15:00 Poster B

Splitting of the magnetic monopole excitation energy in spin ice — •Jacob Hornung[1,2], Tino Gottschall[1], Mathis Antlauf[3], Lars Opherden[1,2], Thomas Herrmannsdörfer[1], and Jochen Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik,TU Dresden, Germany — [3]Institut für Anorganische Chemie, TU Bergakademie Freiberg, Germany

We present a new model for the magnetic monopole excitation process in spin-ice systems. In this approach, we include the interactions of the electric dipole moments which where priviously predicted to emerge in consequence of the formation of magnetic monopoles. By that, the model allows for describing the temperature-dependent spin relaxation time. We compare this relaxation-time behavior with data received for the three spin-ice systems $Dy_2Sn_2O_7$, $Dy_2Ti_2O_7$ and $Dy_2Ge_2O_7$. By that we also determine the magnitude of their electrical dipole interactions.

TT 72.57 Wed 15:00 Poster B

ESR on the $S = 1/2$ triangular magnet $NaYbS_2$ — •Jörg Sichelschmidt[1], Michael Baenitz[1], Philipp Schlender[2], and Thomas Doert[2] — [1]MPI for Chemical Physics of Solids, Dresden — [2]TU Dresden, Dept. of Chemistry and Food Chemistry

$NaYbS_2$ is one of a few spin 1/2 triangular quantum magnets for which a quantum spin-liquid picture is invoked. It has a delafossite structure with a planar triangular spin arrangement which leads to a low-temperature magnetism determined by exchange frustration effects. The crystal electric field (CEF) in $NaYbS_2$ allows an effective spin $S = 1/2$ in contrast to other delafossites materials which contain Cr^{3+} ($S = 3/2$), for instance. There, extensive electron spin resonance (ESR) measurements of Cr^{3+} could verify a Z_2 ordering scenario for triangular Heisenberg antiferromagnets [1].

We present first results of the Yb^{3+}-ESR in single-crystalline $NaYbS_2$. Well-defined spectra could be only observed for temperatures below $\approx$ 70 K because of the increasing influence of the relaxation via the higher CEF levels of Yb^{3+} towards higher temperatures. The spectra show a large anisotropy, as determined by the CEF, similar to what has been observed in other Yb-systems [2]. Towards low temperatures we observed a moderate increase of the linewidth. This may indicate a spin-liquid state in agreement with NMR results where the increase of the spin-spin relaxation towards low temperatures is discussed as a signature of a quantum spin-liquid.

[1] M. Hemmida et al., J. Phys. Soc. Jpn. 80, 053707 (2011)
[2] A. Kutuzov et al., J. Phys. Cond. Mat. 20, 455208 (2008)

TT 72.58 Wed 15:00 Poster B

From Kitaev exchange towards quantum disorder: A pressure dependent optical study on α-$RuCl_3$ — •Tobias Biesner[1], Weiwu Li[1], Yohei Saito[1], Andrej Pustogow[1], Martin Dressel[1], Anja Wolter-Giraud[2], Bernd Büchner[2], Maria Roslova[3], and Thomas Doert[3] — [1]1. Physikalische Institut, Universität Stuttgart, Germany — [2]IFW-Dresden, Germany — [3]Dept. Chem. and Food Chem., TU-Dresden, Germany

The j_{eff}=1/2 Mott insulator α-$RuCl_3$ is a promising Kitaev quantum spin liquid candidate due to its layered, almost ideal honeycomb lattice with a high degree of frustration. While the pure Kitaev physics is commonly hampered by a magnetic state, external pressure could suppress antiferromagnetic order.

We present a comprehensive study of the optical properties of α-$RuCl_3$ powder and single crystals by infrared spectroscopy in a broad range of frequencies down to low temperatures and under hydrostatic pressures in order to elucidate a pressure-induced new quantum state. Due to the large energy scales of α-$RuCl_3$, moderate pressures ($p < 1.8$ GPa) do not significantly affect the Mott insulating state. However, afm order is suppressed by pressure resulting in a transition to a quantum spin liquid like state and unveiling pure Mott physics. In the optical response we see signatures of enhanced symmetric anisotropic exchange, and evolution of the band structure; providing evidence for a strong coupling of electronic and magnetic correlations. The potential of optical studies for pressure-induced exotic quantum states is shown for α-$RuCl_3$ and discussed for other Kitaev candidates.

TT 72.59 Wed 15:00 Poster B

Comparative thermal expansion study on organic quantum-spin-liquid-candidate systems — •S. Hartmann[1], R. S. Manna[2], J. Schlueter[3], Y. Yoshida[4], and M. Lang[1] — [1]Physikalisches Institut, SFB/TR 49, Goethe-Universität Frankfurt, Germany — [2]Dept. of Physics, Indian Institute of Technology Tirupati, India — [3]Div. of Materials Research, National Science Foundation, Arlington, Virginia, USA — [4]Dept. of Chemistry, Kyoto University, Japan

The search for the realization of a quantum spin-liquid (QSL) is a major concern for condensed matter physicists since its proposal in 1973. The entangled QSL ground state lacks magnetic ordering down to lowest temperatures where spins continue to fluctuate even at $T = 0$ K [1]. One way to experimentally realize a QSL is magnetic frustration of geometric origin, inherent to the quasi 2D-triangular lattice of the organic charge-transfer salts κ-(BEDT-TTF)$_2X$. We present a comparative study of ultra-high-resolution thermal expansion measurements on the QSL-candidates $X = Cu_2(CN)_3$ and $X = Ag_2(CN)_3$. The X= $Cu_2(CN)_3$ system shows a mysterious anomaly around 6 K, frequently assigned to a QSL instability, the origin of which is still an open question. The shape and size of this effect are attributed to a second-order phase transition [2]. In contrast, we do not find any indications for a phase transition for X= $Ag_2(CN)_3$. In addition, we discuss effects of applying a magnetic field and pay attention to sample-to-sample variations in the materials' low-temperature lattice effects.

[1] Balents, Nature 2010
[2] Manna et al., PRL 2010

TT 72.60 Wed 15:00 Poster B

Phase diagram of chiral antiferromagnets — •Benjamin Wolba[1], Sebastian Mühlbauer[2], and Markus Garst[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

Chiral antiferromagnets are characterized by a Dyzaloshinskii-Moriya interaction that stabilizes spatially modulated phases of the staggered order parameter. In the framework of a Ginzburg-Landau theory, we determine the phase diagram as a function of temperature and magnetic field. In zero magnetic field, a phase with spiral antiferromagnetic order is present. A finite field naturally leads to an easy-plane anisotropy that induces a spinflop transition into a topological phase consisting of a square-lattice of vortices and antivortices. We discuss the relevance of our results for the chiral antiferromagnet $Ba_2CuGe_2O_7$.

TT 72.61 Wed 15:00 Poster B

Interface-driven Skyrmions in $SrRuO_3$ based heterostructures — •Sven Esser[1], Sebastian Esser[1], Anton Jesche[1], Vladimir Roddatis[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany — [2]Institut für Materialphysik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Formation of Néel-type skyrmions at oxide interfaces is supported by Dzyaloshinskii-Moriya (DM) interaction through introducing a break of inversion symmetry. Recently artificial perovskite bilayers of the ferromagnetic metal $SrRuO_3$ (SRO) and spin-orbit semimetal $SrIrO_3$ (SIO) have been proposed to host two-dimensional Néel-type skyrmions [1].

By using a metal-organic aerosol deposition technique we have grown $[(SrIrO_3)_2/(SrRuO_3)_5]_k$ bilayers with $k = 1, 5, 10$ repetitions on cubic (001)-oriented $SrTiO_3$ substrate to investigate the interface induced changes of the electronic and magnetic properties. The fully epitaxially strained state of the thin films was verified by X-ray diffraction patterns in combination with reciprocal space mapping and TEM images. Measurement of the in-plane magnetization indicate a relation to the number of interfaces between SRO and SIO layers. A contribution of the topological Hall effect to the Hall resistance can be observed near 80K, which may be a hint for the formation of skyrmions.

[1] J. Matsuno *et al.*, Science Adv. **2** (2016) e1600304.

TT 72.62 Wed 15:00 Poster B

High-frequency EPR and magnetization studies on azopyridine-bridged transition metal dinuclear complexes — •Felix Spathelf[1], Marco Hoffmann[1], Changhyun Koo[1], Roland Bischoff[2], Hans-Jörg Krüger[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Faculty of Chemistry, TU Kaiserslautern, Kaiserslautern, Germany

The magnetic properties of azopyridine-bridged transition metal dinuclear complexes $([\{M(L-N_4Me_2)\}_2(\mu-apy^{2-})](SbF_6)_2$ with $M = Fe^{2+}, Cu^{2+}$) are studied by means of high-frequency electron paramagnetic resonance (HF-EPR) and magnetization measurements. Magnetization data show that the Cu_2-complex exhibits a singlet ground state associated with an intra-dimer coupling of $J = 155$ K. Accordingly, at low temperatures we observe no EPR resonances up to 700 GHz. In contrast, magnetic susceptibility of the Fe_2-complex obeys a Curie-Weiss-like behaviour at $T \leq 80$ K. Upon further heating, the data imply spin crossover from the $S = 2$ to a $S = 4$ state. Furthermore, we observe weak antiferromagnetic coupling of the Fe-ions ($J = (1.0 \pm 0.5)$ K). The HF-EPR spectra at $T = 2$ K show two resonance branches ω_1 and ω_2 with effective g-factors of 9.8 ± 0.4 and 1.986 ± 0.008, respectively, and no zero-field splitting. While the ω_1-branch can be attributed to forbidden dimer transitions, the origin of ω_2 is yet unclear. It may be either due to intrinsic transitions or result from paramagnetic impurities.

TT 72.63 Wed 15:00 Poster B

high frequency EPR studies on lanthanide monomers in different ligand structures — •sajedeh shahbazi[1], johannes werner[1], julian butscher[1], changhyun koo[1], asha roberts[2], peter comba[2], denis gorbunov[3], and rüdiger klingeler[1] — [1]Kirshhoff-Institut für Physik, Universität Heidelberg, Heidelberg, Germany — [2]Anorganisch-Chemisches Institut, Universität Heidelberg, Heidelberg, Germany — [3]Hochfeld-Magnetlabor Dresden, Institution Helmholtz-Zentrum, Dresden, Germany

The magnetic properties of lanthanide monomers (Ln=Dy(III) and Tb(III)) in two different ligand structures but similar coordination geometries ([Ln(x-1,2-HOPO)$_2$]PyH (x = 2Li,5Li)) are reported in order to investigate ligand field effects. The ground states of the complexes were estimated by using high-field electron paramagnetic resonance (HF-EPR) and pulsed-field magnetization studies. The slopes of the resonance branches seen in the HF-EPR data on the Tb-complexes correspond to g-factors much larger than 2 implying a forbidden transition. Based on the HF-EPR data and the saturated magnetization value at $B = 58$ T, the ground states of the Tb-complexes are derived. Finite zero-field splitting observed in [Tb(III)(2Li-1,2-HOPO)$_2$]PyH indicates lifting of the degeneracy in a non-Kramers doublet. From the obtained experimental results, the ligand field effect on the ground state in the studied complexes is discussed.

TT 72.64 Wed 15:00 Poster B

Thermal and thermal-Hall conductivity study of $SrCu_2(BO_3)_2$ — •Stevan Arsenijević[1], Hanna Dabkowska[2], Bruce Gaulin[2], Raivo Stern[3], and Jochen Wosnitza[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Brockhouse Institute for Materials Research, McMaster University, Hamilton, Canada — [3]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present measurements of the thermal and the thermal-Hall conductivity as a function of temperature and magnetic field in the two-dimensional dimer spin system $SrCu_2(BO_3)_2$. The thermal conductivity in zero magnetic field shows a pronounced peak around 4 K which is ascribed to a spin-gap opening. The low-temperature maximum is strongly suppressed by the application of magnetic field. This result implies that the majority of heat is conducted by phonons which interact with the magnetic excitations. Furthermore, a theoretical study predicted a strong thermal Hall signature due to anisotropies originating from the Dzyaloshinskii-Moriya interactions which lead to a topological character of triplon excitations [1]. Our detailed experimental investigation did not reveal such effect disproving the existence of topological transitions in the triplon band structure.

[1] J. Romhányi, K. Penc, R. Ganesh, Nat. Commun. **6** (2015) 6805

TT 72.65 Wed 15:00 Poster B

Magnetic and Structural Properties of the Trirutile-type 1D Heisenberg Antiferromagnet $CuTa_2O_6$ — •A. Golubev[1], R. E. Dinnebier[1], A. Schulz[1], R.K. Kremer[1], H. Langbein[2], A. Senyshyn[3], J. M. Law[4], T. Hansen[5], H.-J Koo[6], and M.-H. Whangbo[7] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institut für Anorganische Chemie der Technischen Universität Dresden, Dresden, Germany — [3]Forschungsneutronenquelle Heinz Maier-Leibnitz (FRM II), Garching, Germany — [4]Dresden High Magnetic Field Laboratory (HLD), Dresden, Germany — [5]Institut Laue-Langevin, Grenoble, France — [6]Kyung Hee University, Seoul, Republic of Korea — [7]North Carolina State University, North Carolina, USA

$CuTa_2O_6$ crystallizes with a monoclinically distorted trirutile structure type. By detailed high temperature neutron and x-ray powder diffraction measurements we mapped the structural phase transition to the tetragonal trirutile structure-type at 500 K. The structural phase transition was ascertained by Raman scattering experiments. ab-initio GGA+U density functional calculations of the spin exchange parameters, magnetic susceptibility and isothermal magnetization measurements constitute $CuTa_2O_6$ as one-dimensional Heisenberg quantum antiferromagnet with predominant nearest-neighbor spin exchange interaction $J - nn$ 50 K. Long-range magnetic order was not detected down to 0.4K.

TT 72.66 Wed 15:00 Poster B

NMR of the two-dimensional $S = 1/2$ Heisenberg antiferromagnet CuPOF — •D. Dmytriieva[1,2], Z. T. Zhang[1], M. Uhlarz[1], C. P. Landee[3], J. Wosnitza[1,2], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA

The metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF) is a molecular-based analog of the two-dimensional quantum $S = \frac{1}{2}$ Heisenberg antiferromagnet (2D QHAF) with well-isolated Cu(pz) layers and a very low $k_BT_N/J = 0.21$ ratio ($J/k_B = 6.8$ K, $T_N = 1.38$ K). We present a focus study of the low-temperature phase transition to long-range order performed via ^{1}H and ^{31}P nuclear magnetic resonance (NMR), as well as high-field magnetometry. A low-temperature minimum of the temperature-dependent local and uniform magnetizations at T_{min} indicates a presence of the magnetic order. Within the ordered state, a splitting of the ^{1}H NMR spectra reveals commensurate AF order, presumably of checkerboard type. The phase transition, manifested as a sharp maximum of the temperature-dependent ^{31}P nuclear spin-lattice relaxation rate $1/T_1$, occurs at temperatures slightly lower than T_{min}, indicating an easy-plane anisotropy as well as a crossover between isotropic and XY behavior.

TT 72.67 Wed 15:00 Poster B

Superposition of FM and AFM Cu(II) spin-1/2 chains in $BaAg_2Cu[VO_4]_2$ studied by magnetic resonance spectroscopies — •Y. Krupskaya[1], M. Schäpers[1], A.U.B. Wolter[1], H.-J. Grafe[1], E. Vavilova[1,2], A. Möller[3], B. Büchner[1], and V. Kataev[1] — [1]IFW Dresden, Dresden, Germany — [2]Zavoisky Physical-

Technical Institute, Kazan, Russia — [3]Johannes Gutenberg University Mainz, Mainz, Germany

$BaAg_2Cu[VO_4]_2$ contains Cu(II) S=1/2 ions in a distorted two-dimensional triangular lattice interconnected via non-magnetic $[VO_4]$ entities. The theoretical analysis and the magnetization measurements show that the magnetism of this compound is determined by a superposition of ferromagnetic (FM) and antiferromagnetic (AFM) uniform spin-1/2 chains. In order to probe the local magnetic properties we have performed the study of $BaAg_2Cu[VO_4]_2$ by High-Field/Frequency Electron Spin Resonance (HF-ESR) and Nuclear Magnetic Resonance (NMR) spectroscopies. In the HF-ESR measurements, we observe an anisotropic ESR spectrum typical for the Cu(II) ions and determine the g-tensor. The detailed analysis shows that the shape of the low-temperature ESR spectrum is defined by the development of the anisotropic internal fields corresponding to FM and AFM correlations in the respective Cu spin chains. The NMR study has identified the signals from ^{51}V nuclei in the two types of chains, which strongly supports the ESR results. Altogether, the HF-ESR and NMR results confirm theoretical predictions of the superposition of FM and AFM Cu(II) spin-1/2 chains in $BaAg_2Cu[VO_4]_2$.

TT 72.68 Wed 15:00 Poster B

High-Pressure Transport Studies in 2H-$NbSe_2$ — •Owen Moulding and Sven Friedemann — University of Bristol, Bristol, UK

The transition metal dichalcogenide 2H-$NbSe_2$ has well-documented charge density wave (CDW) and superconducting transitions at 33K and 7K at ambient pressure. The CDW transition is suppressed under high pressure and is absent beyond the quantum critical point (QCP) at 4.6 GPa [1]. The effect of this QCP on superconductivity is of great interest and stimulates discussions on the relation between superconductivity and the CDW order. So far, resistivity and X-ray measurements have explored the vicinity of this QCP, and they indicate only a weak relation between superconductivity and the CDW: either a weak competition between CDW order and superconductivity or a weak promotion of superconductivity by fluctuations at the CDW QCP. Here, we present high-pressure Hall effect measurements as a clear probe of the CDW order. We use patterned moissanite anvil cells for pressures well beyond the QCP.
[1] Feng, Y., et al. PNAS, **109**, 7224 (2012).

TT 72.69 Wed 15:00 Poster B

Resistance peak at the superconducting transition of $SrTiO_3/Al_2O_{3-x}$-heterostructures — •Daniel Arnold, Roland Schäfer, Dirk Fuchs, and Karsten Wolff — Karlsruhe Institute of Technology, Institute for Solid State Physics

When an anisotropic system undergoes a superconducting transition the resistance is often peaking before it drops to zero. This effect is well documented for low- and high-T_c materials.

We have studied the resistive transition in the superconducting interface of (001)-oriented $SrTiO_3$ and Al_2O_{3-x} as a function of temperature and magnetic field using a Van-der-Pauw sample geometry. Our sample shows a distinct difference for the two orthogonal directions of current flow indicating a preferential direction for supercurrents. In one of the direction an especially large peak effect is present.

We discuss our experimental data by comparing it to the results of numerical simulations and analytical calculations.

TT 72.70 Wed 15:00 Poster B

Investigation of LAO/STO nanostructures — •Mithun S Prasad[1], Mohzin Minhas[1], Alexander Müller[1], and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]Interdisziplinäres Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany

The high-mobility two-dimensional electron gas (2DEG) confined at the interface of two insulating complex oxides, $LAlO_3$ (LAO) and $SrTiO_3$ (STO) provides new opportunities to explore nano electronic devices. Recently our group has developed an industry compatible nano patterning technique [1] for the LAO/STO interface. Some recent studies on this interface have revealed that at low temperature the current transport in LAO/STO heterostructures is mainly through the domain boundaries which results in the formation of numerous current carrying filaments [2]. This fact also results massive changes in conductivity when a few filaments are confined in nanostructures. We investigate the dependence of the effect on the orientation of nanostructures with respect to the crystalline structure of the substrate at different temperatures and under application of a back-gate voltage.

TT 72.71 Wed 15:00 Poster B

Tuning the electric interface properties of amorphous $AlO_x/SrTiO_3$ interfaces — •Berengar Leikert[1], Judith Gabel[1], Martin Stübinger[1], Philipp Scheiderer[1], Matthias Schmitt[1], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM) — [2]Diamond Light Source, Beamline I09, Didcot, England

Two dimensional electron systems (2DESs) at the interfaces of oxide heterostructures are considered a promising platform for future microelectronic technology which may utilize the rich electronic behavior of transition metal oxides. A simple and cost-effective method to create a 2DES is to deposit Al on the surface of $SrTiO_3$. It reduces the first oxide layers and leads to an n-doping of the oxide surface. By changing the Al redox potential via growth in oxygen atmosphere we can tune the electronic interface properties, as probed by hard x-ray photoelectron spectroscopy of the film as well as the substrate core levels. Emission angle resolved film and core level spectra are used to determine the band bending behaviour and the sheet carrier concentration as function of growth parameters. By comparison to the spectroscopic data, transport experiments offer information on carrier trapping in this oxygen vacancy dominated material.

TT 72.72 Wed 15:00 Poster B

Investigating the charge transfer in $LaVO_3/SrTiO_3$ heterostructures by photoemission spectroscopy — •Martin Stübinger[1], Judith Gabel[1], Philipp Gagel[1], Christoph Schlueter[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom

Akin to the well known oxide heterostructure $LaAlO_3/SrTiO_3$ (LAO/STO) a conducting interface is found also between the strongly correlated, polar Mott insulator $LaVO_3$ (LVO) and the non-polar band insulator STO. A possible mechanism for this behavior is an electron transfer to the interface caused by the polar discontinuity. Since in LVO/STO the transition metals Ti as well as V can have different oxidation states, they both may act as hosts for the transferred electrons. In particular, a charge transfer to V would lead to a band-filling controlled Mott insulator-to-metal transition. By means of photoemission spectroscopy with synchrotron radiation we investigate the valence band structure of LVO/STO and the band alignment at the interface. In accordance with resonant photoemission at the V-L and the Ti-L edge we arrive at the conclusion that it is energetically more favorable for transferred electrons to occupy Ti than V sites. Therefore, a Mott insulator-to-metal transition is not observed in LVO.

TT 72.73 Wed 15:00 Poster B

Strain-induced metal-to-insulator transition in LiV_2O_4 thin films — •Ulrike Niemann[1], Daigorou Hirai[2], and Hidenori Takagi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan

The spinel compound LiV_2O_4 is well-known for its exotic heavy fermion behaviour and has therefore been subject to several studies, addressing the origin of the heavy fermion phase [1]. Repeatedly, geometric frustration with regard to the charge and spin arrangement on the vanadium sides was discussed as a possible alternative to a dense Kondo system scenario. However, the difficulties in growing significantly large single crystals of high quality, limit the verification of discussed models. We fabricated single-crystalline thin films of LiV_2O_4 on $SrTiO_3$, LSAT and MgO substrates using pulsed laser deposition [2]. The heavy fermion behaviour of bulk LiV_2O_4 is well-reproduced in relaxed films on $SrTiO_3$ substrates, giving the opportunity to explore the heavy fermion phase in area-vice significantly larger single crystals. In contrast, an insulating phase was found in strained LiV_2O_4 thin films on MgO substrates, supporting the importance of geometric frustration for the appearance of heavy fermions in this particular compound. On the poster, we discuss the thin film fabrication and the effect of epitaxial strain on heavy fermions in LiV_2O_4 in detail.
[1] C. Urano et al., Phys. Rev. Lett. 85, 1052 (2000).
[2] U.Niemann, D. Hirai, H. Takagi (submitted)

TT 72.74 Wed 15:00 Poster B

Electronic Structure of Palladium Measured by Compton Scattering and Electron-Positron Annihilation. — •Josef Helmut Schmidbauer[1], Michael Leitner[1], and Christoph Pascal Hugenschmidt[1,2] — [1]Physik Department E21, Technische Universität München, James-Franck-Straße 1, 85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstraße 1, 85748 Garching, Germany

Compton scattering and measurements of the angular correlation of electron-positron annihilation radiation (ACAR) offer two unique possibilities for the investigation of the bulk electronic structure. Although both methods allow the measurement of the electron momentum distribution (EMD) various differences are inherent to the respective technique. While a single ACAR spectrum provides a two-dimensional projection of the EMD a Compton scattering profile corresponds to a one-dimensional projections. Besides dissimilar experimental resolution further differences originate from the influence of the positron wave function and the enhancement of different electron states (probe effects). We applied both techniques to the correlated system Palladium in order to study its electronic structure, and we present the specific features inherent to Compton scattering and ACAR.

TT 72.75 Wed 15:00 Poster B

Electronic structure of the B20 compound CrGe — •J. Klotz[1,2], K. Götze[1,2], J. Bruin[3], C. Geibel[4], K. Weber[4], M. Schmidt[4], H. Rosner[4], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]High Magnetic Field Laboratory, Radboud University, Netherlands — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

CrGe is a nonmagnetic transition-metal germanide with the B20 noncentrosymmetric cubic structure. In contrast, the isostructural MnGe and FeGe both show a helical spin order. We present dHvA-effect data on CrGe that were obtained employing capacitive torque magnetometers in a 18 T/30 mK and a 33 T/340 mK system. In combination with our fplo calculations, we provide a detailed picture of the Fermi-surface topology of CrGe. Furthermore, by comparing the calculated band structures of CrGe and MnGe, we discuss possible reasons for the absence of magnetic order in CrGe. Finally, our calculations indicate that substituting Ge by As or Sn will not lead to magnetic order.

TT 72.76 Wed 15:00 Poster B

Interplay of spin-orbit coupling, crystal-field and electronic correlations in ruthenate oxides — •Esmaeel Sarvestani[1], Guoren Zhang[1], Evgeny Gorelov[1,2], and Eva Pavarini[1,3] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany — [2]European XFEL GmbH, Hamburg, Germany — [3]JARA High-Performance Computing, RWTH Aachen, Aachen, Gemany

We investigate the effects of spin-orbit (SO) coupling, crystal-field and Coulomb interaction on the electronic properties of the t_{2g}^4 layered ruthenates Sr_2RuO_4 and $Sr_3Ru_2O_7$. We calculate effective masses, life-times and optical conductivity via the LDA+DMFT approach, using the general implementation of the continuous-time interaction-expansion QMC impurity solver of Refs.[1,2]. We find that the effect of SO coupling on the mass-enhancements depends on the parameter range. We explain this via a two-site t_{2g} Hubbard model. We additionally find that for a realistic description of the optical conductivity, it is important to include the effects of SO interaction. We show that the effects of low-symmetry terms of Coulomb interaction on the total spectral function and in-plane conductivity are small; however, they have a strong effect on the mass-enhancement anisotropy [3].

[1] E. Gorelov et. al., Phys. Rev. Lett. **104**, 226401 (2010).
[2] G. Zhang et. al., Phys. Rev. Lett. **116**, 106402 (2016).
[3] E. Sarvestani et. al., submitted to Phys. Rev. B.

TT 72.77 Wed 15:00 Poster B

Spin-Orbit Coupling and Electronic Corrleations in Ca_2RuO_4 — •Michael T. Schmid[1], Philipp Hansmann[2], and Maria Daghofer[3] — [1]michael.schmid@fmq.uni-stuttgart.de — [2]p.hansmann@fkf.mpg.de — [3]maria.daghofer@fmq.uni-stuttgart.de

Transition metal oxides of the 4d and 5d series with large spin orbit coupling (SOC) such as Iridates and Ruthenates are currently under intensive investigation [1]. Especially in the 4d systems the absence of a clear hierarchy of energy scales between crystal field (CF) and SOC splittings (e.g. in Ca_2RuO_4) poses a significant challenge for standard methods like the merger of density functional theory with dynamical mean-field theory (DFT+DMFT). With state-of-the-art DMFT impurity solvers [2], however, effective low energy models that include both CF and SOC contributions can be tackled. Here we present most recent results for Ca_2RuO_4 on the level of the magnetic susceptibilities. In contrast to mere single particle spectral functions the magnetic two particle response sheds significantly more light on the nature of the correlated magnetic phases in the considered materials.

[1] C. G. Fatuzzo et al., Phys. Rev. B, **91**, 1155104 (2015)
[2] O. Parcollet et al., Computer Physics Communications, **196**, 398 (2015)

TT 72.78 Wed 15:00 Poster B

Spin dynamics in a honeycomb compound probed by magnetic resonance technique — •Margarita Iakovleva[1,2], Hans-Joachim Grafe[1], Angela Möller[3], T. Taetz[4], Evgeniia Vavilova[2], Bernd Büchner[1], and Vladislav Kataev[1] — [1]IFW Dresden, Dresden, 01069, Germany — [2]KPhTI, Kazan, 420029, Russia — [3]IAAC, JGU Mainz, Mainz, 55128, Germany — [4]Institut für Anorganische Chemie, Universität zu Köln, Köln, 50939, Germany

The S=1/2 Heisenberg antiferromagnet $InCu_{2/3}V_{1/3}O_3$ appears to be a rare model of a honeycomb lattice compound with very weak interlayer couplings. Previous magnetization and Electron Spin Resonance (ESR) studies on this compound have revealed signatures of an antiferromagnetic transition at T_N = 38 K [1,2]. In our study, we used Nuclear Quadrupolar Resonance (NQR) and Nuclear Magnetic Resonance (NMR) techniques to investigate the local magnetic properties of $InCu_{2/3}V_{1/3}O_3$. The ^{115}In NMR as well as NQR spectra show a line splitting at $T<T_N$ which is a signature of the development of local magnetic fields in the vicinity of a magnetic phase transition. The T-dependence of the longitudinal relaxation rate T_1^{-1} shows a characteristic sharp peak upon approaching T_N = 38 K. Remarkably, with further decreasing temperature a second peak develops at T* = 15 K. We discuss this peculiar feature and possible scenarios of magnetic order in $InCu_{2/3}V_{1/3}O_3$.

[1] V. Kataev, et al., JMMM 290-291, 310 (2004)
[2] M. Yehia, et al., Phys. Rev. B, 81, 060414 (2010)

TT 72.79 Wed 15:00 Poster B

Strong electronic correlations: the example of VO_2 — •Elham Khorasani[1], Malte Schüler[2], Bálint Aradi[1], and Peter Deák[1] — [1]BCCMS, Universität Bremen, Bremen, Germany. — [2]Institut für Theoretische Physik, Universität Bremem, Germany.

The metal-insulator transition in VO_2 has been a controversial issue for several decades. It is at the boundary between band theory and many-body physics and forms an important benchmark problem in theoretical solid state physics. To understand the metal-insulator mechanism across the VO_2 in B-phase, GGA+U calculations based on density functional theory have been done. Our results reveal that GGA+U can not predict the proper ground state of VO_2 in the B-phase.

Our study based on static cluster dynamical mean field theory(sC-DMFT), which is proved itself valuable in the M-phase (J. M. Tomczak et .al,J.Phys. Condens Matter, 19, 365206(2007)), did not lead to the experimentally known gap in the insulator VO_2 in B-phase. So, in the next step, in order to elucidate the correlated electronic structure of the B-phase, the full C-DMFT(P. Werner et al, Phys. Rev. Lett., 97, 076405(2006))have been done. Our results for M-phase show that the implementation of Continues-Time Quantum Monte Carlo based on hybridization expansion (CT-Hyb) as a solver makes a sign problem in full C-DMFT.To overcome the sign problem in CT-Hyb , cluster DMFT using exact agonalisation (ED) has been implemented. We compare ED and CT-QMC results for R-phase and explore properties of B-phase using ED.

TT 72.80 Wed 15:00 Poster B

Lattice dynamics of palladium in the presence of many-body effects — •Wilhelm Appelt[1,3], Andreas Östlin[2], Ivan Leonov[2], Michael Sekania[2], and Liviu Chioncel[2,3] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We present theoretical results on the phonon spectrum of palladium. A combination of the local density approximation (LDA) and dynamical mean-field theory (DMFT) is employed in order to investigate the interplay between correlated electrons and lattice degrees of freedom. A

good agreement with experimental dispersion curves is found for the realistic local Coulomb interaction ($U = 1\,\mathrm{eV}$) and the local Hund's rule coupling ($J = 0.3\,\mathrm{eV}$). The Kohn anomaly along the Σ-line is observed on the level of LDA when computed at the experimental volume. When supplement with local electronic interactions, of Hubbard-type, we find that the kink along the Σ-line in the phonon dispersion curve is smoothened. Corrections in lowest order perturbation theory are used in order to study the influence of non-adiabatic self-energy effects on the phonon propagtor. This simple correction to the Born-Oppenheimer approximation allows us to access phonon lifetimes in the LDA+DMFT study.

TT 72.81 Wed 15:00 Poster B

Flavor-twisted Boundary Conditions for calculation of two-particle correlation functions — •Jonas Heverhagen and Maria Daghofer — University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Germany

We generalize the simulation technique flavor-twisted boundary condition (FTBC) combined with exact diagonalization (ED) to gain continuous momentum resolution for two-particle correlation functions. To validate this technique, we compare the results with cluster perturbation theory calculations and identify the strength and weaknesses of both techniques. Hereby, we focus on one-dimensional spin-orbital systems, where first CPT is well established and second results from only ED calculations can easily be compared with FTBC calculations. However, we stress that this technique can also be applied in higher dimensions.

TT 72.82 Wed 15:00 Poster B

CT-1/2-HYB-QMC: a new solver for time-dependent Anderson impurity — •Patryk Kubiczek[1], Alexey N. Rubtsov[2,3], and Alexander I. Lichtenstein[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics, Lomonosov Moscow State University, Moscow, Russia — [3]Russian Quantum Centre, Skolkovo, Russia

We report on the progress of the development of a modified real-time continuous-time hybridization-expansion quantum Monte Carlo solver for a time-dependent single-orbital Anderson impurity model: CT-1/2-HYB-QMC. In the proposed method the diagrammatic expansion is performed only for one out of the two spin channels, while the resulting effective single-particle problem for the other spin is solved explicitly for each diagrammatic term. We show that the CT-1/2-HYB-QMC method alleviates the dynamical sign problem by reducing the order of sampled diagrams and makes it possible to reach twice as long time scales in comparison to the standard CT-HYB method. Moreover, the structure of CT-1/2-HYB perturbative expansion leads to an easier and less computationally expensive measurement of the charge current.

TT 72.83 Wed 15:00 Poster B

Variational approach to models with strongly correlated electrons — •Philip Mirbach[1], Malte Schüler[1,2], Tim Wehling[1,2], and Gerd Czycholl[1] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

Electronic systems with strong interactions are promising materials for a wide variety of applications. These strongly correlated electron systems are often described by lattice models such as the Hubbard model. However, they are difficult to treat numerically.

We use Feynman's Variational Principle to determine optimal effective model systems that can be solved exactly, for example by ED-methods. We divide the original model into exactly solvable clusters, where the partition and the parameters are optimized by the variational principle. Internal correlation effects are correctly considered in these clusters. In addition, they maintain effective influences of the originally neglected interactions through the variation. The trivial case of completely decoupled clusters is equal to the Hartree-Fock (HF) approximation. Therefore, more complex effective model systems lead to systematic improvements beyond HF. By an optimal choice of the representation of the model, e. g. in real or momentum space, particularly effective parameters for describing the original model can be found.

Using the one-dimensional Hubbard model with four sites as an example, we show the possibilities of this method and compare the results with HF and the exact solution.

TT 72.84 Wed 15:00 Poster B

The finite-temperature Lanczos method as solver for the variational cluster approach — •Jan Lotze and Maria Daghofer — Universität Stuttgart, Institut für Funktionelle Materie und Quantentechnologien, Pfaffenwaldring 57, 70569 Stuttgart

The variational cluster approximation (VCA) based on self-energy functional theory (SFT) [1] can be used to study correlated-electron Hamiltonians: Instead of the original systems self-energy, that of a 'reference system' is considered. While full diagonalisation suffices for small reference systems, larger systems require the Lanczos method or a quantum Monte Carlo method [2] to be tractable. Considering systems at finite temperature increases the numerical burden even further. Demanding on top of this the resolution of degenerate states in the reference system requires to switch from the regular Lanczos method to the Band Lanczos method.

Here, thermodynamic and dynamical properties of the one- and two-dimensional Hubbard model at finite temperature are presented to illustrate the finite-temperature Lanczos and Band Lanczos method as solver of the reference system. The effect of degeneracies onto the results is discussed.

[1] M. Potthoff, 'Self-Energy-Functional Theory', in Strongly Correlated Systems – Theoretical Methods (Springer, 2012).
[2] G. Li, W. Hanke, A. N. Rubtsov, S. Bäse, M. Potthoff, Phys. Rev. B **80**, 195118 (2009).

TT 72.85 Wed 15:00 Poster B

Theoretical investigation of excitonic agnetism in $LaSrCoO_4$ — •juan fernandez afonso, andrii sotnikov, and jan kunes — Institute of Solid State Physics TU Wien, Vienna, Austria

We use the LDA+U approach to search for possible ordered ground states of $LaSrCoO_4$. We find a staggered arrangement of magnetic multipoles to be stable over a broad range of Co $3d$ interaction parameters. This ordered state can be described as a spin-density-wave-type condensate of $d_{xy} \otimes d_{x^2-y^2}$ excitons carrying spin $S = 1$. Further, we construct an effective strong-coupling model, calculate the exciton dispersion and investigate closing for the exciton gap, which marks the exciton condensation instability. Comparing the layered $LaSrCoO_4$ with its pseudo cubic analog $LaCoO_3$, we find that for the same interaction parameters the excitonic gap is smaller (possibly vanishing) in the layered cobaltite.

TT 72.86 Wed 15:00 Poster B

Anisotropy crossover in the frustrated Hubbard model on four-chain cylinders — •Georg Ehlers[1], Benjamin Lenz[2,3], Salvatore R. Manmana[3], and Reinhard M. Noack[1] — [1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS UMR 7644, 91128 Palaiseau, France — [3]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany

Motivated by dimensional crossover in Bechgaard and layered organic κ salts, we investigate the metal-insulator transition in the anisotropic frustrated Hubbard model on four coupled Hubbard chains.

Using the hybrid-space density matrix renormalization group (DMRG) and the variational cluster approximation (VCA), we map out the phase diagram as a function of the anisotropy and interaction strength. The phase diagram, as seen by the hybrid-space DMRG, features a quasi-one-dimensional anti-ferromagnetic phase, a two dimensional anti-ferromagnetic phase, a metallic phase, and an incommensurate spin-density wave phase [1]. The phases are characterized through their magnetic ordering, dielectric response, and dominant static correlations.

We use DMRG in a formulation for lattices with cylindrical geometry utilizing the conserved transverse lattice momentum [2] and corroborate our findings with VCA calculations using a cluster geometry corresponding to the cylindrical lattice. As an outlook, we make contact with work studying dimensional crossover in the full two-dimensional system.

[1] G. Ehlers et al., arXiv:1705.04450 (2017)
[2] G. Ehlers et al., Phys. Rev. B 95, 125125 (2017)

TT 72.87 Wed 15:00 Poster B

Doublon Formation by Ions Impacting a Strongly Correlated System — Karsten Balzer, •Niclas Schlünzen, Maximilian Rodriguez Rasmussen, and Michael Bonitz — CAU Kiel, Germany

Strongly correlated systems of fermions have a number of exciting

collective properties. Among them, the creation of a lattice that is occupied by doublons, i.e. two fermions with opposite spins, offers interesting electronic properties. In the past a variety of methods has been proposed to control doublon formation both spatially and temporally. Here, a recently proposed[1] mechanism is described and verified by computer simulations – doublon creation by the impact of energetic ions[1,2]. The theoretical characterization is based on exact diagonalization calculations for small systems and is extended to larger systems via a Nonequilibrium Green Functions description[3]. Finally, we present an idea how this concept can be realized with atoms in an optical lattice.

[1] K. Balzer, M. Rasmussen, N. Schlünzen, M. Bonitz, submitted
[2] K. Balzer, N. Schlünzen, M. Bonitz, Phys. Rev. B 94, 245118 (2016)
[3] S. Hermanns, N. Schlünzen, M. Bonitz, Phys. Rev. B 90, 125111 (2014)

TT 72.88 Wed 15:00 Poster B

Analytical Evidences for Particle Induced Doublons in Strongly Correlated Systems — •Maximilian Rodriguez Rasmussen, Karsten Balzer, Niclas Schlünzen, and Michael Bonitz — CAU Kiel, Germany

Under certain conditions strongly correlated fermions in lattice systems are known to form doublons – quasi-particles consisting of two electrons on the same site. Due to the interesting resulting electronic properties doublon formation processes have been the subject of various studies. Recently, a new mechanism has been proposed[1] – doublon creation by the impact of energetic ions. Here, these processes are described and verified by analytical results for a two-site model that is shown to capture the basic features and allows for a systematic analysis of the main trends[2]. The findings are additionally supported by a Landau–Zener description of the doublon state.

[1] K. Balzer, M. Rasmussen, N. Schlünzen, and M. Bonitz, submitted for publication (2017)

[2] M. Rasmussen, "Particle Induced Doublons in Strongly Correlated Systems", bachelor thesis (2017)

TT 72.89 Wed 15:00 Poster B

Prethermalization after a short electric field pulse — •Marc Alexander and Marcus Kollar — Theoretische Physik III, Universität Augsburg

We study the nonlinear current response to a short electric field pump pulse [1]. For weakly interacting Hubbard models we find that a prethermalization plateau develops after the pulse, in contrast to the noninteracting case. While this behavior is analogous to the prethermalization plateau that occurs after weak interaction quenches [2], the details of the metastable state now depend on the details of the bandstructure and the length, shape, and frequency of the pump pulse.

[1] V. Turkowski and J. K. Freericks, Phys. Rev. B **71**, 085104 (2005)
[2] M. Moeckel and S. Kehrein, Phys. Rev. Lett. **100**, 175702 (2008)

TT 72.90 Wed 15:00 Poster B

Generalized Gibbs ensembles in weakly open quantum systems — •Florian Lange, Zala Lenarcic, and Achim Rosch — Universität zu Köln

We consider weakly driven and weakly open quantum systems in the situation when the unperturbed system has a set of conservation laws. If the perturbation is sufficiently weak the non-equilibrium steady state can be in the thermodynamic limit efficiently described by a generalized Gibbs ensemble (GGE) characterized by one Lagrange parameter for each approximate conservation law. The values of those are determined by rate equations for the approximately conserved quantities. We extend the concept of GGEs by showing that an ensemble with time-dependent Lagrange parameters can capture the relaxation towards the steady state.

TT 72.91 Wed 15:00 Poster B

Single-hole dynamics in two-leg t-J ladder systems with matrix product states (MPS) — •Alexander Osterkorn[1], Fabian Grusdt[2], Sebastian Paeckel[1], Thomas Köhler[1], and Salvatore Manmana[1] — [1]Institut für Theoretische Physik, Universität Göttingen, 37077 Göttingen, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We study the time evolution of a single hole in two-leg t-J-ladder systems at zero temperature using time-dependent matrix product states (MPS). We prepare the system with one fermion per lattice site with neither interaction nor tunneling between the legs. At time t = 0 one particle is removed from one of the legs and the tunneling amplitude between the two legs is set to a nonzero value. This allows us to study the separation of spinons and holons as a function of the rung-tunneling and compare to predictions from effective theories. We discuss implications for realizations with ultracold gases on optical lattices.

TT 72.92 Wed 15:00 Poster B

EPR studies of the triangular-lattice antiferromagnet Cs_2CuBr_4 — •Erik Schulze[1,2], Alexey N. Ponomaryov[1], Jochen Wosnitza[1,2], Hidekazu Tanaka[3], and Sergei A. Zvyagin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [3]Tokyo Institute of Technology, Tokyo, Japan

The spin dynamics of the spin-1/2 triangular-lattice antiferromagnet Cs_2CuBr_4 is probed by means of high-frequency electron paramagnetic resonance (EPR) spectroscopy. Temperature dependences of EPR parameters are studied in a broad temperature range between 1.4 and 200 K for different orientations of the applied magnetic field. In the high-temperature regime ($T \gg J/k_B$), an unusually broad and anisotropic resonance line is detected, suggesting a sizeable Dzyaloshinskii-Moriya interaction. Employing the theory of exchange narrowing, the ratio of the Dzyaloshinskii-Moriya vector components, $Dc/Da \approx 0.3$, is estimated.

This work was partially supported by Deutsche Forschungsgemeinschaft (project ZV 6/2-2) and by the HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 72.93 Wed 15:00 Poster B

NMR study in the expected spin nematic state in Linarite — •Gaël Bastien[1], Quentin Goutaland[1], Hans Joachim Grafe[1], Edwin Kermarrec[2], Fabrice Bert[2], Philippe Mendels[2], Stefan Ludwig Drechsler[1], Satoshi Nishimoto[1], Stefan Süllow[3], Kirrily Rule[4], Anja U. B. Wolter[1], and Bernd Büchner[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, Germany — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay, Orsay, France — [3]Institute for Physics of Condensed Matter, TU Braunschweig, Germany — [4]The Bragg Institute, ANSTO, Kirrawee DC, Australia

The $J_1 - J_2$ Heisenberg chain is a frustrated magnetic system with competing first and second nearest neighbor interactions along a 1D chain. A new exotic state i.e. the spin nematic state is predicted to occur under magnetic field in this model. The linarite $PbCuSO_4(OH)_2$ is such a $J_1 - J_2$ Heisenberg chain with a relatively low saturation field H_{sat} ≈10T. It shows a long range magnetic spiral order below T_N=2.7K. Under a magnetic field applied along the b axis, it is changed into a collinear antiferromagnetic state and then to a collinear spin density wave, which is finally suppressed around 9.4T. We perform NMR measurement in the spin density wave state and in the narrow field interval between this spin density wave state and the saturation down to dilution temperature, to measure both the NMR spectrum and the relaxation rate. The relaxation rate was also measured at higher temperature in the paramagnetic state to investigate the fluctuations around the expected spin nematic state.

TT 72.94 Wed 15:00 Poster B

Non-linear optical response in $SrCuO_2$ — •Philipp Warzanowski[1], Eva Benckiser[2], Dalila Bounoua[3], Paul H. M. van Loosdrecht[1], Christian Hess[4], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]ICMMO-Université Paris Sud — [4]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden

$SrCuO_2$ is regarded as a model system realizing a 1D $S = 1/2$ antiferromagnetic Heisenberg chain with a charge-transfer gap of about 1.6 eV and a large exchange constant of $J > 0.2$ eV. Optical spectroscopy allows us to study spinons by means of phonon-assisted absorption. We find $J = 225$ meV, in good agreement with neutron scattering results [1]. At low temperatures, the optical data reveal an additional non-linear absorption feature around 0.8 eV which originates from photoexcited states and depends on the incident light intensity. From time-resolved measurements we observe the temporal dynamics for the saturation and relaxation of this feature in the order of seconds to minutes. Above 160 K, this feature vanishes. Based on a three-level scheme, we describe the intensity dependence and time dependence in terms of rate equations. Similar findings in $LaSrAlO_4$ by Demsar *et*

al. [2] suggest a scenario of excited carriers trapped in long-lived states related to oxygen vacancies.

[1] I. A. Zaliznyak *et al.*, Phys. Rev. Lett. 93, 087202 (2004)
[2] J. Demsar *et al.*, Phys. Rev. B 76, 054304 (2007)

TT 72.95 Wed 15:00 Poster B

Flat bands in fractal-like geometry — •Biplab Pal and Kush Saha — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

We report the presence of multiple flat bands in a class of two-dimensional (2D) lattices formed by Sierpinski gasket (SPG) fractal geometries as the basic unit cells. Solving the tight-binding Hamiltonian for such lattices with different generations of a SPG network, we find multiple degenerate and non-degenerate *completely flat* bands, depending on the configuration of parameters of the Hamiltonian. Moreover, we find a generic formula to determine the number of such bands as a function of the generation index ℓ of the fractal geometry. We show that the flat bands and their neighboring dispersive bands have remarkable features, the most interesting one being the spin-1 conical-type spectrum at the band center without any staggered magnetic flux, in contrast to the Kagome lattice. We furthermore investigate the effect of the magnetic flux in these lattice settings and show that different combinations of fluxes through such fractal unit cells lead to richer spectrum with a single isolated flat band or gapless electron- or hole-like flat bands. Finally, we discuss a possible experimental setup to engineer such fractal flat band network using single-mode laser-induced photonic waveguides.

TT 72.96 Wed 15:00 Poster B

Automated construction of U(1)-invariant matrix-product operators from graph representations — •Sebastian Paeckel, Thomas Köhler, and Salvatore Manmana — Institut für Theoretische Physik, Georg August Universität Göttingen, Germany

We present an algorithmic construction scheme for matrix-product-operator (MPO) representations of arbitrary $U(1)$-invariant operators whenever there is an expression of the local structure in terms of a finite-states machine (FSM). Given a set of local operators as building blocks, the method automatizes two major steps when constructing a $U(1)$-invariant MPO representation: (i) the bookkeeping of auxiliary bond-index shifts arising from the application of operators changing the local quantum numbers and (ii) the appearance of phase factors due to particular commutation rules. The automatization is achieved by post-processing the operator strings generated by the FSM. Consequently, MPO representations of various types of $U(1)$-invariant operators can be constructed generically in MPS algorithms reducing the necessity of expensive MPO arithmetics. This is demonstrated by generating arbitrary products of operators in terms of FSM, from which we obtain exact MPO representations for the variance of the Hamiltonian of a $S = 1$ Heisenberg chain.

TT 72.97 Wed 15:00 Poster B

Multiferroicity in Ni_3TeO_6 and $PbNi_6Mn_2Te_3O_{18}$ - a comparative Raman study — •Florian Büscher[1], Dirk Wulferding[1,2], Peter Lemmens[1,2], Raman Sankar[3], and Fang-Cheng Chou[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]NTU, Taipei, Taiwan

We report a comparative Raman study on the layered, 2D multiferroic compounds Ni_3TeO_6 and $PbNi_6Mn_2Te_3O_{18}$. The emergence of 2-magnon scattering enables a characterization of their magnetic subsystems. Phonon anomalies below the magnetic ordering temperatures evidence a strong coupling between lattice and spin degrees of freedom in both systems. Work supported by the Quantum- and Nanometrology initiative "QUANOMET" within Project NL-4 and NTH School "Contacts in Nanosystems".

TT 72.98 Wed 15:00 Poster B

Magnetic properties of the spin-1 chain compound $NiCl_3C_6H_5CH_2CH_2NH_3$ — Ferdinand Lipps[1], Anke Arkenbout[2], Alexey Polyakov[2], Marco Günter[3], Timur Salikhov[4], Eugeniia Vavilova[4], Hans-Henning Klauss[3], Bernd Büchner[1], Thomas Palstra[2], and •Vladislav Kataev[1] — [1]IFW Dresden, 01069 Dresden, Germany — [2]University of Groningen, 9747 AG Groningen, The Netherlands — [3]TU Dresden, 01069 Dresden, Germany — [4]Zavoisky Physical Technical Institute, 420029 Kazan, Russia

We report experimental results of the static magnetization, ESR and NMR spectroscopic measurements of the Ni-hybrid compound $NiCl_3C_6H_5CH_2CH_2NH_3$. In this material $NiCl_3$ octahedra are structurally arranged in chains along the crystallographic a-axis. According to the static susceptibility and ESR data Ni^{2+} spins $S = 1$ are isotropic and are coupled antiferromagnetically (AFM) along the chain with the exchange constant $J = 25.5\,\mathrm{K}$. These are important prerequisites for the realization of the so-called Haldane spin-1 chain with the spin-singlet ground state and a quantum spin gap. However, experimental results evidence AFM order at $T_\mathrm{N} \approx 10\,\mathrm{K}$ presumably due to small interchain couplings. Interestingly, frequency-, magnetic field-, and temperature-dependent ESR measurements, as well as the NMR data, reveal an inhomogeneous ground state of co-existent mesoscopically spatially separated AFM ordered and spin-singlet state regions.

TT 73: Quantum Dynamics, Decoherence and Quantum Information (joint session DY/TT)

Time: Wednesday 15:30–18:15 Location: EB 107

TT 73.1 Wed 15:30 EB 107

Modeling Dye-Mediated Photon-Photon Interaction in Condensates of Light — Milan Radonjić[1], •Wassilij Kopylov[2], Antun Balaž[1], and Axel Pelster[3] — [1]Institute of Physics Belgrade, University of Belgrade, Serbia — [2]Department of Physics, TU Berlin, Germany — [3]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany

Based entirely on the Lindblad master equation approach we obtain a microscopic description of photons in a dye-filled cavity, which features condensation of light [1,2]. To this end we generalize the nonequilibrium approach of Ref. [3] such that the dye-mediated contribution to the photon-photon interaction in the light condensate is accessible. We describe the dynamics of the system by analyzing the resulting equations of motion. In particular, we discuss the existence of two limiting cases for steady states: photon BEC and laser-like. In the former case, we determine the corresponding dimensionless interaction strength relying on realistic experimental data and find a good agreement with the previous theoretical estimate [4]. Furthermore, we investigate how the dimensionless interaction strength depends on the respective system parameters such as the effective temperature of the dye and the number of the dye molecules.

[1] J. Klaers et al., Nature 468, 545 (2010)
[2] R. A. Nyman and M. H. Szymanska, Phys. Rev. A 89, 033844 (2014)
[3] P. Kirton and J. Keeling, Phys. Rev. Lett. 111, 100404 (2013)
[4] E. C. I. van der Wurff et al., Phys. Rev. Lett. 113, 135301 (2014)

TT 73.2 Wed 15:45 EB 107

Optimized polarization control in a Central-Spin System — •Alessandro Ricottone[1], Yi Nan Fang[2], Stefano Chesi[2], and William Coish[1] — [1]Department of Physics, McGill University, Montréal, Québec H3A 2T8, Canada — [2]Beijing Computational Science Research Center, Beijing 100084, China

We study the dissipative dynamics of the central-spin system, where one central spin is homogeneously coupled with many ancilla spins. We find that, due to a combination of the quantum Zeno effect and many-body collective behaviour of the ancilla spins, the dissipation rate can be optimized to minimize the time scale for polarization dynamics. An archetypical example of this model is given by an electron spin coupled to nuclear spins in a quantum dot via hyperfine interactions, but the same Hamiltonian can be applied in many other physical scenarios. These results may be important for protocols to quickly polarize nuclear spins in semiconductor quantum dots or to rapidly and efficiently equilibrate a quantum annealer.

TT 73.3 Wed 16:00 EB 107

Quantum heat transport and rectification through anharmonic chains between reservoirs — •Thomas Motz, Joachim Ankerhold, and Jürgen Stockburger — Ulm University, Institute

for Complex Quantum Systems

We present a novel dynamical description of quantum heat transfer through anharmonic chains between thermal reservoirs [1,2]. The approach is non-perturbative in the system-bath coupling and also allows to include disorder and the presence of external driving. Technically, we start from the formally exact stochastic Liouville-von Neumann (SLN) treatment of open quantum dynamics [3] and consider the situation of ohmic dissipation. For purely harmonic chains this leads to a very efficient scheme to study also very long chains and flux-flux correlations. In the anharmonic situation, we particularly study thermal rectification, the impact of disorder, and strong coupling to the heat baths.

[1] J. T. Stockburger and T. Motz, Fortschr. Phys. **65**, 1600067 (2017)
[2] T. Motz et al., New J. Phys. **19** 053013 (2017)
[3] J. T. Stockburger and H. Grabert, PRL **88** 170407 (2002)

TT 73.4 Wed 16:15 EB 107

Stochastic simulation of open-system quantum dynamics: overcoming the curse of non-Hermitian propagation — Konstantin Schmitz[1], Thomas Unden[2], and •Jürgen Stockburger[1] — [1]Ulm University, Institute for Complex Quantum Systems — [2]Ulm University, Intstiute for Quantum Optics

The Stochastic Liouville-von Neumann equation [1] provides an exact numerical simulation strategy for quantum systems coupled to a reservoir with Gaussian fluctuations of arbitrary spectrum (linear dissipation). Individual stochastic samples are propagated with Hamiltonians containing random non-Hermitian terms, leading to poor signal-to noise ratios in some cases. However, the efficiency of this approach has recently improved dramatically through time-domain projection techniques, implemented as reduction operations [2]. In addition, we present two recently developed sampling strategies which show significantly improved scaling with the strength of the dissipative interaction and with the reservoir memory time: a) anticorrelated sampling, exploiting a gauge-like symmetry and b) reducing the non-unitary terms in sample propagation through convex optimization techniques.

[1] J. T. Stockburger and H. Grabert, PRL **88** 170407 (2002)
[2] J. T. Stockburger, EPL **115**, 40010 (2016)

TT 73.5 Wed 16:30 EB 107

Fidelity plateaux from correlated noise in cold-atom quantum simulators — •Scott R Taylor and Chris A Hooley — University of St Andrews, St Andrews, UK

We demonstrate that, in a quantum simulation protocol based on the Hubbard model, correlated noise in the Hubbard parameters leads to arbitrarily long plateaux in the state-preparation fidelity as a function of elapsed time. We argue that this correlated-noise scenario is the generic one in the cold-atom context, since all of the Hubbard-model parameters ultimately depend on the same set of lasers. We explain the formation of such a plateau using the Bloch-sphere representation, deriving analytical expressions for its start and end times and its height.

15 min. break

TT 73.6 Wed 17:00 EB 107

Non-Markovian Quantum Dynamics - On the way to real-time simulations of heat engines — •Michael Wiedmann, Jürgen T. Stockburger, and Joachim Ankerhold — Institute for Complex Quantum Systems, Ulm University, Albert-Einstein- Allee 11, D-89069 Ulm

The experimental miniaturization of heat engines down to the single-atom level questions classical concepts such as work and heat flux. In the regime of higher temperatures, well-established theories from classical thermodynamics apply, where surrounding heat baths exchange energy and particles with a much smaller system of interest. Quantum mechanically, the situation is more intricate though. The non-locality of quantum mechanical wave functions induces system-reservoir correlations and entanglement which may have profound impact on thermodynamic properties, particularly for condensed phase systems at cryogenic temperatures. The fully dynamical approach of the stochastic Liouville-von Neumann equation (SLN) builds an exact, time-local and non-perturbative framework to tackle non-Markovian dynamics at low temperatures, for arbitrarily driven systems and strong coupling [1]. With emphasis on particularities induced by anharmonic potentials, we present an efficient real-time propagation scheme for a single quantum oscillator coupled to dissipative reservoirs. Aspects of work and heat flux are analyzed in the regime of strong system-reservoir couplings and in the context of reservoir fluctuations far from equilibrium.

[1] M. Wiedmann et al., Phys. Rev. A **94**, 052137 (2016).

TT 73.7 Wed 17:15 EB 107

Jump-based feedback control in the Lipkin-Meshkov-Glick model — •Sven Zimmermann — Technische Universität Berlin, Deutschland

We apply a measurement based feedback control scheme to the dissipative Lipkin-Meshkov-Glick model to affect the quantum phase transition [1-3]. Here we use the Wiseman-Milburn control scheme and apply it on the level of the master equation to the system dissipator [4, 5]. Our interest lies in the steady state properties of the Lipkin-Meshkov-Glick system under the feedback action. By numerically calculating the average spin expectation values, we show that the considered control scheme changes the critical point of the phase transition. Furthermore, by investigating the waiting time distribution and the concurrence, we show, that the emission properties of the system and the entanglement can be significantly modified by the considered closed-loop control scheme.

[1] H.J. Lipkin, N. Meshkov and A. Glick, Nucl. Phys., 62, 188 (1965)
[2] S. Morrison and A. S. Parkins PRL 100, 040403 (2008)
[3] W. Kopylov and T. Brandes, NJP 17, 103031 (2015)
[4] H. M. Wiseman and G. J. Milburn, Quantum Measurment Control, Cambrige University Press, Campridge (2010)
[5] G. Kießlich, C. Emary, G. Schaller and T. Brandes, NJP 14, 123036 (2012)

TT 73.8 Wed 17:30 EB 107

Architectures for quantum simulation showing a quantum speedup — •Juan Bermejo-Vega[1], Dominik Hangleiter[1], Martin Schwarz[1], Robert Raussendorf[2], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, 14195 Berlin, Germany — [2]University of British Columbia, Department of Physics and Astronomy, Vancouver, BC, V6T 1Z1, Canada

A main goal in the field of quantum simulation is to demonstrate a quantum speedup (or "quantum computational supremacy"), referring to the experimental realization of a quantum device that computationally outperforms classical computers. In this talk, we present simple and feasible schemes of two-dimensional dynamical quantum simulators with the potential to show such a quantum speedup. In each of the schemes, an initial (potentially disordered) product state is prepared, followed by a short-time evolution under a basic translationally invariant Hamiltonian with nearest-neighbor interactions, and a final measurement in a fixed basis. The correctness of the final state preparation in each scheme is fully efficiently certifiable. Our schemes are tailored to platforms of cold atoms in optical lattices, and cannot be efficiently classically simulated under plausible complexity-theoretic assumptions. This work shows that benchmark settings exhibiting a quantum speedup may require little control in contrast to universal quantum computing. Thus, our proposal puts a convincing experimental demonstration of a quantum speedup within reach in the near term.

TT 73.9 Wed 17:45 EB 107

Analytical results for the non-Markovianity of quantum spin ensembles — •Remy Dubertrand[1,2], Alexandre Cesa[2], and John Martin[2] — [1]Institut für Theoretische Physik Universität Regensburg 93040 Regensburg, Germany — [2]Institut de Physique Nucleaire, Atomique et de Spectroscopie, CESAM, University of Liege, Bat. B15, B - 4000 Liege, Belgium

We study the non-Markovian character of spin ensembles. The ensemble is assumed to be isolated and a subset of spins is taken as the system, while the remaining part of the ensemble is taken as the environment. For a large class of interaction range, we derive analytical expressions for the non-Markovianity [1] following a recently introduced measure [2]. In particular, we investigate the thermodynamic limit and derive conditions to observe a Markovian dynamics or not. For a system of a single spin, it is explicitly shown that our results agree with the other known measures of non-Markovianity. We believe that our work can be used to investigate further the dynamics of fundamental models in condensed matter physics from the new perspective of (non-)Markovianity.

[1] R. Dubertrand, A. Cesa, J. Martin, to be submitted
[2] S. Lorenzo, F. Plastina, and M. Paternostro, Phys. Rev. A 88 (2013)

TT 73.10 Wed 18:00 EB 107

Quantum Dynamics beyond Gaussians: from Coarse Graining to a Tower of Scales via Multiresolution — •Antonina N. Fedorova and Michael G. Zeitlin — Russia, 199178, St.Petersburg, V.O. Bolshoj pr., 61, IPME RAS, Mathematical Methods in Mechanics Group

We present a family of methods which can describe complex behaviour in quantum ensembles. We demonstrate the creation of nontrivial (meta) stable states (patterns), localized, chaotic, entangled or decoherent, from the basic localized modes in various collective models arising from the quantum hierarchy described by Wigner-Moyal-von Neumann-like equations. The advantages of such an approach are as follows: i). the natural description of localized states in any proper functional realization of (Hilbert) space of states, ii). the representation of hidden symmetry of a chosen representation of the functional model describes the (whole) spectrum of possible states via the multiresolution decomposition. Effects we are interested in are as follows: 1. a hierarchy of internal/hidden scales (time, space, phase space); 2. non-perturbative multiscales: from slow to fast contributions, from the coarser to the finer level of resolution/decomposition; 3. the coexistence of the levels of hierarchy of multiscale dynamics with transitions between scales; 4. the manifestation of the key features of the complex quantum world such as the existence of chaotic and/or entangled states with possible destruction in "open/dissipative" regimes due to interactions with quantum/classical environment and transition to decoherent states.

TT 74: Molecular Electronics and Photonics

Time: Wednesday 16:00–18:30 Location: H 3005

TT 74.1 Wed 16:00 H 3005

Unimolecular NAND logic gate with input by single Au atoms — •Dmitry Skidin[1], Justus Krüger[1], Frank Eisenhut[1], Andre Gourdon[2], Gianaurelio Cuniberti[1,3], Christian Joachim[2], and Francesca Moresco[1] — [1]Institute for Materials Science, Max Bergmann Center of Biomaterials, and Center for Advancing Electronics Dresden, TU Dresden, 01069 Dresden, Germany — [2]CEMES, CNRS, 29 rue J. Marvig, 31055 Toulouse Cedex, France — [3]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01069 Dresden, Germany

Design and fabrication of nanoscale functional electronic units remains a main task of molecular electronics. In this study, we combine on-surface synthesis approach with STM manipulation techniques to create a unimolecular NAND logic gate. For this purpose, we use asymmetric starphene, which has a characteristic Y-shape, but with the two branches being one phenyl ring longer than the other one. It is obtained by surface-assisted cyclodehydrogenation on Au(111). As predicted by theoretical calculations, local perturbations of the longer branches (which serve as an input) lead to the electronic changes on the shorter branch (output). The perturbations are provided by the interaction with the single Au atoms created on the surface. Scanning tunneling spectroscopy signal showing the position of the molecular resonance is used as an output. Thus, by carefully bringing the single Au atoms into interaction with the molecule, we induce the shifts of the resonant state in a way that replicates the Boolean truth table of a NAND logic gate.

TT 74.2 Wed 16:15 H 3005

Time-dependent framework for energy and charge currents in nanoscale systems — •Thomas Lehmann[1], Alexander Croy[1,2], Rafael Gutiérrez[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The calculation of time-dependent charge and energy currents in nanoscale systems is a challenging task. Nevertheless it is crucial for gaining a deep understanding of the relevant processes at the nanoscale. We extend the auxiliary-mode approach for time-dependent charge transport to allow for the calculation of energy and heat currents for arbitrary time-dependencies. We apply the approach to illustrative examples, demonstrating its usefulness for a wide-range of problems, such as thermoelectric effects in driven systems.

TT 74.3 Wed 16:30 H 3005

Current-induced bond rupture in molecular junctions — •André Erpenbeck[1], Uri Peskin[2], and Michael Thoss[1,3] — [1]Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, 91058 Erlangen, Germany — [2]Schulich Faculty of Chemistry & Lise Meitner Center for Computational Quantum Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel — [3]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

Coupling between electronic and vibrational degrees of freedom in molecular junctions is an important mechanism, which influences the conductance properties. It also causes current-induced vibrational excitation, which may trigger bond rupture and is thus crucial in the context of the stability of molecular junctions. In this contribution, we study current-induced dissociation in molecular junctions based on representative models. To this end, we apply the hierarchical quantum master equation approach to the electronic transport problem. For the treatment of the nuclear degree of freedom, modeled with dissociative potentials, two different levels of theory are considered, (i) a quantum-classical description within the Ehrenfest approach and (ii) a fully quantum mechanical treatment using a discrete variable representation. Comparing the two approaches, we identify different processes leading to current-induced dissociation such as transient population of anti-bonding states by tunneling electrons or current-induced heating of the nuclear motion. The significance of the processes and their dependence on different model parameters is discussed in some detail.

TT 74.4 Wed 16:45 H 3005

Switching the conductance of molecular junctions by proton transfer — •Dominik Weckbecker[1], Pedro B. Coto[1], and Michael Thoss[1,2] — [1]FAU Erlangen-Nürnberg, Institut für Theoretische Physik, Staudtstrasse 7/B2, 91058 Erlangen, Germany — [2]Universität Freiburg, Physikalisches Institut, Hermann-Herder-Str. 3, 79104 Freiburg

While most experiments on single-molecule junctions have employed metal electrodes, recent works demonstrate that graphene has a number of advantages over metallic leads [1-2]. In this contribution, we investigate charge transport in graphene-molecule junctions employing a theoretical approach that combines first-principles electronic structure methods with nonequilibrium Green's function transport theory [3]. Specifically, we consider zigzag and armchair terminated graphene leads with covalently bonded molecular bridges. We analyze the possibility to use a proton transfer reaction as novel mechanism for switching the conductance of a molecular junction. Our simulations demonstrate that an intramolecular proton transfer can change the conductance of the graphene-molecule junction significantly [4]. While a proton transfer parallel to the transport direction could be used to realize a molecular switch or diode, a junction with a perpendicular proton transfer can resemble a transistor.
[1] K. Ullmann et al., Nano Lett. 15, 3512 (2015)
[2] C. Jia et al., Science 352, 1443 (2016)
[3] M. Brandbyge et al., Phys. Rev. B 65, 165401 (2002)
[4] D. Weckbecker et al., Nano Lett. 17, 3341 (2017)

TT 74.5 Wed 17:00 H 3005

Characteristic excitations in conduction through Ag-CO molecular junctions — •Atasi Chatterjee[1], Jan Philipp Stöckmann[1], Christoph Tegenkamp[1,2], and Herbert Pfnür[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167, Hannover, Germany — [2]Technische Universität Chemnitz, Institut für Physik, 09126, Chemnitz, Germany

Ag metallic nano-electrodes with an initial centre width of approximately 20 nm were fabricated using a combination of e-beam lithography (EBL) and focused ion beam (FIB) milling. These structures

were thinned by electromigration (EM) to generate atomic point contacts. With the help of a 4-tip SEM / STM setup, the visualization of the structural changes as well as conductance measurements were performed at the same time. Conductance histograms exhibit characteristic signatures of atomic point contacts. Conductance of these point contacts was strongly altered by adsorbed CO, which was deposited in-situ after opening the contact. Sub-G_0 plateaus were observed as first signatures of the metal molecule interaction. I-V measurements were performed at sub-G_0 values when the conductance was stable for at least 15 mins. The I-V curves are asymmetric with a slightly rectifying behavior for negative voltages. This asymmetry can be attributed to the fact that CO molecule binds preferably to one side of the metallic electrode. From the characteristic changes of slope, resonance features, and change of noise levels at different voltages in the IV measurements, we explain the properties of these Ag-CO molecular junctions.

15 min. break.

TT 74.6 Wed 17:30 H 3005

Tension related vibrational frequency shifts in helicene molecules — •Yuxiang Gong[1], Chao Jing[1], Peter Hasch[1], Joachim Reichert[1], Ivo Starý[2], and Johannes Barth[1] — [1]Physik Department, Technische Universität München, James-Franck-Str. 1, 85748 Garching, Germany — [2]Institute of Organic Chemistry and Biochemistry ASCR, v.v.i. Flemingovo nám. 2, CZ-166 10 Prague 6, Czech Republic

The investigation of electronic properties of organic molecules is a fundamental aspect in the field of molecular electronics. Molecular transistors, switches and amplifiers have been demonstrated. In this work, a single-molecule junction spectroscopy (MJS) technique is applied to detect the current-voltage characteristics and vibrational properties of 1,7-dithiol-7-helicene molecules simultaneously. The single-molecule junction can be established by approaching the substrate to a gold covered tetrahedral scanning near-field tip, which is monitored via Raman spectroscopy. Afterwards, the substrate is carefully retracted, stretching the molecule. At each step, a Raman spectrum is acquired. One distinct vibrational mode is analyzed, and reveals a systematic red shift corresponding to the applied strain in the single-molecule junction. The experimental results are complemented and explained by DFT simulations which take the electrodes into consideration.

TT 74.7 Wed 17:45 H 3005

Quantum Transport Properties of Silane Molecular Wires — •María Camarasa-Gómez[1], Haixing Li[2], Timothy A. Su[2], Daniel Hernangómez-Pérez[1], Latha Venkataraman[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg (Germany) — [2]Department of Applied Physics and Chemistry, Columbia University, New York, NY 10027 (USA)

In single-molecule junction experiments the conduction of silane wires attached to Au and Ag electrodes has been measured for thiol- and amine-based anchoring groups [1]. The experimental results show that amine-terminated molecules present lower conductance when attached to Ag than Au. The result is in agreement with expectations based on the trends in the metal work function. Surprisingly, the trend is reversed with thiol-linkers.

We present a theoretical analysis employing transport calculations based on the density functional theory that explains this result. Our study shows how the chemical nature of the bonds between anchor groups and metal electrodes can influence the conductance trends. We conclude that the influence of anchor groups can be large and sometimes even dominating over a work function related level mismatch.

[1]H. Li, T. A. Su, M. Camarasa-Gómez et. al., Angew. Chem. Int. Ed. 56, 14145 (2017)

TT 74.8 Wed 18:00 H 3005

Quantum Transport Properties of Polymethine and Polyene Molecular Wires — •Daniel Hernangómez-Pérez[1], Suman Gunasekaran[2], Iryna Davydenko[3], Seth Marder[3], Ferdinand Evers[1], and Latha Venkataraman[2,4] — [1]Institute of Theoretical Physics, University of Regensburg, D-93050 Regensburg, Germany — [2]Department of Chemistry, Columbia University, New York, New York 10027, United States — [3]School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States — [4]Department of Applied Physics and Applied Mathematics, Columbia University, New York, New York 10027, United States

We report recent results on quantum transport properties of polymethine and polyene molecular wires. These wires represent a class of linear conjugated molecules which can be understood in the context of the topological Su-Schrieffer-Heeger model. Here, we present conductance measurements in polymethine dye junctions obtained with the scanning tunneling microscope break junction technique. Supported by tight-binding and ab-initio calculations, we argue that the lack of exponential decay in the conductance trends with the system length is due to the small bond-length alternation present in the polymethine wires. We finally discuss conditions for the observation of topological modes in quantum transport experiments.

TT 74.9 Wed 18:15 H 3005

Rotational dynamics of model molecular gears: non-equilibrium Green's function approach — •Huang-Hsiang Lin[1,2], Alexander Croy[1], Rafael Gutiérrez[1], and Gianaurelio Cuniberti[1,3,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany — [4]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany

The possibility of creating nanoscale molecular gears has opened novel routes to implement true molecule-based mechanical analogs. Here, we investigate, within a model Hamiltonian approach, the rotational dynamics of a molecular gear. For this, we combine Langevin dynamics and non-equilibrium Green's functions to compute current-induced torque and damping, which allows it to study the influence of the electronic system on the rotational dynamics. Our model provides the rotational analog of the Anderson-Holstein Hamiltonian. To demonstrate the typical behavior of the gear, we present analytical and numerical calculations.

TT 75: Superconductivity: Mesoscopic Superconductivity and Quantum Circuits

Time: Wednesday 17:00–18:30 Location: H 2053

TT 75.1 Wed 17:00 H 2053

Reducing phase drift by injection locking a cavity mode driven by a Josephson junction — •Ciprian Padurariu, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany

Circuit QED devices are highly tunable radiation emitters with high photon collection efficiency, leading as candidates for on-demand single photon sources, on-demand entangled photon pairs, and sensitive single photon detectors in the microwave spectrum [1]. The main hurdle on the way to full quantum control of the emitted radiation is phase drift due to electrical noises generated from outside, as well as from within, the device [2].

In quantum optics, a well known technique to reduce phase drift is injection locking to a low intensity, narrow bandwidth laser. We borrow this technique for circuit QED by locking the active mode to a small amplitude near-resonant microwave tone. We describe theoretically the quantum dynamics of injection locking and quantify the effectiveness of the phase drift reduction. When the microwave tone is off-resonant, we describe the phenomenon of frequency pulling, where the frequency of radiation emission is shifted towards that of the microwave tone.

[1] M. Westig *et al*, Phys. Rev. Lett. **119**, 137001 (2017).
[2] S. Dambach *et al*, New J. Phys. **19**, 023027 (2017).

TT 75.2 Wed 17:15 H 2053

Noise switching at a dynamical critical point in a cavity-conductor hybrid — Andrew D. Armour[1], •Björn Kubala[2], and Joachim Ankerhold[2] — [1]School of Physics and Astronomy and Centre for the Mathematics and Theoretical Physics of Quan-

tum Non-Equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, UK — [2]Institute for Complex Quantum Systems and IQST, Ulm University, Albert Einstein-Allee 11, 89069 Ulm, Germany

Coupling a mesoscopic conductor to a microwave cavity can lead to fascinating feedback effects which generate strong correlations between the dynamics of photons and charges. We explore the connection between cavity dynamics and charge transport in a model system consisting of a voltage-biased Josephson junction embedded in a high-Q cavity, focussing on the behavior as the system is tuned through a dynamical critical point. On one side of the critical point the noise is strongly suppressed, signalling the existence of a novel regime of highly coherent transport, but on the other side it switches abruptly to a much larger value. Using a semiclassical approach we show that this behavior arises because of the strongly nonlinear cavity drive generated by the Cooper pairs. We also uncover an equivalence between charge and photonic current noise in the system which opens up a route to detecting the critical behavior through straightforward microwave measurements.

TT 75.3 Wed 17:30 H 2053

Adiabatic Simulation of the Hydrogen Molecule with Superconducting Qubits — •Marco Roth[1], Marc Ganzhorn[2], Nikolaj Moll[2], Stefan Filipp[2], Gian Salis[2], and Sebastian Schmidt[3] — [1]Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [2]IBM Research - Zurich, Zürich, Switzerland — [3]Institute for Theoretical Physics, ETH Zürich, Switzerland

Superconducting circuits are well suited for the adiabatic simulation of Hamiltonians with bosonic as well as fermionic degrees of freedom. Here, we present analytical and numerical results, which demonstrate the feasibility of simulating the groundstate of the hydrogen molecule using two superconducting qubits. In our proposal tunable two-qubit interactions are realised by parametrically modulating the frequency of a tunable bus element with an external magnetic flux. We derive the effective Hamiltonian of the device with tunable XX and YY type interactions using a time-dependent Schrieffer-Wolff transformation. Numerical simulations of a quantum annealing protocol for the groundstate of the hydrogen molecule demonstrate that the time required to reach chemical accuracy lies in the few microsecond range for typical device coherence.

TT 75.4 Wed 17:45 H 2053

A passive on-chip, superconducting circulator using a ring of tunnel junctions — •Clemens Müller[1], Shengwei Guan[1], Nicolas Vogt[2], Jared H. Cole[2], and Thomas M. Stace[1] — [1]ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Australia — [2]Chemical and Quantum Physics, RMIT University, Melbourne, Australia

We present the design of a passive, on-chip microwave circulator based on a ring of superconducting tunnel junctions. We investigate two distinct physical realisations, based on either Josephson junctions (JJ) or quantum phase slip elements (QPS), with microwave ports coupled either capacitively (JJ) or inductively (QPS) to the ring structure. A constant bias applied to the center of the ring provides the symmetry breaking (effective) magnetic field, and no microwave or rf bias is required. We find that this design offers high isolation even when taking into account fabrication imperfections and environmentally induced bias perturbations and find a bandwidth in excess of 500 MHz for realistic device parameters.

TT 75.5 Wed 18:00 H 2053

Semiclassical quantisation of spinning quasiparticles in ballistic Josephson Junctions — •Sebastian Bergeret[1], Ilya Tokatly[2], and François Konschelle[1] — [1]Material Phsyics Center (CSIC) , San Sebastian — [2]Universidad del Pais Vasco

A Josephson junction made of a generic magnetic material sandwiched between two conventional superconductors is studied in the ballistic semiclassic limit. The spectrum of Andreev bound states is obtained from the single valuedness of a particle-hole spinor over closed orbits generated by electron-hole reflections at the interfaces between superconducting and normal materials. The semiclassical quantization condition is shown to depend only on the angle mismatch between initial and final spin directions along such closed trajectories. For the demonstration, an Andreev-Wilson loop in the composite position* particle-hole*spin space is constructed and shown to depend on only two parameters, namely, a magnetic phase shift and a local precession axis for the spin. The details of the Andreev-Wilson loop can be extracted via measuring the spin-resolved density of states. A Josephson junction can thus be viewed as an analog computer of closed-path-ordered exponentials.

[1] Phys. Rev. Lett. 116, 237002 (2016)
[2] Phys. Rev. B. 94, 014515 (2016).

TT 75.6 Wed 18:15 H 2053

Spectroscopy of Two-Level-Systems in an Xmon Qubit — •Alexander Bilmes[1], Georg Weiss[1], Alexey V. Ustinov[1,2], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

Superconducting quantum circuits are close to fulfilling all criteria to realize a quantum processor. However, a severe coherence-limiting factor are Two-Level-Systems (TLS) that reside in substrate-qubit interfaces or dielectric layers such as surface oxides and the tunnel barrier of the Josephson junction. Since TLS possess an electrical dipole moment, they can couple to the oscillating field of the qubit's circuit, making them an energy sink for the qubit. We exploit this sensitivity of qubits to spectroscopically detect individual TLSs, whose transition frequencies are tuned via applied physical strain and an electrical dc field. This experimental platform enables us to investigate coherence properties of individual TLSs in various quantum circuits and to draw conclusions about their density. Here we present the first strain and dc-field dependent spectroscopy of TLSs obtained with an Xmon sample. Especially, we propose a method to distinguish TLSs hosted in Josephson contacts from surface TLSs.

TT 76: Topology: Other Topics

Time: Wednesday 17:00–18:30 Location: A 053

TT 76.1 Wed 17:00 A 053

Robustness and quantum phase transitions of the perturbed 3D toric code — •David A. Reiss[1,2] and Kai P. Schmidt[2] — [1]Dahlem Center for Complex Materials and Physics Department, Free University Berlin — [2]Chair for Theoretical Physics 1, University of Erlangen-Nürnberg

Topological quantum order in 3D represents quantum phases with exotic excitations which are spatially extended and have anyonic statistics different from bosons and fermions. This talk discusses the robustness against quantum fluctuations and the quantum phase transitions of a paradigmatic example, the 3D toric code in a uniform magnetic field. First, the qualitative dynamics of its quasiparticles according to perturbation theory is reviewed: the point excitations are mobile, while the single constituents of spatially extended excitations stay spatially localized to all orders of perturbation theory in a translationally invariant system without disorder. This is similar to excitations in so-called fracton phases, which might be employed as thermally stable topologically-protected quantum memories in contrast to the 3D toric code. Second, a variational ansatz and exact duality relations of special magnetic field cases of the toric code to other models are employed to determine the zero-temperature phase diagram. The main results are that (1) for the breakdown of 3D topological quantum order, the exotic mutual statistics of the point excitations and the spatially extended excitations is not relevant compared to their deconfinement and confinement, respectively, and that (2) the perturbed 3D toric code is robust and features a rich phase diagram.

TT 76.2 Wed 17:15 A 053

Dynamical Equilibration of Topological Properties — Andreas Kruckenhauser[1,2] and •Jan Carl Budich[1,3] — [1]Department of Physics, University of Gothenburg, SE 412 96 Gothenburg, Sweden — [2]Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

We discuss the dynamical process of equilibration of topological properties in quantum many-body systems undergoing a parameter quench between two topologically inequivalent Hamiltonians. This scenario is motivated by recent experiments on ultracold atomic gases, where a trivial initial state is prepared before the Hamiltonian is ramped into a topological insulator phase. While the manybody wave function must stay topologically trivial in the coherent post-quench dynamics, here we show how the topological properties of the single particle density matrix dynamically change and equilibrate in the presence of interactions. In this process, the single particle density matrix goes through a characteristic level crossing as a function of time, which plays an analogous role to the gap closing of a Hamiltonian in an equilibrium topological quantum phase transition. We exemplify this generic mechanism with a numerical case study on one-dimensional topological insulators.

TT 76.3 Wed 17:30 A 053

Quantum Oscillations in Insulators with Neutral Fermi Surfaces — •Inti Sodemann[1], Debanjan Chowdhury[2], and T. Senthil[2] — [1]Max-Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

We describe a theory of quantum oscillations in insulators with a fermi sea of neutral fermions minimally coupled to an emergent U(1) gauge field. In the presence of a physical magnetic field the emergent magnetic field develops a non-zero value leading to Landau quantization for the neutral fermions. We will describe the temperature and magnetic field dependence of oscillations in magnetization and in electrical resistivity and discuss suitable experimental conditions for the observation of these effects in the composite exciton fermi liquid state proposed in mixed valence insulators as well as in the spinon fermi surface state proposed in triangular organic materials.

TT 76.4 Wed 17:45 A 053

Non-Hermitian Hamiltonian for exceptional points of cavity modes — •Heinrich-Gregor Zirnstein and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig, Germany

Recently, the existence of exceptional points in uniaxial optical cavities has been predicted [S. Richter et al., Phys. Rev. A **95**, 023836 (2017)]. In order to pave the way for a topological characterization of these exceptional points, it is desirable to derive an effective non-Hermitian Hamiltonian that describes the corresponding cavity modes. Since open cavities are characterized by their transmission and reflection coefficients, i.e. their S-matrix, we use the Mahaux-Weidenmüller formula together with a partial fraction expansion to connect the S-matrix to a non-Hermitian Hamiltonian. In an exactly solvable toy model with two coalescing resonances, i.e. an exceptional point, we find that the Hamiltonian and the S-matrix describe the exceptional point with excellent agreement. Using a more realistic model for an optical cavity, we demonstrate that two exceptional points with opposite chirality merge into a Dirac point in the hypothetical limit of a decoupled cavity.

TT 76.5 Wed 18:00 A 053

Shining a light on fractional excitations — •Dirk Wulferding[1,2], Peter Lemmens[1,2], Alexander Glamazda[3], Vladimir Gnezdilov[3], A.K. Bera[4], A.T.M.N. Islam[4], Bella Lake[4], Seunghwan Do[5], Youngsu Choi[5], Vladimir Kurnosov[3], Bodo Lobbenmeier[1], and Kwang-Yong Choi[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]ILTPE, NASU, Kharkov, Ukraine — [4]Helmholtz-Zentrum Berlin, Germany — [5]Chung-Ang Univ., Seoul, Korea

Quantum spin liquid ground states host exotic, fractional spinon or Majorana fermion excitations that are notoriously difficult to verify experimentally. Raman scattering is an alternative approach used on Kitaev-, Kagome-, and Haldane-chain materials [1,2,3,4,5] to provide spectroscopic fingerprints of fractional excitations. Work supported by the Quantum- and Nanometrology initiative "QUANOMET" within Project NL-4, the NTH School "Contacts in Nanosystems", and the DFG Project LE967/16-1.

[1] Sandilands et al., PRL 114, 147201 (2015)
[2] Nasu et al., Nat. Phys. 12, 912 (2016)
[3] Glamazda et al., Nat. Commun. 7, 12286 (2016)
[4] Glamazda et al., PRB 95, 174429 (2017)
[5] Wulferding et al., PRB 82, 144412 (2010)

TT 76.6 Wed 18:15 A 053

Tailoring topological features in the excitation spectra of spin chains via their quantum spin number — •Peter Lemmens[1,2], Dirk Wulferding[1,2], Vladimir Gnezdilov[3], Vladimir Kurnosov[3], Yurii Pashkevich[4], A.K. Bera[5], A.T.M.N. Islam[5], and Bella Lake[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]ILTPE, NASU, Kharkov, Ukraine — [4]DonFTI, NASU, Donetsk, Ukraine — [5]Helmholtz-Zentrum Berlin, Germany

We provide a comparative insight into the rich spectrum of magnetic excitations in the isostructural spin chain compounds $SrCo_2V_2O_8$ ($s = 1/2$) and $SrNi_2V_2O_8$ ($s = 1$). Evidence for fractionalization is obtained for the Haldane chain in an anomalous T-dependence of the scattering intensity and other features.

Work supported by DFG Project LE967/16-1.

TT 77: Focus Session: Quantum Turbulence and Imaging of Quantum Flow of Superfluids

Quantum turbulence - turbulent motion of quantum fluids displaying superfluidity, systems such as superfluid helium and atomic Bose-Einstein condensates, which are characterized by quantized vorticity and, at finite temperatures, two-fluid behavior - represents a lively research field linking fluid mechanics, atomic physics, condensed matter, and low-temperature physics. This session covers the central aspects of quantum flows and progress in this field over recent years.

Organization: Ladislav Skrbek, Charles University, Prague; Richard Haley, Lancaster University

Time: Thursday 9:30–12:15 Location: H 0104

Invited Talk TT 77.1 Thu 9:30 H 0104

Quantum Turbulence: New Aspects of an Old Problem — •Carlo F. Barenghi — Newcastle University

Turbulence is everywhere: inside us (aorta flow), in devices which we build (jet engines) and around us (the atmosphere). From a physicist's point of view, turbulence is an old problem; the governing Navier-Stokes equation has been known since the XIX century but predicting solutions is difficult due to the nonlinearity and the huge number of degrees of freedom simultaneously excited. Recent studies have revealed new aspects of the old turbulence problem in superfluid helium and in atomic Bose-Einstein condensates, systems close to absolute zero where quantum mechanics rules the behaviour of macroscopic amounts of matter. In some of the observed regimes, this 'quantum turbulence' is utterly simple (vortex line defects moving in a perfect background) yet it displays the same properties which we observe in ordinary turbulence such as the same distribution of kinetic energy over the length scales. In other regimes quantum turbulence shows different properties, involves unusual forms of energy dissipation or displays turbulent two-fluid behaviour of great complexity. This talk will introduce the problem and its new experimental and theoretical challenges.

[1] C.F. Barenghi, L. Skrbek, and K.R. Sreenivasan, PNAS **111** (Suppl. 1), 4647 (2014).
[2] M.C. Tsatsos, P.E.S. Tavares, A. Cidrim, A.R. Fritsch, M.A. Caracanhas, F.E.A. dos Santos, C.F. Barenghi, and V.S. Bagnato, Phys. Reports **622** 1 (2016).

Invited Talk TT 77.2 Thu 10:00 H 0104

Numerical Simulation of Quantum Turbulence — •Makoto Tsubota — Department of Physics, Osaka City University, Osaka, Japan

Quantum turbulence (QT) is highly nonlinear and nonequilibrium phenomena. Thus numerical simulation is indispensable for studying QT. In this talk, we discuss some important topics of QT in atomic Bose-Einstein condensates (BECs) and superfluid helium. QT in atomic BECs includes several kinds of turbulence like vortex turbulence, wave turbulence, spin turbulence and two-component turbulence. We show these kinds of turbulence, and then focus on the recent confirmation of the cascade flux of QT in BECs trapped by a box potential. Next we discuss the coupled dynamics of the two-fluid model in superfluid helium. Superfluid is described by the vortex filament model and normal-fluid obeys the Navier-Stokes equation, and they are coupled through the mutual friction. Superfluid turbulence makes the normal fluid change its flow profile significantly, which is compared with the recent visualization experiments in thermal counterflow.

The author thanks K. Fujimoto, C. Eigen, J. Zhang, R. Lopes, N. Navon, R. Smith, Z. Hadzibabic, S. Yui and H. Kobayashi for collaboration.

Invited Talk TT 77.3 Thu 10:30 H 0104

Visualising Pure Quantum Turbulence in Fermionic Superfluid — •Viktor Tsepelin — Lancaster University, Lancaster, UK

In this talk, we present experimental and numerical studies of pure quantum turbulence in superfluid ^{3}He-B. While the flow of bulk superfluid must be irrotational, it can mimic classical turbulence by supporting singly quantised vortices. Due to the absence of friction at the lowest temperatures, quantum turbulence is significantly simpler to model than classical turbulence. We demonstrate that, despite stringent requirements to reach one ten-thousandth of a degree from absolute zero, superfluid ^{3}He contains everything required for the generation and study of quantum turbulence. For instance, we do not need to add small tracer particles to visualise turbulence, since the existing ambient thermal excitations, ballistic quasiparticles, can play that role. We explain how to use these ballistic quasiparticles to image vortex tangles produced by a mechanical agitation of the superfluid at velocities above critical. Next we discuss, numerical simulations of a realistic 3D vortex tangle and propagation of quasiparticles through it. This simulation validates the experimental visualization of turbulence and highlights interesting properties of pure quantum turbulence.

The author thanks S. Ahlstrom, A. Baggaley, C.F. Barenghi, D.I. Bradley, S.N. Fisher, E.A. Guise, R. Haley, M. Jackson, G.R. Pickett, Y. Sergeev, N.G. Suramlishvili and A. Woods for collaboration.

15 min. break.

Invited Talk TT 77.4 Thu 11:15 H 0104

Experimental Exploration of Intense Quantum Turbulence with He-II — •Philippe-E. Roche — CNRS, Grenoble, France

The exotic properties of quantum fluids open numerous opportunities to test our understanding of classical turbulence, for example on the role of dissipation and vorticity. However, each type of quantum fluids pose specific experimental challenges when it comes to generate and probe its turbulence. One quantum fluid, superfluid 4He (He-II) has favourable properties that allows to generated very intense quantum turbulence in classical wind-tunnels and stirring cells. In such conditions, a one-to-one direct comparison between classical and quantum turbulences becomes possible. We will present the recent progresses (and stumbling blocks) along this route.

Support from ANR SHREK/ECOUTURB and EC Euhit project is acknowledged

Invited Talk TT 77.5 Thu 11:45 H 0104

Visualization of Superfluid Helium Flows — •Marco La Mantia — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

The investigation of flows of superfluid helium (He II) constitutes an active and challenging research field. Flow visualization techniques, which allow following the motion of relatively small particles suspended in the fluid, have been specifically giving in recent years significant contributions to our understanding of the underlying physics. It has been shown, for example, that the derived flow-induced properties, such as the velocity statistical distribution, depend on the length scale probed by the particles, for both thermally and mechanically driven flows of He II. Quantum features appear indeed at small enough length scales, smaller than the quantum length scale of the flow, the average distance between quantized vortices, while, at larger scales, a classical (viscous-like) picture emerges, especially in the case of mechanically driven flows. The visualization results obtained to date firmly support the view that the investigation of particle dynamics in quantum flows is not only interesting in its own right but it may also lead to the deeper understanding of fluid turbulence in general.

The author thanks L. Skrbek, M. Rotter, D. Duda, E. Varga, P. Švančara and P. Hrubcová for fruitful discussions and valuable help; the support of the Czech Science Foundation under grant GAČR 16-00580S is acknowledged.

TT 78: Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions I (joint session MA/TT)

This session will focus on the novel direction of spintronics, often called spin-orbitronics, that exploits the Spin-Orbit Coupling (SOC) in nonmagnetic materials instead of the exchange interaction to open fascinating new roads for basic research and new line of technologies. A first aim of this symposium will be to review both fundamental and theoretical recent advances made in using spin-orbit effects for generating or detecting spin-polarized currents either through bulk contributions e.g. the Spin Hall Effect or at interfaces through Rashba effects or topological surface states in topological insulators. Spin-orbit coupling can also be used in magnetic materials to create new types of topological objects such as chiral domain walls or magnetic skyrmions, that have generated a strong interest in the last couple of years. The second objective of this focused session will be to review the most recent significant results obtained to generate and characterize strong interfacial Dzyaloshinskii-Moriya Interactions (DMI). Beyond the stabilization of Néel domain walls in perpendicular magnetic layers with great promises for a new generation of race track memories, it has been recently that this chiral interaction plays a crucial role in the observation of magnetic skyrmions at room temperature. The goal will be here also to gather the key advances on the physics of magnetic skyrmions as well as on the potential applications and concept devices that shall leverage on their fascinating topological properties.

Organized by: Vincent Cros (Université Paris-Sud), Giovanni Finocchio (University of Messina)

Time: Thursday 9:30–12:30 Location: H 1012

Invited Talk TT 78.1 Thu 9:30 H 1012

Understanding Spin-Charge Conversion in Topological Insulators — •Aurelien Manchon — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

The interface between TI and 3d transition metal ferromagnets (3d-

TM) represents a powerful platform for the realization of spin-charge conversion processes such as, but not limited to, spin pumping and spin-orbit torques. Uncovering the impact of 3d-TM overlayers on the surface states of TI and evaluating the resulting interfacial spin-momentum locking will undoubtedly open promising avenues for the efficient control of spin and charge currents mediated by spin-orbit coupling.

After a short review of the experimental results available, I will first discuss the spin-charge conversion processes expected from an ideal model. I will show that the very symmetry of the spin-orbit torques expected from topological surface states is quite different from the one observed experimentally. In a second part, based on recent density functional theory calculations, I will discuss the nature of interfacial orbital hybridization in 3d-TM adsorbed on Bi2Se3. Finally, based on these considerations I will present a minimal tight-binding model that allows us to inspect the transition between surface-dominated and bulk-dominated spin-orbit torque in 3d-TM/Bi2Se3 bilayers. This last model demonstrates that spin Hall effect arising from the bulk states of the topological insulator are unlikely to contribute to the last torque observed in experiments.

TT 78.2 Thu 10:00 H 1012

Impact of disorder on interfacial DMI for skyrmionics: intermixing and dusting — •Bernd Zimmermann[1], William Legrand[2], Nicolas Reyren[2], Vincent Cros[2], Stefan Blügel[1], and Albert Fert[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Unité Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay, Plaiseau, France

The spin-orbit (SOC) based Dzyaloshinskii-Moriya interaction (DMI) is of utmost importance for future nanotechnological devices, e.g. for the stabilization of small magnetic skyrmions in heterostructures such as magnetic multilayers. Additionally, the problematic role of disorder in such systems, e.g. leading to pinning of skyrmions, needs to be overcome making production processes tedious and expensive.

Here, we at first reveal from *ab initio* calculations for the important example of Co-Pt bilayers a surprisingly profound robustness of the DMI against interfacial intermixing. We incorporate disorder realistically by employing the coherent-potential approximation in combination with the Korringa-Kohn-Rostoker method. The robustness of DMI is a result of compensation, which turns out to follow simple arguments. We also explore the possibility to tune the DMI by dusting the interface with various impurities, including noble and transition metals, and elements with low and high SOC (bismuth and boron).

We acknowledge funding by a postdoc fellowship from DAAD, the EU's H2020 FET-open project "MAGicSky", and computing time on JURECA of JSC and JARA-HPC of RWTH Aachen University.

TT 78.3 Thu 10:15 H 1012

Control of the skyrmion Hall angle by combining spin-Hall effect, breathing mode and in-plane field — •Riccardo Tomasello[1], Anna Giordano[2], Roberto Zivieri[2], Vito Puliafito[3], Stefano Chiappini[4], Bruno Azzerboni[3], Mario Carpentieri[5], and Giovanni Finocchio[2] — [1]Dept. Engineering, Polo Scientifico e Didattico di Terni, University of Perugia, Terni, Italy — [2]Dept. Mathematical and Computer Sciences, Physical Sciences and Earth Sciences, University of Messina, Messina, Italy — [3]Dept. Engineering, University of Messina, Messina, Italy — [4]Istituto Nazionale di Geofisica e Vulcanologia, Roma, Italy — [5]Dept. Electrical and Information Engineering, Politecnico di Bari, Bari, Italy

The spin-Hall effect(SHE)-driven skyrmion motion is characterized by an in-plane angle, i.e. the skyrmion Hall angle (SHA)[1].

Here, we micromagnetically report, for the first time, the SHE-driven dynamics of a breathing skyrmion. In particular, we can excite the breathing mode by applying an ac perpendicular-polarized current[2] and we can control the SHA by an in-plane external field Hy. Our results show that the SHA depends on the SHE current only under the simultaneous presence of Hy and breathing mode. Our achievements can be important for understanding the origin of the SHA current dependence when the field-like torque comes from the SHE and the breathing mode is due to temperature and/or disordered parameters[3].

[1]G. Chen, Nat. Phys. 13, 112 (2017). [2]G. Finocchio et al., Appl. Phys. Lett. 107, 262401 (2015). [3]J.-V. Kim and M.-W. Yoo, Appl. Phys. Lett. 110, 132404 (2017).

TT 78.4 Thu 10:30 H 1012

Electric-field-induced and magneto-optic response properties of chiral magnetic solids — •Sebastian Wimmer, Sergiy Mankovsky, Svitlana Polesya, and Hubert Ebert — Dept. Chemie, LMU, München, Deutschland

Chiral magnetism and its manifestation in response properties such as Hall effects are one of the most attractive topics in current solid state science owing to their fascinating fundamentals as well as promising potential for application. This talk will report on the space-time symmetry restrictions on the tensor shapes of charge and spin conductivity, spin-orbit torque and (Rashba-)Edelstein effect and accompanying first-principles calculations of the respective response coefficients in Mn-based compounds experimentally known to exhibit large chirality-induced Hall effects. The numerical work has been performed using the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) multiple-scattering-based band structure method and Kubo's linear response formalism. The focus will be on chirality-driven or topological contributions arising due to a nonvanishing scalar spin chirality. Discussions will be based on computational studies of a spin texture smoothly varying between the collinear and noncollinear coplanar limits and manipulation of the spin-orbit coupling strength. Complementary results for orbital moments and current distributions as well as X-ray magnetic dichroism will be presented in addition.

30 minutes break

Invited Talk TT 78.5 Thu 11:15 H 1012

Interfacial spin-orbitronic: Rashba interfaces and topological insulators as efficient spin-charge current converters — •Juan-Carlos Rojas-Sanchez — Insitut Jean Lamour, Univ. Lorraine -CNRS, Nancy, France

New materials with large efficiency of spin-charge current interconversion are highly desirable to study new physical phenomena as well as for spintronics applications. The spin-orbit coupling (SOC) in the 2DEG states at Topological Insulator (TI) or Rashba Interfaces (RI) is predicted to be more efficient than their 3D counterparts for such interconversion. We have found the highest efficiency at room temperature using the topological insulator α-Sn [1]. The spin-to-charge current conversion in such 2D systems is called Inverse Edelstein Effect (IEE), or spin galvanic effect. I will show results of spin-to-charge conversion by spin pumping experiments and their analysis in term of inverse Edelstein Length in RI TI [1-3]. Experimental results based on ARPES and spin pumping indicate that direct contact of metallic ferromagnetic layer is detrimental for the surfaces states of topological insulators but we can keep the surfaces states of α-Sn using Ag spacer [1]. I will use the conversion parameter obtained at room temperature with α-Sn to demonstrate the very large advantage of the SOC effects in 2D interface states with respect to the Spin Hall Effect (SHE) of 3D metals and the resulting perspective for low power spintronic devices.

[1]J.-C. R-S et al. PRL 116, 096602 (2016). [2]J.-C. R-S et al. Nat. Comm 4, 2943 (2013). [3]E. Lesne, J.-C. R-S et al. Nat. Mat. 15, 1261 (2016).

TT 78.6 Thu 11:45 H 1012

Dynamical spin-orbitronic effects in exchange-bias bilayers from first-principles — •Filipe Souza Mendes Guimarães, Manuel dos Santos Dias, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The interplay between charge and spin has been extensively studied in ferromagnetic systems. Recently, the focus has shifted to antiferromagnets, which are insensitive to external magnetic fields and offer much faster dynamics. When ferromagnets and antiferromagnets are coupled through the exchange bias, we can combine the best of both worlds [1]. For a deep understanding of such complex structures, a microscopic material-specific dynamical theory, such as the one we developed, is crucial [2,3]. In this work, we apply our theory to an idealized FePt/PtMn bilayer, to identify how the ferromagnet/antiferromagnet interface contributes to the dynamical magnetization and transport properties. We demonstrate how the resonances, reaching the THz range, may enhance the currents flowing through the system. The layer-resolved magnetic interactions and spin-orbit torques can also be used to understand switching processes of this type of heterostructures.

[1] S. Fukami *et al.*, Nature Materials **15**, 535–541 (2016)
[2] F. S. M. Guimarães *et al.*, Phys. Rev. B **92**, 220410(R) (2015)
[3] F. S. M. Guimarães *et al.*, Sci. Rep. **7**, 3686 (2017)
– Funding from the European Research Council (ERC) under the Euro-

pean Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 – DYNASORE).

TT 78.7 Thu 12:00 H 1012

Determination of the Dzyaloshinskii-Moriya interaction in epitaxial asymmetric trilayers — •Fernando Ajejas[1], Adrian Gudin[1], Ruben Guerrero[1], Diane Chaves[2], Viola Křižáková[2], Jan Vogel[2], Stefania Pizzini[2], Paolo Perna[1], and Julio Camarero[1] — [1]IMDEA Nanociencia, Campus Universidad Autónoma de Madrid, Spain — [2]CNRS, Institut Néel, Université Grenoble Alpes, 38042 Grenoble, France

We will address the issue of domain wall velocity limitations in ultra-thin magnetic films in symmetric and non-symmetric stacks. The DW wall speed is in general limited by the breakdown. This limitation is overcome in asymmetric trilayer systems in which Co is deposited on a heavy metal: in this case the Dzyaloshinskii-Moriya interaction (DMI) favours chiral Néel walls that are more stable against precession. It has been shown that in asymmetric thin layer systems the domain wall speed saturates above the Walker field, which is in general not the case for symmetric samples. Using magneto-optical Kerr magnetometry and microscopy, we measured domain wall velocities driven by magnetic field pulses in Pt/Co/Pt and Pt/Co/M (M=Al, Cu, Ir,) Typical Co thicknesses is 0.6 nm. The main result is that the saturation velocity of the DWs in the Pt/Co/M trilayers is strongly dependent on the nature of the top interface. We attribute this variation to the different contribution of the Co/M interfaces to the total DMI strength. The largest saturation velocities (typically 300m/s) are obtained for the samples covered by Al, Cu, or an oxyde, while much smaller velocities (typicaly 100m/s) are obtained for Ir or Ta top layers.

TT 78.8 Thu 12:15 H 1012

The spin-Hall stationarity conditions in the light of the second law of thermodynamics — •Jean-Eric Wegrowe[1], Rober Benda[1], Jean-Michel Dejardin[2], and Miguel Rubi[3] — [1]LSI, Ecole polytechnique, Palaiseau, France — [2]Laboratoire de Mathématique et Physique, Université de Perpignan, France — [3]Facultat de Fisica, Universitat de Barcelona, Spain

The determination of the stationary states for the bulk spin-Hall effect are discussed in the context of the two spin-channel model. It is shown that the usual stationarity condition (namely no explicit time-dependence) leads to an indeterminacy: different stationary states can equally be defined [1]. A first state S1 is characterized by a transverse pure spin current and no electric field while a second stationary state S2 is characterized by spin-dependent electric fields and no transverse current. The two states have the same properties with respect to spin-accumulation and spin-Hall angle, but not with respect to the total power dissipated.

The application of the second law of thermodynamics allows a reformulation of the problem in the form of a variational principle under constraints (Kirchhoff-Helmholtz principle). The constraints include charge accumulation and spin-flip scattering. The stationary state is then defined univocally: the first state S1 is found for the Corbino disk while the second state S2 is found for the Hall bar [2].

[1] J.-E. Wegrowe, J. Phys.: Cond Matter 29, 485801 (2017). [2] J.-E. Wegrowe, R. Benda, M. J. Rubì, Europhys. Lett. 18, 67005 (2017).

TT 79: Superconductivity: Superconducting Electronics - Circuit QED

Time: Thursday 9:30–12:45 Location: H 2053

TT 79.1 Thu 9:30 H 2053

Anharmonic quantum oscillator under field drive: probing the AC Stark shift of higher levels — •Martin Weides[1,2], Andre Schneider[1], Patrizia Stehle[1], Jochen Braumueller[1], Hannes Rotzinger[1], Lingzhen Guo[3], Michael Marthaler[3], and Alexey Ustinov[1] — [1]Institute of Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Materials Science in Mainz, University Mainz, Germany — [3]Institute for Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

We report on the investigation of a superconducting anharmonic multilevel circuit under the influence of a detuned and strong microwave drive. The AC Stark shift of higher level transition frequencies caused by the applied drive is investigated. We demonstrate that this shift depends on the anharmonicity, the drive amplitude and the detuning between drive and transition frequency. For large detunings we find the shift to be linear to the power of the drive. Experimentally, multi-photon transitions via virtual energy levels of our system up to the third excited state are observed. The measured AC Stark shift of higher order multi-photon transitions under increasing drive amplitude is demonstrated to be in good agreement with the analytic model and numerical simulations. Having a detailed model of the qudit behavior, we can take the qudit as a sensor for high excitation numbers in coupled harmonic systems like microwave resonators or magnonic systems by observing the shift of the qudit levels.

TT 79.2 Thu 9:45 H 2053

Quasiparticle dynamics in microwave resonators from granular aluminum close to the superconductor to insulator transition — •Lukas Grünhaupt[1], Nataliya Maleeva[1], Sebastian T. Skacel[1], Florence Lévy-Bertrand[2], Alexey V. Ustinov[1,3], Hannes Rotzinger[1], Alessandro Monfardini[2], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut Néel, CNRS and Université Grenoble Alpes, Grenoble, France — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

Superconducting high kinetic inductance elements constitute a valuable resource for quantum circuit design and millimeter-wave detection. Granular aluminum (GrAl) is a particularly interesting material since it has already shown a kinetic inductance in the range of nH/□ and its deposition is compatible with conventional $Al/AlO_x/Al$ Josephson junction fabrication. We characterize microstrip resonators in the GHz range fabricated from GrAl thin films with resistivity and geometry dependent kinetic inductances between 0.3 and 2.0 nH/□. Our results suggest that non-equilibrium quasiparticles limit their internal qualitiy factors at a level of 10^5. We extract quasiparticle relaxation times on the order of 1 s and we observe quasiparticle producing events approximately every 30 s. The current level of coherence of GrAl resonators makes them attractive for integration in quantum devices, while it also evidences the need to reduce the density of non-equilibrium quasiparticles.

TT 79.3 Thu 10:00 H 2053

Circuit quantum electrodynamics of granular Aluminum resonators — •Nataliya Maleeva[1], Lukas Grünhaupt[1], Florence Levy-Bertrand[2], Martino Calvo[2], Patrick Winkel[1], Wolfgang Wernsdorfer[1], Alexey Ustinov[1,3], Hannes Rotzinger[1], Alessandro Monfardini[2], Mikhail Fistul[3], and Ioan Pop[1] — [1]Physikalisches Institut, KIT, Karlsruhe, Germany — [2]Institut Neel, CNRS, Universite Joseph Fourier Grenoble I, Grenoble, France — [3]RQC, National University of Science and Technology MISIS, Moscow, Russia

Granular Aluminum (GrAl) thin film structures can be used as superinductors in superconducting qubits, or as high kinetic inductance detectors for mm wavelength radiation. Their microstructure consists of pure aluminum grains of 2-5 nm diameter, separated by thin aluminum oxide barriers, forming a self-assembled network of Josephson junctions (JJ). We model microwave resonators made of GrAl as a 1D array of effective Josephson junctions, directly relating their dispersion relation and nonlinearity to GrAl microstructure. Below 20 GHz, we can measure the dispersion relation of GrAl stripline resonators using a circuit QED setup. We observe self-Kerr coefficients in the range of $10^{-1} - 10^4$ Hz/photon, depending on the resonator geometry and the sheet resistance of the film. Using an optical setup designed for mm wave spectroscopy we measure the plasma frequency of the film around 75 GHz. These results are in agreement with values calculated using our effective JJ chain model, and they are encouraging for the design of cQED elements such as qubits or parametric amplifiers using GrAl.

TT 79.4 Thu 10:15 H 2053

Echo trains in pulsed electron spin resonance — •Stefan Weichselbaumer[1,2], Petio Natzkin[1,2], Christoph W.

Zollitsch[1,2], Martin S. Brandt[2,3], Rudolf Gross[1,2,4], and Hans Huebl[1,2,4] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Walter Schottky Institut, Technische Universität München, Garching, Germany — [4]Nanosystems Initiative Munich, Munich, Germany

Strong coupling between a spin ensemble and a microwave resonator is essential for a coherent exchange of excitation. While today experiments mostly focus on continuous wave experiments, we investigate the dynamics of the coupled spin-resonator system in the strong coupling regime by pulsed ESR measurements. In particular, we use Hahn echos and observe multiple unexpected echo signatures after the first conventional echo. Experimentally, we study an ensemble of phosphorus donor spins in isotopically purified ^{28}Si with ms coherence times. With a static magnetic field, we tune their transition frequency into resonance with a superconducting lumped element microwave resonator. We present experimental data within and outside the strong coupling regime and discuss a model predicting and corroborating the amplitude evolution of the echos based on the echo separation time, the dephasing rate of the spin ensemble, and the linewidth of the microwave resonator.

We acknowledge financial support from the DFG via SPP 1601.

TT 79.5 Thu 10:30 H 2053

Strong coupling between a carbon nanotube based quantum dot circuit and a microwave cavity — •Tino Cubaynes, Laure Bruhat, Jeremie Viennot, Matthieu Dartiailh, Matthieu Desjardins, Audrey Cottet, and Takis Kontos — Laboratoire Pierre Aigrain, ENS, Paris 75005, FRANCE

Circuit quantum electrodynamics allows one to probe, manipulate and couple superconducting quantum bits using cavity photons at an exquisite level. One of its cornerstones is the possibility to achieve the strong coupling which allows one to hybridize coherently light and matter. Mesoscopic-QED inherits the c-QED toolbox and applies it to nano-circuits. I will present cavity transmission and simultaneous transport measurements on a quantum dot circuit -a Cooper pair splitter- embedded in a microwave cavity. By using a new cavity-DQD coupling scheme, the strong coupling of a photonic system to a hybrid circuit has been reached [1]. Our findings open the path to ultra-long distance entanglement of quantum dot based qubits. They could be adapted to many other circuit designs, shedding new light on the roadmap for scalability of quantum dot setups. I will also present current development on a nanofabrication technique allowing integration of prisitine carbon nanotube in mesoscopic-QED devices. From this perspective we can envision carbon nanotube based circuit with high tunability and very low decoherence.

[1] L. E. Bruhat , T. Cubaynes, et al. arXiv:1612.05214 (2016)

TT 79.6 Thu 10:45 H 2053

Non-degenerate Parametric Resonance in Superconducting Cavity — Waltraut Wustmann[1] and •Vitaly Shumeiko[2] — [1]Laboratory for Physical Sciences, College Park, Maryland 20740, USA — [2]Chalmers University of Technology, S-41296 Göteborg, Sweden

We present a theory for non-degenerate parametric resonance in a tunable superconducting cavity. We consider both regimes of down- and up- conversion. In the first, parametric amplification regime we focus a nonlinear gain close to the parametric instability threshold. Here the quantum noise undergoes four-mode squeezing and less efficient amplification than the coherent signal. This results in enhancement of output signal-to-noise ratio compared to the input.

Above the instability threshold, the system enters the parametric oscillation regime with two correlated beams having uncertain phase difference. Continuous degeneracy of the oscillator state is in drastic contrast to the two-fold degeneracy of the degenerate parametric oscillator. This property leads to a broadening of the output radiation spectrum, and divergence of the linear response at the oscillation frequencies. Application of a small on-resonance input lifts the degeneracy and locks the radiation phases.

For the frequency conversion regime we evaluate a nonlinear conversion coefficient, and identify an optimum pump strength at which a full inter-mode conversion can be achieved.

[1] W. Wustmann, V. Shumeiko, Phys. Rev. Appl. 8 (2017) 024018.

15 min. break.

TT 79.7 Thu 11:15 H 2053

Time-Translation Symmetry Breaking and Reentrant First Order Transition in Periodically Driven Quantum Oscillators — •Jennifer Gosner[1], Yaxing Zhang[2], Mark Dykman[3], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Germany — [2]Department of Physics, Yale University, USA — [3]Department of Physics and Astronomy, Michigan State University, USA

Breaking of discrete time-translation symmetry is a well-known phenomenon in dissipative periodically driven systems. Such systems reveal generic properties, which apply to all multiple-period transitions, but do not occur in period doubling. Here, we investigate a nonlinear oscillator, that is driven at three times the eigenfrequency [1]. Multiple crossings of eigenstates occur with varying parameters of the driving field. Physically, they result from interference of the Floquet wave functions in the classically inaccessible region. We discuss time-translational symmetry breaking, and develop a detailed analysis of the phase-space structure and its symmetries.

In the presence of dissipation, a quantum oscillator can support three states of period-three vibrations that co-exist with the state of no vibrations. With varying detuning a reentrant first-order transition appears, where the populations of these states change exponentially strongly. We study tunneling as well as switching via quantum activation. The results allow revealing "time crystals" in simple quantum systems, including the systems studied in circuit QED.

[1] Y.Zhang et al., PRA **96**, 052124 (2017)

TT 79.8 Thu 11:30 H 2053

Enhancing photon squeezing one Leviton at a time — •Flavio Ronetti[1,2], Dario Ferraro[3], Jérôme Rech[2], Thibaut Jonckheere[2], Thierry Martin[2], and Maura Sassetti[1] — [1]Università di Genova and CNR-SPIN, Via Dodecaneso 33, 16146, Genova, Italy — [2]Aix Marseille Univ, Université de Toulon, CNRS, CPT, Marseille, France — [3]Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, I-16163 Genova, Italy

A mesoscopic device in the simple tunnel junction or quantum point contact geometry emits microwaves with remarkable quantum properties, when subjected to a sinusoidal drive in the GHz range. In particular, single and two-photons squeezing as well as entanglement in the frequency domain have been recently reported [1]. By revising the photo-assisted noise analysis developed in the framework of electron quantum optics [2], we present a detailed comparison between the cosine drive case and other experimentally relevent periodic voltages like rectangular and Lorentzian pulses [3]. We show that the latter drive is the best candidate in order to enhance quantumness and purity of the outgoing single and two-photons states in view of quantum information perspectives.

[1] G. Gasse, et al., Phys. Rev. Lett. 111, 136601 (2013).
[2] J. Dubois, et al., Nature 502, 659 (2013).
[3] D. Ferraro, et al., in preparation (2017)

TT 79.9 Thu 11:45 H 2053

Remote state preparation with propagating quantum microwaves — •Stefan Pogorzalek[1,2], Kirill G. Fedorov[1,2], Behdad Ghaffari[1,2], Minxing Xu[1,2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Edwar Xie[1,2,3], Achim Marx[1], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Propagating two-mode squeezed (TMS) microwave states enable applications of quantum communication and sensing with superconducting quantum circuits [1]. In our work, we perform experimental studies of TMS microwave states, which are generated by the means of flux-driven Josephson parametric amplifiers and linear circuit elements [2, 3]. We use the TMS states for the demonstration of a basic quantum communication protocol, namely, remote state preparation (RSP) in which the sender has knowledge of a to-be-teleported quantum state. In particular, we experimentally demonstrate the feasibility of the continuous variable RSP protocol with analog feed-forward by remotely preparing single-mode squeezed states.

The authors acknowledge support from DFG through FE 1564/1-1.

[1] R. Di Candia *et al.*, EPJ Quantum Technol. **2**, 25 (2015).
[2] K. G. Fedorov *et al.*, Phys. Rev. Lett. **117**, 020502 (2016).
[3] K. G. Fedorov *et al.*, arXiv:1703.05138 (2017).

TT 79.10 Thu 12:00 H 2053

New Spectroscopic Methods in Quantum Microwave Photonics: Accessing Correlated Noise, and Multiphoton Processes — •Tomás Ramos and Juan José García-Ripoll — Instituto de Física Fundamental IFF CSIC, Calle Serrano 113b, Madrid 28006, Spain

In this talk, we present new methods for characterizing correlated noise and multiphoton scattering processes in experiments with propagating photons in superconducting circuits.

First, we study how correlated dephasing noise is manifested in single-photon scattering experiments. We introduce a general noise model that describes correlated gaussian and non-gaussian noise, 1/f noise, white noise, telegraph noise, etc, and we study how the transmission lineshapes are modified on each case. Only for white noise, the dephasing can be characterized by a constant 'dephasing rate', but a general dephasing response depends on the photon's detuning. In addition, we demonstrate a general relation between these spectroscopic measurements and standard time-resolved Ramsey measurements, allowing one to infer the effect of correlated noise in one experiment from the knowledge of the other.

Second, we provide a spectroscopic protocol to characterize photon-photon interactions mediated by a qubit in a transmission line. The experimental method requires coherent state inputs and homodyne detection at the qubit's output, and it can be generalized to determine the multiphoton scattering matrix of any quantum object [1].

[1] T. Ramos, J.J. García-Ripoll, PRL 119, 153601 (2017).

TT 79.11 Thu 12:15 H 2053

Probing the strongly driven spin-boson model in a superconducting quantum circuit — L. Magazzù[1], P. Forn-Diaz[2], Ron Belyansky[2], J.-L. Orgiazzi[2], M.A. Yurtalan[2], M.R. Otto[2], A. Lupascu[2], C. Wilson[2], and •M. Grifoni[3] — [1]Institute of Physics, University of Augsburg, Universitätsstrasse 1, D-86135 Augsburg, Germany — [2]Institute for Quantum Computing, University of Waterloo, Waterloo N2L 3G1, Canada — [3]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

Quantum two-level systems interacting with the surroundings are ubiquitous in nature. The interaction suppresses quantum coherence and forces the system towards a steady state. Such dissipative processes are captured by the paradigmatic spin-boson model, describing a two-state particle, the "spin", interacting with an environment formed by harmonic oscillators. A fundamental question to date is to what extent intense coherent driving impacts a strongly dissipative system. Here we investigate experimentally and theoretically a superconducting qubit strongly coupled to an electromagnetic environment and subjected to a coherent drive. This setup realizes the driven Ohmic spin-boson model. We show that the drive reinforces environmental suppression of quantum coherence, and that a coherent-to-incoherent transition can be achieved by tuning the drive amplitude. An out-of-equilibrium detailed balance relation is demonstrated. These results advance fundamental understanding of open quantum systems in the case of strong light-matter interaction.

[1] arXiv:1709.01157

TT 79.12 Thu 12:30 H 2053

Quasiparticle dynamics in Andreev quantum dots — •Leandro Tosi, Marcelo Goffman, Cristian Urbina, and Hugues Pothier — Quantronics group, SPEC, CEA Saclay, France

In contrast with a bulk superconductor, a single-channel phase-biased superconducting weak link hosts a discrete subgap quasiparticle state, called "Andreev state". It can be seen as a sort of quantum dot in which zero, one or two quasiparticles can be trapped, not due to electrostatic barriers, but to the phase drop. This "Andreev quantum dot" constitutes a very simple playground to explore the foundations of mesoscopic superconductivity.

I will present experiments on Andreev quantum dots obtained at one-atom contacts between aluminum electrodes, in which we probe the dynamics of quasiparticles trapping and un-trapping using circuit-QED like techniques [1]. I will focus in particular on the effect of the cavity on this dynamics.

[1] C. Janvier et al., Science 349, 1199 (2015)

TT 80: Graphene

Time: Thursday 9:30–13:00 Location: H 3005

TT 80.1 Thu 9:30 H 3005

Transport in systems with nodal degeneracy — •Andreas Sinner and Klaus Ziegler — Institut für Physik, Theorie II Universität Augsburg Universitätsstr. 1 D-86159, Augsburg, Germany

We study the DC conductivity of a weakly disordered 2D electron gas with two bands and spectral nodes, employing the field theoretical version of the Kubo-Greenwood conductivity formula. Disorder scattering is treated within the standard perturbation theory by summing up ladder and maximally crossed diagrams. The emergent gapless (diffusion) modes determine the behavior of the conductivity on large scales. We find a finite conductivity with an intermediate logarithmic finite-size scaling towards smaller conductivities but do not obtain the logarithmic divergence of the weak-localization approach. Our results agree with the experimentally observed logarithmic scaling of the conductivity in graphene with the formation of a plateau near the universal conductivity. We extend our analysis by including effects of anisotropy on hexagonal lattices.

[1] A. Sinner, K. Ziegler, Phys. Rev. B 90, 174207 (2014).
[2] A. Sinner, K. Ziegler, J. Phys. Condens. Matter. 28, 305701 (2016).
[3] A. Sinner, K. Ziegler, Europhys. Lett. 119, 27001 (2017).

TT 80.2 Thu 9:45 H 3005

Echoes of zitterbewegung in graphene — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Viktor Krueckl[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, Germany — [2]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle Upon Tyne, UK

In the last decade, Zitterbewegung (ZB) – the trembling motion of (effectively) relativistic particles – has attracted the attention also in the solid state community [1], e.g. in graphene [2]. The advantage of solid state systems is the lower energy difference of particle- and antiparticle-like states that defines the frequency of the ZB, which is the reason for a supposedly easier experimental detection.

However, the ZB of a wave packet decays over time because of the separation of the two sub-wave packets in the two bands and the according loss of interference. On the other hand, Quantum Time Mirrors in graphene have been recently proposed to invert the motion of wave packets [3]. Here, we discuss the application of the Quantum Time Mirrors on the sub-wave packets after the ZB has decayed, which is supposed to make the separated sub-wave packets interfere again and accordingly, to create an echo of the ZB.

[1] J. Schliemann, D.Loss, R. M. Westervelt, Phys. Rev. Lett. **94**, 206801 (2005)
[2] W.Zawadzki and T.M. Rusin , J. Phys.: Condensed Matter **23**, 143201 (2011)
[3] P. Reck, C. Gorini, A. Goussev, V. Krueckl, M. Fink, K. Richter, Phys. Rev. B **95**, 165421 (2017)

TT 80.3 Thu 10:00 H 3005

Tunable quantum random walks in graphene — •Vanessa Junk, Phillipp Reck, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

One of the many fascinating aspects connected to quantum computing are quantum random walks [1] which can be used to speed up classical algorithms.

We show that such a quantum walk can be physically implemented in graphene by extending a recently proposed Quantum Time Mirror [2]. The pulse used in Ref. [2] for the time reversal can be tuned such that an initial wave-packet is split into two parts moving in opposed directions. By adjusting the pulse length, the amplitudes of the two resulting packets can be chosen arbitrarily. Hence, applying such a pulse is equivalent to the coin toss in descrete time quantum walks [3] with the advantage of having additional degrees of freedom in the "coin". Moreover, the system we are dealing with is continuous in space. This allows for arbitrary timing of the pulses which leads to further variety in the probability distribution of the wave-packet in space.

In this talk we will discuss the described system and show the influence of the coin parameters on the resulting quantum walk of charge carriers in graphene.

[1] Y. Aharonov, L. Davidovich, and N. Zagury, Phys. Rev. A **48**, 1687-1690 (1993)
[2] P. Reck, C. Gorini, A. Goussev, V. Krueckl, M. Fink, K. Richter, Phys. Rev. B **95**, 165421 (2017)
[3] J. Kempe, Contemporary Physics **44**, 307-327 (2003)

TT 80.4 Thu 10:15 H 3005

Quantum interference assisted spin-filtering in graphene nanoflakes — •Angelo Valli[1,2], Adriano Amaricci[1,2], Valentina Brosco[1,2], and Massimo Capone[1,2] — [1]Scuola Superiore di Studi Avanzati (SISSA), Trieste, Italy — [2]Democritos National Simulation Center, CNR-IOM, Trieste, Italy

We present a theoretical investigation of the transport properties through magnetic zigzag graphene nanoflakes. In the ballistic regime, we identify transmission antiresonances as clear fingerprints of destructive quantum interference (QI), analogous to those observed in molecular junctions. The QI antiresonances are remarkably robust and can be rationalized in terms of symmetries. In the presence of short-range magnetic ordering, the interplay of QI and magnetism results in spin-resolved QI features and in a nearly-perfect QI-assisted spin-filtering effect. We also devise a protocol to achieve electrostatic control over the efficiency of the spin filter. Such a device benefits of the extraordinary conduction properties of graphene, and operates without any external magnetic field, paving the path toward QI-assisted spintronics.

TT 80.5 Thu 10:30 H 3005

Valleytronics in elastically defomed graphene — •Nikodem Szpak[1], Thomas Stegmann[2], and Ralf Schützhold[1] — [1]Faculty of Physics, University of Duisburg-Essen, Germany — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca, Mexico

Electrons in graphene obey at low energies the 2D-Dirac equation with two psuedospin (valley) degrees of freedom. Manipulation of the valley polarization of the electronic current has potential applications in nanoelectronics, known as valleytronics. We discuss systems based on elastically deformed graphene in which the Dirac equation couples to effective curvature and pseudo-magnetic field introduced by strain. We introduce the basic theory and special approximations developed to enable an efficient design of intended valleytronic systems. We present results of numerical simulations of the current flow and compare different models. Finally, we present particular systems for efficient manipulation of the valley polarization which, among others, can act as ultrasensitive nanosensors.

TT 80.6 Thu 10:45 H 3005

Hybrid Monte Carlo simulations the electronic Lifshitz transition in monolayer graphene — •Michael Körner[1], Dominik Smith[1], Pavel Buividovich[2], Maksim Ulybyshev[2], and Lorenz von Smekal[1] — [1]Institut für theoretische Physik, Justus Liebig Universität Gießen, 35392 Gießen, Germany — [2]Institut für theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

We report on Hybrid-Monte-Carlo simulations at finite spin density of the pi-band electrons in monolayer graphene with realistic interelectron interactions. Unlike simulations at finite charge-carrier density, these are not affected by a fermion-sign problem. We nevertheless observe effects that are quite similar to observations in angle resolved photoemission spectroscopy experiments on charge doped graphene, such as an interaction-induced warping of the Fermi contours or a reduction of the bandwidth. Furthermore, we find evidence that the neckdisrupting Lifshitz transition, which occurs when the Fermi level traverses the van Hove singularity (VHS), might become a true quantum phase transition due to interactions. This is in-line with an instability of the VHS towards the formation of electronic ordered phases, which has been predicted by a variety of different theoretical approaches.

TT 80.7 Thu 11:00 H 3005

Lifshitz transition and thermoelectric properties of bilayer graphene — Dominik Suszalski, Grzegorz Rut, and •Adam Rycerz — Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland

This is a numerical study of thermoelectric properies of ballistic bilayer graphene in the presence of trigonal warping term in the effective Hamiltonian. We find, in mesoscopic samples of the length exceeding 10 micrometers at sub-Kelvin temperatures, that both the Seebeck coefficient and the Lorentz number show anomalies (the additional maximum and minimum, respectively) when the electrochemical potential is close to the Lifshitz energy, which can be attributed to the presence of the van Hove singularity in a bulk density of states. At higher temperatures the anomalies vanish, but measurable quantities characterizing remaining maximum of the Seebeck coefficient still unveil the presence of massless Dirac fermions. Behavior of the thermoelectric figure of merit (ZT) is also discussed.

15 min. break.

TT 80.8 Thu 11:30 H 3005

Suppression of high magnetic-field-induced electronic transitions in graphite micro flakes — •J. Barzola Quiquia[1], C. Precker[1], M. Stiller[1], M. Zoraghi[1,3], T. Förster[2], Th. Herrmannsdörfer[2], and P. Esquinazi[1] — [1]Felix-Bloch Institute for Solid State Physics, University of Leipzig, 04103 Leipzig, Germany — [2]Forschungszentrum Dresden-Rossendorf, PF 510119, D-01314 Dresden, Germany — [3]MPI for Human Cognitive and Brain Sciences, 04103 Leipzig, Germany

We report a detailed study of the magnetoresistance (MR) in bulk and microflakes of highly oriented pyrolytic graphite samples. Measurements have been done at different temperatures with stationary (7 T) and pulsed magnetic fields to 62 T applied parallel to the c-axis. We found that at low temperature, the MR increases rapidly from 0 to $\approx$ 20 T, and then it saturates at fields to $\approx$ 50 T. At higher fields the MR decreases. At temperatures $T \geq 50$ K, the MR increases rapidly from 0 to $\approx$ 20 T, at higher fields it increases further but with a smaller slope. In thick samples we found also the well-known sudden jumps in the MR in a restricted field region that were interpreted in the past as field-induced electronic phase transitions in graphite associated with a charge density wave. In the case of the thin graphite flakes the jumps in the MR nearly vanish. Our present results indicate that the field-induced electronic transitions observed in bulk graphite are not intrinsic but originate at the two-dimensional (2D) metallic system formed at the interfaces between the different stacking orders or twisted graphite crystalline regions only.

TT 80.9 Thu 11:45 H 3005

Extreme magneto resistance in Ar^+ ion radiated graphene — •Paul Linsmaier[1], Lorenz Weiss[1], Tobias Weinberger[1], Ferdinand Kisslinger[2], Heiko B. Weber[2], and Christoph Strunk[1] — [1]Inst. f. Exp. and Appl. Physics, University of Regensburg — [2]Fac. of Physics, F.-A. University Erlangen-Nürnberg

We report on magnetotransport measurements of epitaxial graphene on SIC [1], bombarded with Ar^+ ions. For different strength of disorder, $\rho_\square(300\text{K}) = 15 - 30\text{k}\Omega$, an Arrhenius temperature dependence of the resistance is found at low temperatures and zero magnetic field. In perpendicular magnetic field, we see a drastic change in the conductivity from Arrhenius ($B = 0$T) to Efros-Shklovskii ($B_\perp = 12$T) Coulomb-gap-like behavior, with an extreme negative magnetoresistance (NMR) of $\rho(B_\perp)/\rho(0) < 0.01$ at $B = 12$T and 300mK. This might indicate a gap, resulting from magnetic interactions in graphene. In parallel magnetic field, we find a much smaller magnetoresistance with a sign change from a NMR at low temperatures to a positive magnetoresistance with increasing temperature and magnetic field.
[1] K. V. Emtsev et al., Nat. Mat. 8, 203 - 207 (2009).

TT 80.10 Thu 12:00 H 3005

Mechanisms of magnetoconductance oscillations in graphene pn junctions — •Ming-Hao Liu[1] and Klaus Richter[2] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

Two-terminal conductance of a graphene pn junction may oscillate with various dependencies, such as carrier density, magnetic field, or even the position of the pn junction. In this talk, various mechanisms giving rise to the oscillation are discussed, focusing on the recent two experiments supported by our quantum transport simulations, one at intermediate magnetic fields [1] and the other at high magnetic fields [2]. The former corresponds to a regime with high filling factors and shows an unusual even-odd effect of the Landau levels, with the underlying mechanism not completely clear. The latter corresponds to a regime with low/lowest filling factors, showing first experimental evidence of valley-isospin-dependent conductance oscillation [3].
[1] H. Overweg et al., Nano Lett. **17**, 2852 (2017)
[2] C. Handschin et al., Nano Lett. **17**, 5389 (2017)

[3] J. Tworzydło et al., Phys. Rev. B **76**, 035411 (2007)

TT 80.11 Thu 12:15 H 3005

Husimi Projections in Graphene: Measuring Klein Tunneling — •George Datseris, Theo Geisel, and Ragnar Fleischmann — Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany

One of the most intriguing electronic properties of graphene is the occurrence of Klein Tunneling: ballistic conduction electrons are expected to show full transmission on normal incidence on almost arbitrary potential barriers. On oblique incidence the transmission decays rapidly, leading to a collimation effect at the barrier. Recently graphene experiments have reached the ballistic regime and measurements confirmed collimated transmission, but measuring the characteristic transmission versus the angle of incidence $T(\theta)$ directly seems to be still out of reach. One reason for this is that it is hard to define an angle of incidence (and even hard to measure) in both experiments and tight-binding calculations.

In order to analyse $T(\theta)$ in a tight-binding quantum transport model we modify and employ the Husimi projection. We combine this approach with a Landauer-Büttiker type description of e.g. a graphene pn-junction. This allows us to observe $T(\theta)$ in a controlled but experimentally relevant model. In the absence of a magnetic field our results almost perfectly match the semi-classically derived formulas for transmission found in the literature. In the presence of a magnetic field, however, our results show strong differences from the semi-classical predictions.

TT 80.12 Thu 12:30 H 3005

Logarithmic Low-Bias Anomalies in the Differential Conductance of Graphene Structures — •Matthias Popp, Ferdinand Kisslinger, and Heiko B. Weber — Friedrich-Alexander-Universität Erlangen-Nürnberg Lehrstuhl für Angewandte Physik Staudtstraße 7 91058 Erlangen

We measured the voltage-dependent differential conductance of graphene-graphene tunneling junctions at low temperatures in order to probe electron-electron interaction corrections on the density of states (DOS). As predicted by Altshuler and Aronov [1] a logarithmic voltage dependence was observed [2]. Tunneling junctions provide a sharp voltage drop, therefore their differential conductance is a good measure for the DOS. To our surprise we also found logarithmic voltage dependencies in the differential conductance of graphene stripes where no sharp voltage drop is present. We explain this with a model involving voltage dependent heating of electrons in combination with electron-electron interaction as well as weak localization corrections to conductivity, both of which exhibit a logarithmic temperature dependence. We give an overview how to differentiate between these effects which all manifest themselves in logarithmic low-bias anomalies in differential conductance.

[1] B. Altshuler, A. Aronov, *Electron-Electron Interactions in Disordered Systems*, North Holland (1985)
[2] F. Kisslinger, et al., Annalen der Physik 1700048 (2017)

TT 80.13 Thu 12:45 H 3005

Interplay between the moiré superlattice and a npn-junction in a graphene-hBN heterostructure — •Rainer Kraft[1], Pranauv Balaji Selvasundaram[1,2], Ralph Krupke[1,2], Klaus Richter[3], Ming-Hao Liu[3,4], and Romain Danneau[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University Darmstadt, Darmstadt, Germany — [3]Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany — [4]Department of Physics, National Cheng Kung University, Tainan, Taiwan

Here, we present measurements on a device based on a graphene/hexagonal boron nitride van der Waals heterostructure with a moiré superlattice. The superlattice structure modulates the electronic band structure featuring interesting physics, such as new moiré minibands for Dirac electrons in graphene. With the combination of overall back-gate and local top-gate forming a npn-junction we are able to probe the effect of the superlattice by measuring complex sets of Fabry-Pérot interferences of confined charge carriers in several cavities as functions of bias or magnetic field. The decoding of the resulting interference patterns gives insight into the effects of the moiré superlattice on the band structure and as well on the nature of the cloned Dirac fermions.

TT 81: Nonequilibrium Quantum Many-Body Systems III

Time: Thursday 9:30–11:15 Location: H 3010

TT 81.1 Thu 9:30 H 3010

Dynamical Quantum Phase Transitions in Systems with Continuous Symmetry Breaking — •Simon Weidinger[1], Markus Heyl[2,1], Alessandro Silva[3], and Michael Knap[1] — [1]Department of Physics and Institute of Advanced Study, Technical University of Munich, 85748 Garching, Germany — [2]Max-Planck-Institute für Physik komplexer Systeme, 01187 Dresden, Germany — [3]SISSA - International School for Advanced Studies, via Bonomea 265, 34136 Trieste, Italy

Interacting many-body systems that are driven far away from equilibrium can exhibit phase transitions between dynamically emerging quantum phases, which manifest as singularities in the Loschmidt echo. Whether and under which conditions such dynamical transitions occur in higher-dimensional systems with spontaneously broken continuous symmetries is largely elusive thus far. Here, we study the dynamics of the Loschmidt echo in the three dimensional O(N) model following a quantum quench from a symmetry breaking initial state. The O(N) model exhibits a dynamical transition in the asymptotic steady state, separating two phases with a finite and vanishing order parameter, that is associated with the broken symmetry. We analytically calculate the rate function of the Loschmidt echo and find that it exhibits periodic kink singularities when this dynamical steady-state transition is crossed. The singularities arise exactly at the zero-crossings of the oscillating order parameter. As a consequence, the appearance of the kink singularities in the transient dynamics is directly linked to a dynamical transition in the order parameter.

TT 81.2 Thu 9:45 H 3010

Constructing effective free energies for dynamical quantum phase transitions in the transverse-field Ising chain — •Daniele Trapin and Markus Heyl — Max-Planck-Institut fur Physik komplexer Systeme, Nothnitzer Strasse 38, 01187-Dresden, Germany

Phase transitions play a central role in equilibrium many-body systems. The theory of dynamical quantum phase transitions represents an attempt to extend the notion of phase transition to the far from equilibrium regime. As opposed to conventional transitions which are driven by a control parameter such as temperature of pressure, these dynamical transitions occur as a function of time with physical quantities becoming nonanalytic at critical times. While there are many formal analogies to conventional transitions, it is a major question to which extent it is possible to formulate a nonequilibrium counterpart to a Landau-Ginzburg theory. In this work we address this problem for quantum quenches in a one-dimensional transverse-field Ising model. We construct an effective free energy which due to unitary time evolution becomes a complex quantity. This transforms the conventional minimization principle into a saddle-point equation in the complex plane of the order parameter. We study this effective free energy in the vicinity of the dynamical quantum phase transition by performing an expansion in terms of the complex magnetization.

TT 81.3 Thu 10:00 H 3010

Non-Markovian Decay of Nuclear Spins Coupled to Itinerant Electrons — •Stephanie Matern and Bernd Brauncker — SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, United Kingdom

We study the full time evolution of a nuclear spin coupled to itinerant electrons through the hyperfine interaction, with a particular focus on memory effects leading to a non-Markovian behaviour. We show that even a noninteracting electron system causes a notable memory effect due to the restriction of fluctuations by the Fermi surface. The resulting short time dynamics of the nuclear spin is dominated by a

logarithmic, temperature independent decay before crossing over to the standard, thermally induced exponential decay. But even at the longer time scales the initial non-Markovian decay causes a systematic reduction of the decay amplitude that should be detectable. Our approach is based on an expansion of the exact Nakashima-Zwanzig equation in the hyperfine coupling constant, set up to preserve the analytical structure of the memory kernel that causes the non-Markovian behaviour. Our results are analytical and describe the full time range from the novel non-Markovian contributions to the well-known exponential decay expressions.

TT 81.4 Thu 10:15 H 3010

Quantum Quench Dynamics in the bond-alternating Heisenberg Model — •Mirco Marahrens — University of Stuttgart, Institute for Functional Matter and Quantum Technologies

We studying the bond-alternating Heisenberg model regarding its quench dynamics between different symmetry protected topological phases, namely the odd and even degenerated Haldane phases, and quenches to the trivial phase. Therefore we are using the Density Matrix Renormalization Group in the formalism of uniform matrix product states and a time evolution scheme purely based on matrix product operators constructed by finite state machines.

TT 81.5 Thu 10:30 H 3010

Boundary-driven Heisenberg chain in the long-range interacting regime: Robustness against far-from-equilibrium effects — Leon Droenner and •Alexander Carmele — Technische Universität Berlin, Institut für Theoretische Physik, Hardenbergstr. 36, 10623 Berlin

The discovery of disorder induced localization in the presence of interactions,known as many-body localization, opened a new field of theoretical and experimental investigations. A common generic model to study such effects is the disordered isotropic Heisenberg spin-chain [1]. By applying two magnetic boundary reservoirs, we drive the system out of equilibrium and induce a nonzero steady-state current [2]. The long-range coupled chain shows nearly ballistic transport and linear response for all potential differences of the external reservoirs. In contrast, the common isotropic nearest-neighbor coupling shows negative differential conductivity and a transition from diffusive to subdiffusive transport for a far-from-equilibrium driving. We find for the disordered long-range coupled XXZ chain, any change in the transport behavior is independent of the potential difference and the coupling strengths of the external reservoirs [2]. Therefore, to distinguish many-body localization as an effect of disorder from the spin-blockade, long-range coupling provides a clear understanding of MBL for boundary-driven systems as it is robust against far-from-equilibrium effects.
[1] M. Znidaric et al, Phys. Rev. Lett. 117, 040601 (2016).
[2] L. Droenner and A. Carmele Phys. Rev. B 96, 184421 (2017).

TT 81.6 Thu 10:45 H 3010

Non-equilibrium Real-space DMFT for correlated heterostuctures — •Irakli Titvinidze, Max Sorantin, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Institute of theoretical and computational physics, Graz Univeristy of Technology, 8010 Graz, Austria.

We consider a system consisting of correlated monoatomic layers, sandwiched between two metallic leads. In addition to the local Hubbard interaction we also take the long-range Coulomb interaction into account, which causes electronic charge reconstruction not only in the correlated layers but also in the leads. The non-equilibrium situation is driven by applying a bias-voltage to the leads. We investigate the steady-state behavior of the system. In particular, we present results for the steady-state current, spectral functions, and electronic charge reconstruction. Depending on the particular parameters we either observe a capacitor-like behavior or one dominated by charge transport.

In order to investigate steady-state properties we use Non-equilibrium real-space dynamical mean-field theory (R-DMFT) [1-3] combined with the Poisson equation, both solved in a self-consistent fashion. To account for the charge reconstruction in the leads we include some lead layers explicitly in R-DMFT in addition to the correlated layers.
[1] E. Arrigoni, M. Knap, and W. von der Linden, Phys. Rev. Lett **110**, 086403 (2013).
[2] I. Titvinidze, A. Dorda, W. von der Linden, and A. Arrigoni, Phys. Rev. B **94**, 245142 (2016).
[3] J.K. Freericks, Phys. Rev. B **70**, 195342 (2004).

TT 81.7 Thu 11:00 H 3010

From two Algebraic Bethe Ansätze to the dynamics of Dicke-Jaynes-Cummings-Gaudin quantum integrable models through eigenvalue-based determinants — Hugo Tschirhart[1], •Alexandre Faribault[2], and Thierry Platini[3] — [1]Université du Luxembourg, Luxembourg, Luxembourg — [2]Université de Lorraine, Nancy, France — [3]Coventry University, Coventry, United Kingdoms

The work in question was inspired by precedent results on the Gaudin models (which are integrable) for spins-1/2 only which, by a change of variables in the algebraic Bethe equations, manage to considerably simplify the numerical treatment of such models.

This numerical optimisation is carried out by the construction of determinants, only depending on the previously mentioned variables, for every scalar products appearing in the expression of the mean value of an observable of interest at a given time.

By showing it is possible to use the Quantum Inverse Scattering Method, even when the vacuum state is not eigenstate of the transfer matrix, the previous results concerning spins-1/2 only are generalised to models including an additional spin-boson interaction.

A numerical treatment of systems describing the interaction of many spins-1/2 with a single bosonic mode has been done. We studied through it the time evolution of bosonic occupation and of local magnetisation for two different Hamiltonians, the Tavis-Cummings Hamiltonian and a central spin-like Hamiltonian. We learn that the dynamics of these systems, relaxing from an initial state to a stationary state, leads to a superradiant-like state for certain initial states.

TT 82: Topological Insulators II (joint session TT/MA)

Time: Thursday 9:30–13:00 Location: A 053

TT 82.1 Thu 9:30 A 053

Robust spin-polarized midgap states at step edges of topological crystalline insulators — •Domenico Di Sante[1], Paolo Sessi[2], Martin Greiter[1], Titus Neupert[3], Giorgio Sangiovanni[1], Tomasz Story[4], Ronny Thomale[1], and Matthias Bode[2] — [1]Institut fuer Theoretische Physik, Universitaet Wuerzburg — [2]Experimentelle Physik II, Universitaet Wuerzburg — [3]Physik Institut, Universitaet Zuerich, Switzerland — [4]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Topological crystalline insulators are materials in which the crystalline symmetry leads to topologically protected surface states with a chiral spin texture, rendering them potential candidates for spintronics applications. In this talk, I report on the discovery of one dimensional midgap states at odd atomic surface step edges of the three dimensional topological crystalline insulator (Pb,Sn)Se. A minimal toy model and realistic tight-binding calculations identify them as spin polarized flat bands connecting two Dirac points. The midgap states inherit stability through the two dimensional Dirac metal from the three dimensional bulk insulator. This makes (Pb,Sn)Se the first example for a crystal symmetry protected hierarchy of one and two dimensional topological modes, which we experimentally prove to result in a striking robustness to defects, strong magnetic fields, and elevated temperature.
[1] P.Sessi, D. Di Sante et. al, Science 354 1269 (2016)

TT 82.2 Thu 9:45 A 053

Quantum capacitance measurements in $BiSbTeSe_2$ 3D topological insulators — •Jimin Wang[1], Zhiwei Wang[2], Yoichi Ando[2], and Dieter Weiss[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937, Köln, Germany

We conducted low temperature quantum capacitance measurements in high quality bulk-insulating 3D topological insulators $BiSbTeSe_2$ flakes, with h-BN as protective capping layers. The density of states extracted from the gate voltage dependence of the quantum capac-

itance is asymmetric with respect its minimum, indicating a partly nonlinear energy dispersion. Our results can be well fitted using a linear dispersion with superimposed parabolic contributions, which are in agreement with literature [1, 2]. At magnetic fields higher than 10 T, we clearly resolve the zeroth Landau level, which can be observed at least up to 85 K. Due to impurity broadening, higher Landau levels cannot be resolved.

[1] A. A. Taskin, et al., PRL 107, 016801 (2011)
[2] T. Arakane et al., Nat. Commun. 3:636 (2012)

TT 82.3 Thu 10:00 A 053

Gate-Training Effects and Enhanced Transparency in HgTe Quantum Spin Hall Edge Channels — •Lukas Lunczer[1], Philipp Leubner[2], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]Experimentelle Physik 3, Physikalisches Institut, Universität Würzburg — [2]Technische Universität Eindhoven

HgTe quantum wells are the most intensively studied 2D topological insulators. The key property of these systems is the existence of helical edge channels, which has been investigated in detail in various experiments [1,2,3]. However, the experimental observation of quantized conductance in these edge channels is limited to only very small sample dimensions (in the range of a few μm), which is not yet entirely understood. In this talk I will first discuss the influence of the size of the band gap to this limitation. One finds that an enlarged band gap does not result in a more stable quantization, as one would naively expect. We suggest that this the approach of gating affects our devices i.e. potential fluctuations prevent the sample from the bulk insulating state homogeneously. I will show that the non-quantized conductance in large samples can be influenced by hysteretic gate training and thus smoothening the potential landscape in the quantum well. On a 58 μm long pair of edge channels, this leads to a yet unseen conductance of 1.6 e^2/h, almost reaching the theoretically predicted value of 2 e^2/h.

[1] M. König et al., *Science* **318**, 766 (2007)
[2] A. Roth et al., *Science* **325**, 5938 (2009)
[3] C. Brüne et al., *Nature Physics* **8**, 485 (2012)

TT 82.4 Thu 10:15 A 053

Spectroscopy of 1D Edge States and Rashba-Split Valence Bands in Bismuthene on SiC(0001) — •Felix Reis[1], Gang Li[2,3], Raul Stühler[1], Lenart Dudy[1,4], Maximilian Bauernfeind[1], Stefan Glass[1], Werner Hanke[3], Ronny Thomale[3], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany — [4]Tempo Beamline, Synchtron Soleil, L'Orme des Merisiers, 91190 Saint-Aubin, France

Recently, the realization of bismuthene on the wide-gap substrate SiC(0001) was reported [1]. Theoretical analysis shows that Bi/SiC(0001) is a large-gap quantum spin Hall system, and demonstrates the pivotal role of the substrate not just for the stabilization of the monolayer film, but also for its topological properties. We investigate the spectroscopic properties with scanning tunneling spectroscopy (STS), photoemission and density-functional theory. We find a characteristic Rashba-split valence band due to the inversion symmetry breaking by the substrate. A metallic density of states exists at the bismuthene film edges near substrate steps. We will report STS investigations of the narrow 1D spatial confinement, and of the metallic spectra which show a zero-bias anomaly.

[1] F. Reis, G. Li, L. Dudy et al., *Science* **357**, 287 (2017).

TT 82.5 Thu 10:30 A 053

Probing the topological nature of SmB_6 by dynamical mean field theory — Patrik Thunström[1,2] and •Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 751 20 Uppsala, Sweden

Experiments on the presumptive topological insulator SmB_6 remain controversial and hotly debated, with largely conflicting physical interpretations. We present reliable density functional theory plus dynamical mean field theory calculations that yield a mixed valence ($4f^{5.5}$) state with a tiny bulk band gap and a $\Gamma_1+\Gamma_8$ ground state. The bulk states and the emerging topological surface states well agree with angular resolved photoemission spectra. Strong electronic correlations and the mixed valency severely modify the simple topological Kondo insulator picture, and explain, among others, the unusual spin texture of the topological surface states.

TT 82.6 Thu 10:45 A 053

Wigner oscillations and fractional Wigner oscillations in Luttinger liquids — •Niccolo Traverso Ziani and Bjoern Trauzettel — Institut für Theoretische Physik, Universität Würzburg

In finite electronic systems, when electron-electron interactions dominate over kinetic energy, electrons tend to form regular lattices, called Wigner molecules. While the study of the Wigner molecule in three and two spatial dimensions is most often carried out numerically, in one dimension the Luttinger liquid theory allows for analytical results. In one dimension, when interaction strength is increased from the non-interacting regime, a crossover between finite size Friedel oscillations (with wavevector $2k_F$) and Wigner oscillations (with wavevector $4k_F$) is found in the average density. Moreover, in a range of intermediate interactions, increasing temperature favours Wigner oscillations over Friedel ones. Importantly, for strong interactions, the Wigner molecule becomes an almost classical state and any dependence on the spin degree of freedom is lost. This behaviour is antithetical to the concept of spin-momentum locking characterizing the helical edges of two-dimensional topological insulators (helical Luttinger liquids). The compromise between strong interactions and spin-momentum locking leads, in helical systems, to a Wigner oscillation of fermions with fractional charge e/2. This fractional oscillation is also characterized by strongly anisotropic spin-spin correlations. In a finite size setup the fractional charges have a nontrivial interplay with Jackiw-Rebbi fractional solitons.

TT 82.7 Thu 11:00 A 053

Magnetotransport properties of 3D topological insulator (TI) nanowire structures — •Kristof Moors[1], Peter Schüffelgen[2,3], Daniel Rosenbach[2,3], Tobias Schmitt[2], Thomas Schäpers[2,3], and Thomas Schmidt[1] — [1]University of Luxembourg, Luxembourg, Luxembourg — [2]Peter Grünberg Institut, Jülich, Germany — [3]Helmholtz Virtual Institute for Topological Insulators (VITI), Jülich, Germany

3D TIs host gapless spin-momentum locked surface states with great potential for applications in spin electronics or quantum computing. When confined to the surface of a straight nanowire however, a confinement-induced gap appears and the topological protection is lost. Interestingly, this protection can be restored by a magnetic field with a half-integer magnetic flux piercing the cross section of the wire. To further explore the magnetotransport properties of nanowire structures, e.g. kinks or Y-junctions, we present a 3D tight-binding model, based on the $k \cdot p$ Hamiltonian introduced by Zhang. This model allows us to study structures made of different TI materials with a potentially anisotropic and/or particle-hole asymmetric surface state spectrum. Based on band structure and ballistic transport simulations, we demonstrate a rescaling of the magnetoconductance oscillations as a function of the surface state thickness, the protection of gapless surface states from a perpendicular magnetic field and special angles of the magnetic field for which nanowire kinks and Y-junctions feature conductance resonances. These properties could be relevant in future quantum transport experiments of TI nanowire structures.

15 min. break.

TT 82.8 Thu 11:30 A 053

Direct phase transitions between $Z_n \times Z_n$ bosonic topological phases in 1+1D — •Julian Bibo[1], Ruben Verresen[1,2], and Frank Pollmann[1] — [1]Technische Universiät München — [2]Max-Planck-Institut für komplexe Systeme, Dreseden

Symmetry protected topological (SPT) phases are phases of matter without local order parameters. Instead, they are classified by how a global symmetry G acts projectively on the edges. For $G = Z_n \times Z_n$, there are $n-1$ non-trivial SPT phases. For $n \leq 4$, it has been proven that within a certain class of models there are direct transitions between adjacent phases. For $n \geq 5$, however, the expectation was that there are intermediate gapless phases instead of direct transitions. Contrary to this expectation, we argue analytically that there are direct transitions in case n is divisible by 2, 3 or 4. We numerically confirm that these transitions are not fine-tuned.

TT 82.9 Thu 11:45 A 053

Signatures of hydrodynamic transport in ribbons of Dirac material — •Oleksiy Kashuba[1], Laurens Molenkamp[2], and Björn Trauzettel[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg — [2]Physikalisches Institut (EP3), Universität Würzburg, D-97074 Würzburg

Charge transport in ribbon-shaped 2D Dirac systems is studied employing the Boltzmann equation. The dependence of the resistivity on temperature and bias is investigated. An accurate understanding of the influence of electron-electron interaction and material disorder allows us to identify a parameter regime, where the system reveals hydrodynamic transport behaviour. We point out the conditions for three Dirac fermion specific features: two-liquid hydrodynamics, pseudo-diffusive transport, and the electron-hole scattering dominated regime. It is demonstrated that for the very clean samples the Gurzhi effect, a definite indicator of hydrodynamic transport, can be observed.

TT 82.10 Thu 12:00 A 053

Helical Andreev bound states and non-sinusoidal current-phase relationship at the surface of topological insulators — •Niklas Krainovic, Grigory Tkachov, and Ewelina Maria Hankiewicz — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

When a conventional superconductor is brought in close proximity to a three-dimensional topological insulator (3D TI), an unconventional triplet pairing is generated at the TI surface. Josephson junctions based on such hybrids support Andreev bound states (ABSs) that inherit the helical spin polarization of the normal TI, resulting in the non-sinusoidal Josephson current-phase relationship (CPR) [1,2]. Here, we present detailed analytic calculations of the non-sinusoidal CPR in the metallic regime and close to the Dirac point. The CPR exhibits strong forward skewness caused by a reflectionless transport channel perpendicular to the junction interface.

This work has been supported by the DFG Grant No TK60/4-1, by SFB 1170 8220 ToCoTronics 8221 and the ENB Graduate School on Topological Insulators.

[1] G. Tkachov, E. M. Hankiewicz, Phys. Rev. B 88, 075401 (2013).
[2] I. Sochnikov, L. Maier, C. A. Watson, J. R. Kirtley, C. Gould, G. Tkachov, E. M. Hankiewicz, C. Bruene, H. Buhmann, L. W. Molenkamp, and K. A. Moler, Phys. Rev. Lett. 114, 066801 (2015).

TT 82.11 Thu 12:15 A 053

Electrically induced quantum vortices and anyons in three-dimensional topological insulators — •Flavio Nogueira and Jeroen van den Brink — IFW Dresden

The electromagnetic response of a three-dimensional topological insulator is well known to be given by a so called axion electrodynamics, which features a magnetoelectric topological term $\alpha\theta/(4\pi^2)\mathbf{E}\cdot\mathbf{B}$ in the Lagrangian density, where θ is a 2π-periodic parameter and α the fine-structure constant. We show that a point electric charge induces a quantized vortex on the surface of a topological insulator, even if the system is not a superfluid. We derive the exact expressions for the electrically induced magnetic field and angular momentum. It is shown that the dynamics of charged particles on the surface obeys fractional statistics. We briefly discuss different experimental probes to detect this behavior.

TT 82.12 Thu 12:30 A 053

Controlling the Topological Properties of Stanene by Substrate Engineering: Realistic Modelling and Experimental Approaches — •Philipp Eck[1], Maximilian Bauernfeind[2], Marius Will[2], Domenico Di Sante[1], Lenart Dudy[2], Ronny Thomale[1], Jörg Schäfer[2], Ralph Claessen[2], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg — [2]Physikalisches Institut and Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg

Although two-dimensional (2D) group IV (C-, Si-, Ge-, Sn-) honeycomb lattices have been successfully grown on a vast number of substrates, strain, deformation and/or hybridization often destroy their topological properties. Focusing on stanene, a promising strategy is the growth on passivated SiC(0001) with a buffer layer saturating the SiC dangling bonds. We present a systematic density functional theory study of group III and V buffer layers and shed light on the buffer-stanene hybridization physics influencing the vertical stanene distance and the stanene deformation. We find for some buffer layers large equilibrium distances leading to a freestanding-stanene-like topological band structure. The theoretical study will be supported by experimental data on an Al buffer layer.

TT 82.13 Thu 12:45 A 053

Magnetization current and anomalous Hall effect for massive Dirac electrons — •Peter Silvestrov[1] and Patrik Recher[1,2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, 38106 Braunschweig, Germany

Existing investigations of the anomalous Hall effect, *i.e.* a current flowing transverse to the electric field in the absence of an external magnetic field, are concerned with the transport current. However, for many, *e.g.* optical, applications one needs to know the total current, including its pure magnetization part. In this paper, we employ the two-dimensional massive Dirac equation to find the exact universal total current flowing along a potential step of arbitrary shape. For a slowly varying electric field, we find the current density $\mathbf{j}(\mathbf{r})$ and the energy distribution of the current density $\mathbf{j}^{\varepsilon}(\mathbf{r})$. The latter turns out to be unexpectedly nonuniform, behaving like a δ-function at the border of a classically accessible area at energy ε. To demonstrate explicitly the difference between the magnetization and transport currents, we consider the transverse shift of an electron ray in an electric field.

TT 83: Superconductivity: (General) Theory

Time: Thursday 9:30–12:45 Location: HFT-FT 101

TT 83.1 Thu 9:30 HFT-FT 101

High-field superconductivity in ultra-thin films, interfaces, and superlattices — •Gertrud Zwicknagl[1], Lukas Debbeler[1,2], Simon Jahns[1], and Peter Fulde[3] — [1]Institut f. Mathemat. Physik, TU Braunschweig, Germany — [2]Dept. of Physics, University of Oregon, Eugene, OR 97403 (USA) — [3]MPI f. Physik komplexer Systeme, Dresden, Germany

In recent years, the manufacturing of controlled ultra-thin superconducting films has made impressive progress. Important examples are monoatomic or monomolecular layers on a substrate, superconducting layers in a superlattice, or superconducting interfaces and surfaces. These systems have in common the absence of inversion symmetry and hence the presence of Rashba-type spin-orbit interaction which can be tuned to some extent.

We discuss the superconducting properties of ultra-thin superconducting films with Rashba spin-orbit interaction in the presence of a parallel magnetic field. Thereby we cover the range from small to large spin-orbit interactions compared with the gap parameter. We find abrupt changes in the superconducting state at a critical value spin-orbit energy λ_c. We speculate that this might give rise to new phenomena.

TT 83.2 Thu 9:45 HFT-FT 101

Quantum Theory of Linear Magnetoresistance and Linear-in-Temperature Resistance — •Vincent Sacksteder — Royal Holloway University of London, UK

The physical mechanisms responsible for Linear Magnetoresistance (seen in many settings) and Linear-in-Temperature resistance (seen in cuprates and pnictides) are not yet fully understood. We propose that these phenomena are manifestations of quantum interference processes, similar to the logarithmic conductivity corrections known to be caused by weak antilocalization. We submit that the linear-in-temperature resistance is caused not by increased scattering but instead by scatterings interfering coherently to control the resistance. Strong correlations may be responsible for providing the coherence required by the quantum interference processes. We propose a numerically precise approach to analyzing and interpreting magnetotransport data which allows firm conclusions to be made about the length scales and quantum interference processes contributing to transport.

TT 83.3 Thu 10:00 HFT-FT 101

Higgs Spectroscopy of Superconductors in Nonequilibrium — •Benedikt Fauseweh and Dirk Manske — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

In previous studies it has been shown, that the non-equilibrium response of superconductors allows for probing of the amplitude-, or Higgs-, mode of the superconducting condensate [1]. This feature was predicted in theory with different quenching protocols [2,3] and found in experiments using ultra-short laser pulses in the THZ Regime [4]. So far only s-wave superconductors with a constant energy gap as a function of momentum have been investigated.

In our contribution we present a systematic study of Higgs oscillations using a combination of non-equilibrium excitation and symmetry analysis. This allows for a full characterization of the superconducting gap function, similar to Phonon spectroscopy. By investigating the non-equilibrium response of s- and d-wave superconductors we show, that non-equilibrium Higgs-spectroscopy opens a unique approach to distinguish between different symmetries of the condensate. Finally, we propose new methods to implement these ideas in experiments.

[1] Yuzbashyan, Dzero, Phys. Rev. Lett. 96 (2006) 230404
[2] Krull, Manske, Uhrig, Schnyder, Phys. Rev. B 90 (2014) 014515
[3] Krull et al., Nat. Commun. 7 (2016) 11921
[4] Matsunaga, Shimano Phys. Rev. Lett. 109 (2012) 187002,

TT 83.4 Thu 10:15 HFT-FT 101

Multiband superconductivity in noncentrosymmetric YPtBi — •Carsten Timm[1], Andreas P. Schnyder[2], Daniel F. Agterberg[3], and Philip M. R. Brydon[4] — [1]Institute of Theoretical Physics, Technische Universität Dresden, Germany — [2]MPI for Solid State Research, Stuttgart, Germany — [3]Department of Physics, University of Wisconsin, Milwaukee, U.S.A. — [4]Department of Physics, University of Otago, Dunedin, New Zealand

Half-Heusler superconductors such as YPtBi combine two aspects of high current interest: they display noncentrosymmetric and multiband superconductivity. We study bulk and surface states in two exemplary nodal superconducting phases, which transform as the A_1 and T_2 irreducible representations of the crystallographic point group, respectively. The A_1 phase preserves time-reversal symmetry. We find that flat surface bands persist in the presence of multiband pairing. In addition, there are symmetry-protected Fermi arcs of surface states. On the other hand, the T_2 phase breaks time-reversal symmetry. In the bulk, point and line nodes coexist with two-dimensional Bogoliubov Fermi surfaces. The surface exhibits Fermi arcs associated with the bulk point nodes.

TT 83.5 Thu 10:30 HFT-FT 101

Electromagnetic response of spiral magnetic states in two-dimensional metals — •Johannes Mitscherling and Walter Metzner — Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The superconductivity and the normal state of cuprates are not yet fully understood. In a seminal paper [1], Badoux et al. suppressed the superconductivity with high magnetic fields making the normal ground state accessible. Varying the doping in YBCO they found a rapid change of the Hall number near optimal doping indicating a Fermi surface reconstruction. A spiral magnetic ground state was shown to be a possible candidate for such a reconstruction [2]. A full treatment of the electromagnetic response for a two-dimensional metal with a spiral magnetic ground state beyond the long lifetime limit is necessary at the relevant experimental temperatures. In a systematic approach we extend the well-known results of Voruganti et al. [3] including all inter-band effects for arbitrary lifetime which leads to corrections to the conductivity and Hall conductivity. We clarify the conditions under which the well-known results are applicable, discuss the relation between the Hall number and the occupation number and apply it to the experiments mentioned above.

[1] Badoux et al., Nature 531, 210 (2016)
[2] Eberlein et al. PRL 117, 187001 (2016)
[3] Voruganti et al., PRB 45, 13945 (1992)

TT 83.6 Thu 10:45 HFT-FT 101

Spin pumping in a ferromagnet/superconductor/normal-metal trilayer in presence of spin-orbit coupling and Fermi-liquid effects. — •Xavier Montiel and Matthias Eschrig — Royal Holloway University of London, Egham, United Kingdom

The injection of spin current into superconducting (S) layer is of primary importance for superconducting spintronics [1]. The precession of a ferromagnet magnetization close to the ferromagnetic resonance (FMR) "pumps" spins from the ferromagnet (FM) layer into adjacent layers. The injected spin current into superconducting (S) layer is expected to decrease below Tc because singlet Cooper pairs do not carry spin and the addition of a metallic layer does not change this result [2]. Here we show that if an FM-S bilayer is capped on the superconducting side by a normal metal with strong spin-orbit coupling (Nso), as for example in a Py/Nb/Pt trilayer, then an additionnal spin current exists in the superconducting state associated with Fermi liquid corrections, and spin-triplet correlations are induced in the entire structure that are long-range within the F layer. We calculate the spin current accross a F/S/Nso structure as a function of temperature. We show that this effect is sensitive to the F/S and S/N proximity effect and depends on the S layer thickness. We discuss the magnitude of the injected spin current as function of the magnitudes of the spin-orbit coupling and of the Fermi-liquid parameters.

[1] M. Eschrig, Rep. Prog. Phys. 78, 104501 (2015)
[2] J. Morten.et al., Europhys. Lett. 84, 57008 (2008)

TT 83.7 Thu 11:00 HFT-FT 101

Nonunitary triplet pairing from the Edelstein effect in noncentrosymmetric superconductors — •Grigory Tkachov — Wuerzburg University

The search for new forms of spin-triplet pairing is an important goal in superconductivity. The purpose of this contribution is to point out a surprising connection between the Edelstein effect in noncentrosymmetric superconductors [1] and the nonunitary (spin-polarized) pairing in triplet superfluids with a complex $\mathbf{d}$ vector [2]. It will be shown that the Edelstein effect leads to a new form of the nonunitary spin-triplet pairing [3] which is generated electrically by a supercurrent in an initially TR-invariant (unpolarized) system. Such a nonunitary state can be induced in a wide class of noncentrosymmetric superconductors, including those with a real $\mathbf{d}$ vector and proximity structures with $\mathbf{d} = 0$. I will also discuss how to detect the nonunitary spin-triplet pairing by Andreev reflection. These results indicate an unexplored route for electrical manipulation of spin-triplet superconductivity in noncentrosymmetric materials.

This work has been supported by the German Research Foundation (DFG grant No TK60/4-1).

[1] V. M. Edelstein, Phys. Rev. Lett. **75**, 2004 (1995).
[2] A. J. Leggett, Rev. Mod. Phys. **47**, 331 (1975).
[3] G. Tkachov, Phys. Rev. Lett. **118**, 016802 (2017).

15 min. break.

TT 83.8 Thu 11:30 HFT-FT 101

Multi-particle theory of superconductivity — •Gareth Conduit and Thomas Whitehead — Cavendish Laboratory, J.J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom

A spin-imbalanced Fermi gas with an attractive contact interaction forms a superconducting state whose underlying components are multi-particle instabilities, each involving more than two fermions. This multi-particle superconducting state is energetically favourable to Fulde-Ferrell-Larkin-Ovchinnikov superconductivity, because it includes correlations between all available fermions. The ratio of the number of up- and down-spin fermions in the instability is a function of the ratio of the up- and down-spin densities of states in momentum at the Fermi surfaces, to fully utilise the accessible fermions.

TT 83.9 Thu 11:45 HFT-FT 101

Pair density waves from coexistence: properties and experimental signatures — •Pavel A. Volkov[1], Mikhail Malakhov[2], and Konstantin B. Efetov[1,3] — [1]Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Institute of Physics, Kazan (Volga Region) Federal University, 420008 Kazan, Russian Federation — [3]National University of Science and Technology MISiS, 119049 Moscow, Russian Federation

Pair density wave (PDW) is a state of matter where the amplitude of superconducting pairing oscillates in space. One of the cases where PDW is expected to arise is in a system where uniform superconductivity coexists with a charge density wave. This situation is realized in underdoped cuprates, where PDW has been recently discovered in a scanning Josephson tunneling microscopy (SJTM) experiment [1]. In this regard, we consider a mean-field model with the Gor'kov formalism to study the structure of the PDW. We find that the PDW amplitude

has an intricate momentum dependence that bears information about the order parameters as well as the underlying Fermi surface. We also consider the implications of our results for the SJTM experiments and discuss applications to other materials where coexistence of superconductivity and charge density waves has been reported.
[1] M. H. Hamidian et al., Nature 532, 343 (2016).

TT 83.10 Thu 12:00 HFT-FT 101

The Concept of Superconducting Fitness — •Aline Ramires[1], Manfred Sigrist[2], and Daniel Agterberg[3] — [1]Institute for Theoretical Studies, ETH Zurich, 8092 Zurich, Switzerland — [2]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — [3]Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, WI 53201, USA

In this talk, we present a general scheme to probe the compatibility of arbitrary pairing states with a given normal state Hamiltonian by the introduction of a concept called Superconducting Fitness. This quantity gives a direct measure of the suppression of the superconducting critical temperature in the presence of key symmetry-breaking fields and can be used as a tool to identify nontrivial mechanisms to suppress superconductivity in complex multi-orbital systems. This concept can also be employed as a guide to engineer normal state Hamiltonians in order to favor or suppress different order parameters. We discuss the application of this idea to Sr_2Ru0_4, $CePt_3Si$, KFe_2As_2 and $Cu_xBi_2Se_3$.

TT 83.11 Thu 12:15 HFT-FT 101

Renormalization group studies of supeconducting ordering in nickelates — •Michael Klett[1], David Riegler[1], Gang Li[2], and Ronny Thomale[1] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians University of Würzburg, 97074 Würzburg, German — [2]School of Physical Science and Technology, ShanghaiTech University, Shanghai 201210, China

Since the discovery of high T_c superconductivity in the cuprates by Bednorz and Müller, materials bearing similarities to copper oxide compounds have merged as a contemporary research topic of high interest. Although nickelates share many similarities with the cuprates, they exhibit no superconducting phase down to lowest temperatures. In this talk we sketch a simple two-band DFT model of the nickelates and argue why, based on renormalization group calculations competing superconducting ordering propensities make the nickelates belong to the class of low T_c materials

TT 83.12 Thu 12:30 HFT-FT 101

Chiral superconductivity in germanene on molybdenum disulfide — •Xianxin Wu, Domenico Di Sante, Mario Fink, Werner Hanke, and Ronny Thomale — Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

We investigate competing orders for germanene on molybdenum disulfide (Ge/MoS_2), where the Van Hove singularity point is close to the Fermi level, and can already be achieved by moderate electron doping. We find that the system harbors a d+id or f wave superconducting state depending on the electron doping and interaction profile. Our study indicates that Ge/MoS_2 promises to be a prototypical system to realize chiral superconductivity.

TT 84: Fluctuations and Noise

Time: Thursday 9:30–11:15 Location: HFT-FT 131

TT 84.1 Thu 9:30 HFT-FT 131

Thermodynamic Bounds on Dissipation in Open Quantum Systems — •Paul Menczel, Christian Flindt, and Kay Brandner — Department of Applied Physics, Aalto University, 00076 Aalto, Finland

Given today's rapid experimental advances in quantum engineering, it becomes increasingly important to understand the laws that govern thermodynamic processes far from equilibrium in nano-scale devices. For an open quantum system under weak coupling conditions, we derive universal lower bounds on the total dissipation accompanying such a process. Going beyond the second law, our bounds are expressed in terms of the photon exchange between the system and its environment. As a key application of our approach, we obtain a new trade-off relation between power and efficiency of periodically driven quantum heat engines. This bound becomes weakest for semi-classical engine cycles that do not involve superpositions between the energy levels of the working substance. Showing that cycles with coherence inevitably come at the price of increased dissipation, our results are relevant for current experimental efforts to realize thermal machines in the quantum realm.

TT 84.2 Thu 9:45 HFT-FT 131

Electron waiting times of a periodically driven single-electron turnstile — •Elina Potanina and Christian Flindt — Department of Applied Physics, Aalto University, 00076 Aalto, Finland

We investigate the distribution of waiting times between electrons emitted from a periodically driven single-electron turnstile [1]. To this end, we develop a scheme for analytic calculations of the waiting time distributions for arbitrary periodic driving protocols. We illustrate the general framework by considering a driven tunnel junction before moving on to the more involved single-electron turnstile. The waiting time distributions are evaluated at low temperatures for square-wave and harmonic driving protocols. In the adiabatic regime, the dynamics of the turnstile is synchronized with the external drive. As the nonadiabatic regime is approached, the waiting time distribution becomes dominated by cycle-missing events in which the turnstile fails to emit within one or several periods. We also discuss the influence of finite electronic temperatures. The waiting time distributions provide a useful characterization of the driven single-electron turnstile with complementary information compared to what can be learned from conventional current measurements.
[1] E. Potanina and C. Flindt, Phys. Rev. B **96**, 045420 (2017)

TT 84.3 Thu 10:00 HFT-FT 131

Hierarchical quantum master equation approach to current fluctuations in vibrationally coupled charge transport through nanosytems — •Christian Schinabeck[1] and Michael Thoss[1,2] — [1]Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany. — [2]Physikalisches Institut, Universität Freiburg, Freiburg, Germany.

We investigate vibrationally coupled charge transport in nanosytems using the hierarchical quantum master equation (HQME) approach [1-3]. This method allows a systematic convergence of the reduced dynamics of open quantum systems and thus generalizes traditional perturbative master equations. In this contribution, we present an extension of the HQME approach to calculate current fluctuations within the framework of full counting statistics. The method is applied to a model of a single-molecule junction including an electronic level coupled to fermionic leads as well as a vibrational mode in nonequilibrium. In the regime of strong electronic-vibrational coupling, we analyze the influence of higher-order cotunneling processes on avalanche-like transport [4,5]. Furthermore, in the off-resonant transport regime, inelastic corrections to shot noise are studied in some detail.
[1] Y. Tanimura *et al.*, J. Phys. Soc. Jpn. **75**, 082001 (2006).
[2] J. Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407 (2016).
[4] J. Koch *et al.*, Phys. Rev. B **74**, 205438 (2006).
[5] C. Schinabeck *et al.*, Phys. Rev. B **90**, 075409 (2014).

TT 84.4 Thu 10:15 HFT-FT 131

Noninvasive Quantum Measurement of Arbitrary Operator Order by Engineered Non-Markovian Detectors — Johann Bülte[1], •Adam Bednorz[2], Christoph Bruder[3], and Wolfgang Belzig[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Faculty of Physics, University of Warsaw, ul. Pasteura 5, PL02-093 Warsaw, Poland — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

The development of solid-state quantum technologies requires the understanding of quantum measurements in interacting, non-isolated quantum systems. In general, a permanent coupling of detectors to a quantum system leads to memory effects that have to be taken into account in interpreting the measurement results. We analyze a generic setup of two detectors coupled to a quantum system and derive a com-

pact formula in the weak-measurement limit that interpolates between an instantaneous (text-book type) and almost continuous - detector dynamics-dependent - measurement. A quantum memory effect that we term system-mediated detector-detector interaction is crucial to observe non-commuting observables simultaneously. Finally, we propose a mesoscopic double-dot detector setup in which the memory effect is tunable and that can be used to explore the transition to non-Markovian quantum measurements experimentally [arXiv:1711.11347].

TT 84.5 Thu 10:30 HFT-FT 131

Continuous-Variable Entanglement Test in a Driven Quantum Contact — •Hongxin Zhan[1], Mihajlo Vanević[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Department of Physics, University of Belgrade, 11158 Belgrade, Serbia

The standard entanglement test [1] using Clauser-Horne-Shimony-Holt inequality is known to fail in mesoscopic junctions at finite temperatures [2]. Since this is due to the bidirectional particle flow, a similar failure is expected to occur in an ac-driven contact. We develop a continuous-variable entanglement test suitable for electrons and holes that are created by the ac drive [3]. The generalized Bell inequality [4] is violated in junctions with low conductance or small number of transport channels and with ac voltages which create few electron-hole pairs per cycle. Our ac entanglement test depends on the total number of electron-hole pairs [5] and on the distribution of probabilities of pair creations similar to the Fano factor.

[1] N. M. Chtchelkatchev, G. Blatter, G. B. Lesovik, T. Martin, Phys. Rev. B **66**, 161320(2002).
[2] W. R. Hannes, M. Titov, Phys. Rev. B **77**, 115323(2008).
[3] H. Zhan, M. Vanević, W. Belzig, arXiv:1711.11461.
[4] A. Bednorz and W. Belzig, Phys. Rev. B **83**, 125304(2011).
[5] M. Vanević, Y. V. Nazarov, W. Belzig, Phys. Rev. Lett **99**, 076601(2007); Phys. Rev. B **78**, 245308(2008).

TT 84.6 Thu 10:45 HFT-FT 131

Detection of spin precessions in a quantum-dot spin valve via counting statistics — •Philipp Stegmann, Jürgen König, and Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We propose to use the full counting statistics of electron transport to reveal spin precessions in a quantum-dot spin valve, i.e., a quantum dot tunnel coupled to two ferromagnets with noncollinear magnetizations. The spin precession has an unique impact on the statistics which can be identified by generalized factorial cumulants [1,2]. Quantities like the current noise, the waiting time distribution, or ordinary cumulants are affected by the spin precession only for strongly spin-polarized ferromagnets. In contrast, our detection scheme succeeds even for arbitrary small polarizations and especially for the experimentally most favored materials [3].

[1] P. Stegmann and J. König, Phys. Rev. B **92**, 155413 (2015).
[2] P. Stegmann and J. König, New J. Phys. **19**, 023018 (2017).
[3] A. D. Crisan et al., Nat. Commun. **7**, 10451 (2016).

TT 84.7 Thu 11:00 HFT-FT 131

Single-electron thermal devices coupled to a mesoscopic gate — •Rafael Sánchez[1], Holger Thierschmann[2], and Laurens W. Molenkamp[3] — [1]Universidad Autónoma de Madrid — [2]Delft University of Technology — [3]Universität Würzburg

Fluctuations are strong in mesoscopic systems and have to be taken into account for the description of transport. We show that they can even be used as a resource for the operation of a system as a device. We use the physics of single-electron tunneling to propose a bipartite device [1,2] working as a thermal transistor[3,4]. Charge and heat currents in a two terminal conductor can be gated by thermal fluctuations from a third terminal to which it is capacitively coupled. The gate system can act as a switch that injects neither charge nor energy into the conductor hence achieving huge amplification factors. Non-thermal properties of the tunneling electrons can be exploited to operate the device with no energy consumption.

[1] R. Sánchez, M. Büttiker, Phys. Rev. B 83, 085428 (2011)
[2] H. Thierschmann et al., Nature Nanotech. 10, 854 (2015)
[3] R. Sánchez, H. Thierschmann, L. W. Molenkamp, Phys. Rev. B 95, 241401 (2017)
[4] R. Sánchez, H. Thierschmann, L. W. Molenkamp, New J. Phys. 19, 113040 (2017)

TT 85: Focus Session: Emergent Phenomena in Driven Quantum Many-Body Systems (joint session DY/TT)

In the past years, driven quantum many-body systems have been demonstrated to offer a huge playground for emergent states of matter. These range from light-induced switching of phases in solids and laser-modified chemical reactions via Floquet topological states in photonic crystals to artificial gauge fields in optical lattices and Floquet time crystals in many-body localized systems. The goal of the proposed session Emergent phenomena in driven quantum many-body systems is to bring together distinguished scientists from a variety of fields who work on driven quantum systems from different perspectives, both theoretically and experimentally, to stimulate interdisciplinary discussions and guide future research directions. For the general audience, this is an opportunity to gain a broad overview of a growing research field with great potential and many open questions.

Coordinator: France Manghi (Modena)

Time: Thursday 9:30–11:30 Location: EB 107

Invited Talk TT 85.1 Thu 9:30 EB 107

Nuclear and electronic dynamics in ultrafast photoinduced charge separation — •Carlo Andrea Rozzi — CNR-NANO, Modena, Italy

The sub-ps dynamics of photoinduced charge separation is studied in several prototypical photovoltaic materials by combining TDDFT and molecular dynamics simulations. The results are validated against high time resolution pump-probe spectroscopy, and ultrafast electron diffraction. The role of coherent coupling between electronic and nuclear degrees of freedom is shown to be of key importance in triggering charge delocalization and transfer both in covalently bonded molecules[1] and non-bonded bulk heterojunctions[2]. The possible exploitation of our findings in order to design and synthesize novel molecular scaffolds[3] for photovoltaic applications is discussed. Further work in progress on ultrafast photoexcitation of polymer-copolymer aggregates and perovskites is presented.

[1] C. A. Rozzi et al., Nat. Comm 4, 1602 (2013) [2] S. Falke et al., Science 344, 1001 (2014) [3] S. Pittalis et al., Adv. Func. Mat. 25, 2047 (2015) [4] G. M. Vanacore et al., arXiv:1801.03731

Invited Talk TT 85.2 Thu 10:00 EB 107

Theory of pump-probe spectroscopy: Ultrafast laser engineering of ordered phases and microscopic couplings — •Michael Sentef — Max Planck Institut für Struktur und Dynamik der Materie (CFEL), Hamburg

Intense femtosecond laser pulses, spanning a large range of photon energies from the X-ray to the THz regime, allow for controlled excitations ("pump") and monitoring ("probe") of the nonequilibrium dynamics of all the relevant microscopic degrees of freedom in solids. The field of ultrafast materials science is currently evolving towards ultrafast laser engineering of nonthermal phases of matter with novel properties. I will discuss recent theoretical progress in understanding these diverse phenomena from microscopic models and nonequilibrium simulations. I will show examples of light-enhanced superconductivity

in an electron-phonon system from classical nonlinear phononics [1] and laser-controlled order competition between superconductivity and charge-density waves [2]. I will discuss laser engineering of microscopic couplings in graphene [3] based on quantum nonlinear phononics [4]. Finally, I will show ab initio time-dependent density functional theory results for laser-engineered Hubbard U in NiO [5].

[1] M. A. Sentef et al., Phys. Rev. B 93, 144506 (2016). [2] M. A. Sentef et al., Phys. Rev. Lett. 118, 087002 (2017). [3] E. Pomarico et al., Phys. Rev. B 95, 024304 (2017). [4] M. A. Sentef, Phys. Rev. B 95, 205111 (2017). [5] N. Tancogne-Déjean et al., arXiv:1712.01067.

This work was supported by Deutsche Forschungsgemeinschaft through the Emmy Noether Programme (SE 2558/2-1).

TT 85.3 Thu 10:30 EB 107

Transient dynamics in an excitonic insulator: Fast computation of nonequilibrium Green's functions — •Riku Tuovinen[1], Denis Golež[2], Michael Schüler[2], Martin Eckstein[3], and Michael Sentef[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [3]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany

A standard approach to nonequilibrium many-body problems is the Keldysh Green's function technique [1]. Information about the studied system, e.g. photoemission spectra etc., is encoded into the Green's function. To access this, we have to consider coupled integro-differential equations (Kadanoff-Baym equations), whose efficient solution is not trivial [2]. The Generalized Kadanoff-Baym Ansatz (GKBA) offers a simplification by decomposing the two-time-propagation of the Green's function into the time-propagation of a time-local density matrix [3]. We discuss the time-propagation method à la GKBA and present some benchmark simulations against the full solution of the Kadanoff-Baym equations, concentrating on a simple model for an excitonic insulator [4]. We investigate the dynamics of competing orders and how the balance between them could be controlled by laser driving.

[1] G. Stefanucci and R. van Leeuwen, Nonequilibrium many-body theory of quantum systems, CUP (2013) [2] A. Stan et al., J. Chem. Phys. 130, 224101 (2009) [3] P. Lipavský et al., Phys. Rev. B 34, 6933 (1986) [4] D. Golež et al., Phys. Rev. B 94, 035121 (2016)

TT 85.4 Thu 10:45 EB 107

Entanglement growth and thermalisation after a spatially inhomogeneous quench — Maximilian Schulz[1,2], •Chris Hooley[1], Roderich Moessner[2], and Frank Pollmann[3] — [1]SUPA, University of St Andrews, UK — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Technische Universität München, Germany

We consider a system of spinless fermions in a strong optical lattice plus a harmonic trap and uncorrelated disorder. We subject them to a quantum quench that consists of an instantaneous displacement of the trap centre.

In [1] we presented an analysis of the behaviour of the non-interacting version of the problem. We observe that (a) even weak disorder strongly breaks the parity symmetry of the clean problem, qualitatively changing the nature of the infinite-time steady state, and (b) the approach to this long-time state is extremely slow, since it involves the fermions' tunnelling across a broad 'Bragg-forbidden' region.

Here we show that the ingredients in the above study also present a way to realise slow logarithmic entanglement growth as usually observed in many-body localized systems without disorder and even without interactions. We present evidence for this by a time-evolving block decimation and exact diagonalization analysis of the interacting and non-interacting cases.

[1] M. Schulz, C.A. Hooley, and R. Moessner, Phys. Rev. A. 94, 063643 (2016).

TT 85.5 Thu 11:00 EB 107

Creating a superfluid by kinetically driving a Mott insulator — Gregor Pieplow, Fernando Sols, and •Charles Creffield — Universidad Complutense, Madrid, Spain

We study the effect of time-periodically varying the hopping amplitude (which we term "kinetic driving") in a one-dimensional Bose-Hubbard model, such that its time-averaged value is zero. By using Floquet analysis, we derive a static effective Hamiltonian in which nearest-neighbor single-particle hopping processes are suppressed, but all even higher-order processes are allowed. Unusual many-body features arise from the combined effect of non-local interactions and correlated tunneling. At a critical value of the driving, the system passes from a Mott insulator to a superfluid formed by two quasi-condensates with opposite nonzero momenta. A many-body cat state combining the two macroscopically occupied momentum eigenstates emerges even with hard-wall boundary conditions. This work shows how driving of the hopping energy provides a novel form of Floquet engineering, which enables atypical Hamiltonians and exotic states of matter to be produced and controlled.

TT 85.6 Thu 11:15 EB 107

Time evolution, dynamics and control of edge states in laser-driven graphene nanoribbons — •Matteo Puviani[1] and Andrea Bertoni[2] — [1]Università degli Studi di Modena e Raggio Emilia, Modena, Italy — [2]CNR Institute of NanoSciences - S3, Modena, Italy

An intense laser field in the high-frequency regime drives carriers in graphene nanoribbons out of equilibrium and creates topologically-protected edge states. Based on a solution of the Floquet Hamiltonian we have studied these states in different regimes of intensity and polarization. We show that the time-dependent band structure contains many unconventional features that are not captured by considering the Floquet eigenvalues alone. By analyzing the evolution in time of the state population we have identified regimes for the emergence of time-dependent edge states responsible of charge oscillations across the ribbon. Furthermore, we show that they exhibit a robust dynamics also in the presence of very localized lattice defects, which is characteristic of topologically non-trivial behaviour. We eventually reveal how it is possible to control them applying an electrostatic potential barrier or creating a Quantum Point Contact, making them promising candidates for flying qubits architectures.

TT 86: Ferroics and Multiferroics (joint session KFM/TT/MA)

Time: Thursday 9:30–13:30 Location: EMH 225

TT 86.1 Thu 9:30 EMH 225

A piezoresponse force microscopy study of Bi(Fe,Sc)O3 multiferroic ceramics — •Vladimir Shvartsman[1], Andrei Salak[2], Dmitry Khalyavin[3], and Doru Lupascu[1] — [1]Institute for Material Science, University of Duisburg-Essen, Essen, Germany — [2]Department of Materials and Ceramic Engineering/CICECO, University of Aveiro, Aveiro, Portugal — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, UK

Bismuth ferrite (BFO) has attracted an immense attention as a rare room-temperature single-phase multiferroics. The magnetic and ferroelectric structure of BFO can be tuned by cationic substitutions. In particular, using the high-pressure synthesis method BiFe(1-x)Sc(x)O3 ceramics can be sintered. The material appears in different polymorphs. The phase obtained by quenching under pressure is antipolar, but can be irreversibly turned into a polar one by thermal cycling at normal pressure. The resulting modification is a rare example of coexistence of canted ferroelectric and ferromagnetic states. We have addressed ferroelectric properties of these materials by piezoresponse force microscopy (PFM). The post-annealed Bi(Fe0.5Sc0.5)O3 ceramics show a strong PFM signal and posses a well-developed domain pattern typical of a ferroelectric state. The quenched ceramics, however, demonstrate no piezoresponse that is in line with its antiferroelectric state. We found that this state can be transferred to a ferroelectric one by application of a strong enough electric field. The temporal and temperature stability of the induced states are studied.

TT 86.2 Thu 9:50 EMH 225

Electronic Ferroelectricity in Organic Charge-Transfer Salts — •Jonas K. H. Fischer[1], Peter Lunkenheimer[1], Rudra Manna[2,3], Harald Schubert[3], Jens Müller[3], Michael Lang[3], Stephan Krohns[1], John A. Schlueter[4], Cecile Mézière[5],

Patrick Batail[5], and Alois Loidl[1] — [1]Experimental Physics V, EKM, University of Augsburg, Augsburg, Germany — [2]Department of Physics, IIT Tirupati, Tirupati 517506, India — [3]Phys. Inst. Univ. Frankfurt, SFB/TR 49, Frankfurt, Germany — [4]Materials Research, National Science Foundation, Arlington, Virginia, United States — [5]Laboratoire MOLTECH, UMR 6200 CNRS-Université d'Angers, Bt. K, UFR Sciences, Angers, France

The often intriguing dielectric properties of the EDT-TTF-based charge-transfer salts have attracted considerable attention in recent years [1]. Examples are κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, which exhibits multiferroicity [2], as well as α-(BEDT-TTF)$_2$I$_3$, which shows the signature of relaxor-ferroelectric behavior [1].
Here, we will present an overview of the dielectric properties of the above systems and provide new results on κ-(BEDT-TTF)$_2$Hg(SCN)$_2$Cl, which also shows ferroelectric behavior in its charge-ordered state. In addition, further organic candidates for ferroelectricity as well as recent results on δ-(EDT-TTF-CONMe$_2$)$_2$Br are presented. The latter compound exhibits charge order but lacks dimerization. It displays interesting glasslike relaxation dynamics.
[1] P. Lunkenheimer and A. Loidl, J. Phys.: Condens. Matter **27**, 373001 (2015). [2] P. Lunkenheimer *et al.*, Nat. Mater. **11**, 755 (2012).

TT 86.3 Thu 10:10 EMH 225

Superconductivity and ferroelectric quantum criticality in KTaO3 — •Tobias Esswein, Awadhesh Narayan, and Nicola Spaldin — Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland

Electron doped cubic perovskite KTaO3 has recently been shown to become superconducting [1]. In the closely related material SrTiO3, a ferroelectric quantum critical point was proposed to be the origin of superconductivity [2]. In this work, using first-principles calculations, we show that a ferroelectric quantum critical point emerges with electron doping in KTaO3, lying at doping values close to the top of the superconducting dome. We examine the effects of larger spin-orbit coupling and absence of crystal field splitting in KTaO3, in comparison to SrTiO3, on the phonon spectrum, electron-phonon coupling and quantum oscillations. Our findings contribute to the growing understanding of superconductivity around quantum critical points and could help in designing materials with higher superconducting critical temperatures.

[1] Ueno, K. et al. Discovery of Superconductivity in KTaO3 by Electrostatic Carrier Doping. Nature Nanotechnology 6, 408 (2011). [2] Edge, J. M., Kedem, Y., Aschauer, U., Spaldin, N. A. & Balatsky, A. V. Quantum Critical Origin of the Superconducting Dome in SrTiO3. Physical Review Letters 115, 247002 (2015).

TT 86.4 Thu 10:30 EMH 225

In-operando study of polarization reversal in ferroelectric thin films — •Christelle Kwamen[1], Matthias Rössle[2], Matthias Reinhardt[1], Wolfram Leitenberger[2], Flavio Zamponi[2], Marin Alexe[3], and Matias Bargheer[1,2] — [1]Helmholtz Zentrum Berlin — [2]Institute of physics and astronomie, University of Potsdam — [3]Department of physics, University of Warwick

The mechanisms associated with polarization reversal in ferroelectric materails are still under investigations because the microscopic dynamics are not yet fully understood. The permanent quest for energy efficient technologies drives investigations on making a ferroelectric operational under lowest switching voltage. There are many studies which investigate either the electrical signature of the switching or the structural changes of the crystal lattice associated with the switching. We present here a simultaneous study of the electrical and structural responses of a lead-zirconate-titanate-based capacitor heterostructure during charging, discharging, and polarization reversal, using time-resolved X-ray diffraction. Concomitant with the ferroelectric current peak, we observe the switching is characterized by a transient disorder evidenced by a decrease of the Bragg peak intensity. A peak width increase reveals the domain dynamics during the reversal. Our investigations show how the incomplete screening of the depolarization charges affect the piezoelectric response, measured via the Bragg peak position. We examine the interplay between charge flow, atomic motion in real time during device operation. We investigate how ultrashort laser pulse excitation can increase the charge flow in a biased device.

TT 86.5 Thu 10:50 EMH 225

Domains Properties in Thin Ferroelectric Films Related to Surface Screening, Flexoelectric and Vegard Effects — •Ivan S. Vorotiahin[1,2], Anna N. Morozovska[2], Eugene A. Eliseev[3], Sergei V. Kalinin[4], Qian Li[4], Yevhen M. Fomichov[3,5], and Yuri A. Genenko[1] — [1]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institute of Physics, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [3]Institute for Problems of Materials Science, National Academy of Sciences of Ukraine, Kyiv, Ukraine — [4]The Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, USA — [5]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Ferroelectric domains is a topic of undying interest in the research community, since their properties and formation conditions still remain not fully understood. Among those conditions, surface screening charges, flexoelectric effect and chemical stresses can be named. Their influence is well observable in films of several to several tens of nanometres thicknesses, i.e. in the forefront of the phenomenological theories.

A series of modelling experiments has been performed to predict the effects that those physical qualities can make on a shape of ferroelectric domains in the most well-known perovskite materials, as well as their impact on the electromechanical properties, phase diagrams, and field distributions. Their influence has been numerically and analytically estimated to provide a roadmap for future measurements and compared with each other to obtain a stronger understanding of the physical processes occurring in perovskites.

TT 86.6 Thu 11:10 EMH 225

Screening in metallized ferroelectrics — •Hongjian Zhao[1], Alessio Filippetti[2,3], Carlos Escorihuela-Sayalero[1], Pietro Delugas[4], Enric Canadell[5], Laurent Bellaiche[6], Vincenzo Fiorentini[2,3], and Jorge Íñiguez[1] — [1]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Luxembourg — [2]Dipartimento di Fisica, Università di Cagliari, Cittadella Universitaria, Italy — [3]CNR-IOM SLACS, Cittadella Universitaria, Italy — [4]Scuola Internazionale Superiore di Studi Avanzati, Italy — [5]Institut de Ciència de Materials de Barcelona, Spain — [6]Physics Department and Institute for Nanoscience and Engineering, University of Arkansas, USA

Ferroelectric materials are characterized by spontaneous polar distortions. The behavior of such distortions in the presence of free charge is the key to the physics of metallized ferroelectrics in particular, and of structurally-polar metals more generally. Using first-principles simulations, here we show that polar distortions resist metallization and the attendant suppression of long-range dipolar interactions in the vast majority of a sample of eleven representative ferroelectrics. We identify a novel meta-screening effect, occurring in the doped compounds as a consequence of the charge rearrangements associated to electrostatic screening, as the main factor determining the survival of a non-centrosymmetric phase. Our findings advance greatly our understanding of the essentials of structurally-polar metals, and offer guidelines on the behavior of ferroelectrics upon field-effect charge injection or proximity to conductive device elements.

20 min. break

TT 86.7 Thu 11:50 EMH 225

Pressure-induced insulator-metal transition in EuMnO$_3$ — •Andres Cano — CNRS, Univ. Bordeaux, ICMCB, Bordeaux, France

We study the influence of external pressure on the electronic and magnetic structure of $EuMnO_3$ from first-principles calculations. We find a pressure-induced insulator? metal transition at which the magnetic order changes from *A*-type antiferromagnetic to ferromagnetic with a strong interplay with Jahn?Teller distortions. This unexpected pressure-induced insulator-to-metal transition, although similar to the observed in CMR $LaMnO_3$, is unprecedented within the multiferroic $RMnO_3$ series. In addition, we find that the non-centrosymmetric $E^?$-type antiferromagnetic order can become nearly degenerate with the ferromagnetic ground state in the high-pressure metallic state. These features make $EuMnO_3$ an unique compound among the manganites because it behaves differently with respect to physical and "chemical" pressure, and hosts a genuinely new type of ferroelectric-like metallic state.

[1] *Pressure-induced insulator-metal transition in EuMnO3*, R. Qiu, E. Bousquet and A. Cano, J. Phys.: Condens. Matter 29, 305801 (2017).

TT 86.8 Thu 12:10 EMH 225

Far infrared studies on a diluted rare-earth langasite — •Lorenz Bergen[1], Evan Constable[1], Lukas Weymann[1], Alexander A. Mukhin[2], Nadezhda Kostyuchenko[1], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

Rare-earth langasites demonstrate fascinating structural and magnetic effects such as geometric frustration and are possible candidates for the spin-liquid state. To better understand the interplay between the structural and magnetic properties it is important to study the phonon and crystal electric field spectra that can be observed in the far infrared (FIR) range. The langasite structure crystallizes in the P321 space group with a general formula $A_3BC_3D_2O_{14}$. Here we present spectra of the diluted rare-earth langasite $La_{2.91}Ho_{0.09}Ga_5SiO_{14}$ using polarized far infrared radiation along different crystallographic directions and under a broad temperature range. The observed phonon frequencies are compared with model calculations. We compare the results on the holmium doped crystal and on pure $La_3Ga_5SiO_{14}$ langasite.

TT 86.9 Thu 12:30 EMH 225

Magnetic Excitations and High-Order Magnetoelectric Effect in Holmium Langasite — •Lukas Weymann[1], Thomas Kain[1], Alexey Shuvaev[1], Artem Kuzmenko[2], Alexander Mukhin[2], Evan Constable[1], Lorenz Bergen[1], Nadezhda Kostyuchenko[1], Anna Pimenov[1], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Prokhorov General Physics Institute, Russian Academy of Sciences, 119991 Moscow, Russia

Recently, compounds of the langasite family (prototype $La_3Ga_5SiO_{14}$) have attracted considerable attention due to their intriguing magnetic and magnetoelectric properties. The geometric frustration of the magnetic ions lies in the focus of the investigation of rare-earth langasites, since this makes them promising candidates for spin liquids.

In this work we show that in diluted rare-earth langasite $La_{2.91}Ho_{0.09}Ga_5SiO_{14}$ (3%Ho-LGS), where no magnetic frustration is present, unusual properties can be observed. 3%Ho-LGS single crystals reveal a substantial magnetoelectric effect comparable with other rare-earth langasites. The symmetry and the field dependence of the effect can only be explained by taking into account the higher order expansions of the crystal field theory. Terahertz measurements with a Mach-Zehnder interferometer reveal a series of characteristic magnetic excitations and a strong zero-field mode of presently unknown origin.

TT 86.10 Thu 12:50 EMH 225

Structural phase transition and domain formation in the hybrid improper ferroelectric $Ca_3Mn_{1.9}Ti_{0.1}O_7$ — •Mads C. Weber[1], Thomas Lottermoser[1], Morgan Trassin[1], Bin Gao[2], Sang-Wook Cheong[2], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]Rutgers University, Piscataway, New Jersey, USA

One of the bottlenecks for the application of magneto-electric multiferroics is the lack of materials with both, a robust coupling between ferroelectricity and magnetism, and a sufficiently large polarization. This problem may be overcome in layered perovskite systems, where octahedral rotations can give rise to improper ferroelectricity as well as a net-magnetization. Accordingly, ferroelectricity and magnetic order are linked by non-polar structural distortions. Essential for the understanding of the potential coupling of both parameters is an in-depth comprehension of the structural distortions and the formation of domains. In this work, we present a combined Raman spectroscopy (RS) and optical second harmonic generation (SHG) study of the improper ferroelectric phase transition and the related domain formation. Using RS, we trace the evolution of the non-polar structural distortions across the phase transition by probing the lattice vibrations of the system. Furthermore, we investigate the emergence of ferroelectricity by SHG a technique highly sensitive to breaking of inversion symmetry. Hence, RS and SHG represent a unique combination to investigate improper ferroelectric phase transitions.

TT 86.11 Thu 13:10 EMH 225

Lead Palladium Titanate: A new room-temperature magnetoelectric multiferroic — •Elzbieta Gradauskaite[1,2], Jonathan Gardner[3], Rebecca M. Smith[3], Finlay D. Morrison[3], Stephen L. Lee[1], Ram S. Katiyar[4], and James F. Scott[1,3] — [1]School of Physics and Astronomy, University of St Andrews, United Kingdom — [2]Present address: Department of Materials, ETH Zürich, Zürich, Switzerland — [3]School of Chemistry, University of St Andrews, United Kingdom — [4]Department of Physics, SPECLAB, University of Puerto Rico, USA

Magnetoelectric multiferroic materials combine the advantages of FeRAMs (speed, low power) and MRAMs (non-destructive readout) due to the linear (magnetoelectric) coupling between ferroelectricity and ferromagnetism. Despite the worldwide interest and effort, very few single-phase materials have been discovered that exhibit magnetoelectric coupling at room temperature. Until very recently $BiFeO_3$ was the only one, however it is not suitable for real practical device applications due to high leakage currents and weak coupling. Here, we demonstrate that $PbTi_{1-x}Pd_xO_3$ ($0 < x < 0.3$) is multiferroic up to 400 K and possesses a strong magnetoelectric coupling. This observation is remarkable because Pd is difficult to substitute into ABO_3 perovskite oxides and it is magnetic only under unusual conditions (strain or internal electric fields). Dielectric spectroscopy and magnetization studies will be discussed in detail, while paying particular attention to secondary phases present in the bulk specimen, identified as PdO, $PbPdO_2$ and Pd_3Pb using PXRD, SEM, EDX and XPS.

TT 87: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VI (joint session O/MM/DS/TT/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 10:30–12:45 Location: HL 001

TT 87.1 Thu 10:30 HL 001

Core-level spectroscopy with the *GW* approximation — •Dorothea Golze and Patrick Rinke — Department of Applied Physics, Aalto University, Espoo, Finland

Inner-shell spectroscopy is an important tool to characterize molecules, liquids and adsorption processes at surfaces. We present a new, accurate method for computing X-ray photoelectron spectra based on the *GW* approximation that overcomes the limitations of density functional theory based approaches. Green's function theory in the *GW* approximation has become the method of choice for addition and removal energies of valence electrons in solids and is now increasingly being applied to molecules. However, *GW* core-level spectroscopy has thus far not received any attention. In most *GW* implementations, the self-energy is computed in the imaginary frequency domain followed by an analytic continuation to the real frequency axis. However, our calculations show that the analytic continuation becomes highly inaccurate for frequencies far away from the Fermi level and is not suitable for the computation of core excitations. Thus, we evaluate the self-energy on the real-frequency axis using the contour deformation (CD) technique. We implemented CD in combination with a resolution-of-the-identity approximation for the screened Coulomb interaction in the FHI-aims program package. Test calculations reveal that our implementation reproduces Turbomole reference calculations [1] perfectly. Furthermore, we present benchmark studies of small and medium-sized gas-phase molecules and discuss the potential of our method for more complex systems. [1] M. J. van Setten et al. JCTC, 2013, 232

TT 87.2 Thu 10:45 HL 001

***GW* and beyond from matrix resolvents** — •Jan Gesenhues[1], Dmitrii Nabok[2], Michael Rohlfing[1], and Claudia Draxl[2] —

[1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany — [2]Theoretische Festkörperphysik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Typically GW calculations make use of either plasmon pole models or numerical integration in order to determine the screened Coulomb interaction W. We demonstrate how to obtain an analytical representation of W with the help of a matrix resolvent and present some standard GW results which have been obtained with the method. The analytical W is a useful starting point for subsequent calculations involving vertex corrections. On the other hand, the matrix resolvent technique itself can be applied upon a BSE-like equation of motion for the polarizability to include vertex corrections.

TT 87.3 Thu 11:00 HL 001

Electron-Magnon Scattering in Elementary Ferromagnets from First Principles: Lifetime Broadening and Kinks — Mathias C. T. D. Müller, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We study the electron-magnon scattering in bulk Fe, Co, and Ni within the framework of many-body perturbation theory implemented in the full-potential linearized augmented-plane-wave method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the two-particle (electron-hole) Green function, where single-particle Stoner excitations and collective spin-wave excitations (magnons) are treated on the same footing. We employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. The resulting renormalized electronic band structures exhibit strong spin-dependent lifetime effects close to the Fermi energy, which are strongest in Fe. In the case of Co and Ni, the renormalization gives rise to kinks in the electronic band dispersion at low binding energies, which we attribute to electron scattering with spatially extended spin waves. Furthermore, we find a band anomaly at larger binding energies in iron, which results from a coupling of the quasihole with single-particle excitations that form a peak in the Stoner continuum. This band anomaly has, in fact, been observed in recent photoemission experiments at the same energy and momentum.

TT 87.4 Thu 11:15 HL 001

Effects of the Tamm-Dancoff approximation on the optical spectra of organic molecules — •Tobias Lettmann and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

When calculating excited state properties of electronic systems within the many-body perturbation theory (MBPT), the Bethe-Salpeter equation (BSE) needs to be solved. This is often done within the so called Tamm-Dancoff approximation (TDA), neglecting the coupling of resonant and anti-resonant excitations.

It is generally accepted that the TDA is justified for large, extended systems e.g. bulk crystals. However it has been shown that the TDA may no longer hold for some organic semiconductors[1]. In this talk we discuss the effects of the TDA on the resulting optical spectra of organic molecules of different sizes and investigate for which cases the TDA may still be justified.

[1] B. Baumeier et al: *J Chem. Theory Comput.*, 2012, **8**, 997

TT 87.5 Thu 11:30 HL 001

Ab-initio treatment of non-local electronic correlations with the dynamical vertex approximation — •Anna Galler[1], Patrik Thunström[2], Patrik Gunacker[3], Josef Kaufmann[3], Matthias Pickem[3], Jan M. Tomczak[3], and Karsten Held[3] — [1]Centre de Physique Theorique, Ecole Polytechnique, 91128 Palaiseau, France — [2]Department of Physics and Astronomy, Materials Theory, Uppsala University, 75120 Uppsala, Sweden — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Recently, approaches such as the dynamical vertex approximation (DΓA) or dual-fermion method have been developed. These diagrammatic approaches are going beyond dynamical mean-field theory (DMFT) by including non-local electronic correlations on all length scales as well as the local DMFT correlations. Here we present our efforts to extend the DΓA methodology to ab-initio materials calculations (AbinitioDΓA). Our approach is a unifying framework which includes both, GW and DMFT-type of diagrams, but also important non-local correlations beyond, e.g. non-local spin fluctuations. In our multi-band implementation we are using a worm sampling technique within continuous-time quantum Monte Carlo in the hybridization expansion to obtain the DMFT vertex, from which we construct the reducible vertex function in a ladder approximation. As a first application we show results for transition metal oxides. Support by the ERC project AbinitioDGA (306447) is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, Jan M. Tomczak, and K. Held, Physical Review B 95, 115107 (2017)

TT 87.6 Thu 11:45 HL 001

Non-local correlations in effectively reduced spatial dimensions — •Jan M. Tomczak[1], Matthias Pickem[1], Benjamin Klebel[1], Anna Galler[2], Josef Kaufmann[1], Patrik Gunacker[1], Patrik Thunström[3], Thomas Schäfer[2], Alessandro Toschi[1], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, Austria — [2]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France — [3]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Using the dynamical vertex approximation and its recent extension for electronic structure calculations, AbinitioDΓA[1], we explore the impact of spatial dimensions onto non-local correlations: (a) we compare magnitude and manifestations of non-local self-energies in ultra-thin films of transition-metal oxides to those in the bulk material. (b) we track the evolution of non-local correlations in the doped Hubbard model when continuously going from 3D to 2D. In particular we probe the limits of the "space-time separation" of electronic correlations evidenced in 3D[2]. Support by the ERC project AbinitioDGA (306447) and the Austrian Science Fund (FWF) projects I 2794-N35 and P 30213-N36 is acknowledged.

References: [1] A. Galler, P. Thunström, P. Gunacker, JMT, K. Held, PRB 95, 115107 (2017), [2] T. Schäfer, A. Toschi, JMT, PRB 91, 121107R (2015)

TT 87.7 Thu 12:00 HL 001

Does the optical signature of oxidized polyethylene stem from saturated or unsaturated carbonyl defects? — •Guido Roma[1], Fabien Bruneval[1], and Layla Martin-Samos[2] — [1]DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif sur Yvette, France — [2]CNR-Demokritos, Trieste, Italy

Polyethylene (PE), one of the simplest and most used aliphatic polymers, is generally provided with a number of additives, in particular antioxidants, because of its tendency to get oxidized. Carbonyl defects, a product of the oxidation of PE, are occurring in various forms, in particular saturated ones, known as ketones, where a C=O double bond substitutes a CH_2 group, and various unsaturated ones, i.e., with further missing hydrogens. Many experimental investigations of the optical properties in the visible/UV range mainly attribute the photoluminescence of PE to one specific kind of unsaturated carbonyls, following analogies to the emission spectra of similar small molecules. However, the reason why saturated carbonyls should not be optically detected is not clear. We investigated the optical properties of PE with and without carbonyl defects using perturbative GW and the Bethe-Salpeter equation in order to take into account excitonic effects. We discuss the calculated excitonic states in comparison with experimental absorption/emission energies and the stability of both saturated and unsaturated carbonyl defects. We conclude that the unsaturated defects are indeed the best candidate for the luminescence of oxidized PE, and the reason is mainly due to oscillator strengths.

TT 87.8 Thu 12:15 HL 001

Bethe-Salpeter equation beyond the Tamm-Dancoff approximation at finite momentum transfer: Absorption and loss spectra including excitonic effects — •Benjamin Aurich, Caterina Cocchi, and Claudia Draxl — Humboldt-University, Berlin, Germany

The state-of-the-art ab-initio method for computing optical properties of semiconductors is based on the Bethe-Salpeter equation (BSE) which describes the excitations of the system in terms of interacting electron-hole (e-h) pairs. For absorption spectra, typically no momentum transfer from light to the e-h pairs is considered, and the coupling between excitations and de-excitations of e-h pairs is usually neglected by using the Tamm-Dancoff approximation (TDA). This approach yields excellent agreement with experiment for many materials, but may break down for confined systems [1]. The TDA is also known to fail to describe the electron energy loss spectra for materials as simple as silicon [2]. We report on the extensions of the open-source code `exciting` [3] allowing for BSE calculations beyond the TDA and at finite momentum transfer using an exact diagonalization scheme [4]. We demonstrate the differences between TDA and non-TDA spectra

at vanishing and finite momentum transfer for periodic molecular systems.

[1] M. Grüning et al., Nano Lett **9**, 2820 (2009)
[2] V. Olevano and L. Reining, Phys. Rev. Lett. **86**, 5962 (2001)
[3] A. Gulans et al., J. Phys. Condens. Matter **26**, 363202 (2014)
[4] T. Sander et al., Phys. Rev. B **92**, 045209 (2015)

TT 87.9 Thu 12:30 HL 001

Calculations of charge and spin susceptibilities and quasiparticle energy shifts within the CASTEP plane-wave DFT code — •Vincent Sacksteder[1], Evgeny Plekhanov[2], Phil Hasnip[3], Matt Probert[3], Stewart Clark[4], Keith Refson[1], and Cedric Weber[2] — [1]Royal Holloway University of London, UK — [2]Kings College London, UK — [3]University of York, UK — [4]University of Durham, UK

CASTEP is a pseudopotential based plane wave code which scales to the largest supercomputers and offers a wide feature set. Within CASTEP we have implemented calculation of the charge and spin susceptibility tensor, which describes the response to a perturbing charge or spin. We present corrections to the Kohn-Sham energies obtained by using the susceptibility tensor to screen Hartree-Fock exchange. In the static limit this is the SEX part of the COHSEX approximation, and if instead the dynamic susceptibility is used one obtains the GW approximation.

Our memory and CPU consumption scales linearly with the plane wave basis size, allowing thorough exploration of convergence with basis size, not only of the susceptibility itself, but of the SEX and GW quasiparticle shifts. We emphasize that our calculations are heavily parallelized, in exactly the same way as a standard DFT ground state calculation.

This work will allow first principles calculations of magnon spectra, exchange couplings, ionization potentials, and KKR and DMI coefficients.

TT 88: Quantum-Critical Phenomena III

Time: Thursday 11:30–13:00 Location: H 3010

TT 88.1 Thu 11:30 H 3010

Holography and criticality in matchgate tensor networks — •Alexander Jahn, Marek Gluza, Fernando Pastawski, and Jens Eisert — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The AdS/CFT correspondence conjectures a holographic duality between gravity in a bulk space and a critical quantum field theory on its boundary. Tensor networks have come to provide toy models to understand such bulk-boundary correspondences, shedding light on connections between geometry and entanglement. We introduce a versatile and efficient framework for studying tensor networks, extending previous tools for Gaussian matchgate tensors in 1+1 dimensions. Using regular bulk tilings, we show that the critical Ising theory can be realized on the boundary of both flat and hyperbolic bulk lattices. Within our framework, we also produce translation-invariant critical states by an efficiently contractible network dual to the multi-scale entanglement renormalization ansatz. Furthermore, we explore the correlation structure of states emerging in holographic quantum error correction. We hope that our work will stimulate a comprehensive study of tensor network models capturing bulk-boundary correspondences.

TT 88.2 Thu 11:45 H 3010

Fermion-induced quantum critical points with two length scales — •Emilio Torres[1], Laura Classen[2], and Michael Scherer[1] — [1]Institute of theoretical Physics, University of Cologne, Germany — [2]Physics Department, Brookhaven National Laboratory, NY, USA

The quantum phase transition to a Z3-ordered Kekule phase in two-dimensional Dirac semimetals is governed by a fermion-induced quantum critical point, which renders the putative discontinuous transition continuous. We study the resulting universal, critical behavior in terms of a functional RG approach, which permits to access scaling behavior also on the symmetry-broken side of the phase transition. We show that the fermion-induced criticality leads to a scaling form with two divergent length scales, due to the breaking of the discrete Z3 symmetry. This provides a second source for scaling corrections besides the proximity to the first order transition.

TT 88.3 Thu 12:00 H 3010

Quantum critical behavior of Dirac systems at higher-loop order — •Bernhard Ihrig[1], Michael Scherer[1], Luminita Mihaila[2], and Nikolai Zerf[2] — [1]Universität Köln — [2]Universität Heidelberg

Dirac fermions appear as quasi-particle excitations in many different condensed-matter systems. They display various quantum transitions which represent unconventional universality classes related to variants of Gross-Neveu-Yukawa models. For the first time, we study these models – at three- and four-loop order, and compute critical exponents in $4-\epsilon$ dimensions for general number of fermion flavors.We apply the computed series for the exponents and their Padé approximants to several phase transitions of current interest: metal-insulator transitions of spin-1/2 and spinless fermions on the honeycomb lattice, emergent supersymmetric surface field theory in topological phases, as well as dualities in a deconfined quantum criticality scenario. Comparison with the results of other analytical and numerical methods is discussed.

TT 88.4 Thu 12:15 H 3010

Avalanche of entanglement and correlations at quantum phase transitions — •Andreas Osterloh, Konstantin V. Krutitsky, and Ralf Schützhold — Universität Duisburg-Essen, Duisburg, Deutschland

We study the two, three, and four-point correlations in the ground-state of the quantum Ising model in a transverse field with nearest neighbor ferromagnetic coupling J and find a partial inversion of their hierarchy. Namely, the four-point correlation exceeds the three- and two-point correlations, well before the critical point is reached. Qualitatively similar behavior is also found for the Bose-Hubbard model, suggesting this change in hierarchy to be a general feature of a quantum phase transition. It should be taken into account in approximations starting from a mean-field limit.

In addition, we find a sequential increase of entanglement depth d with growing J, hence an avalanche that starts with two-point entanglement, as measured by the concurrence, and continues via the three-tangle and four-tangle, until finally, deep in the ferromagnetic phase for $J=\infty$, the exact model would arrive at a pure L-partite (GHZ type) entanglement of all L spins.

TT 88.5 Thu 12:30 H 3010

Quantum phase transition with dissipative frustration — •Dominik Maile[1,2], Sabine Andergassen[2], Wolfgang Belzig[1], and Gianluca Rastelli[1,3] — [1]Fachbereich Physik, Universität Konstanz, D-78457, Germany — [2]Institut für Theoretische Physik and Center of Quantum Science, Auf der Morgenstelle 14, Universität Tübingen, D-72076 Tübingen, Germany — [3]Zukunftskolleg, Universität Konstanz, D-78457, Konstanz, Germany

We study the quantum phase transition of the one dimensional phase model in presence of dissipative frustration, provided by an interaction of the system with the environment through two non-commuting operators [1]. Such a model can be realized in Josephson junction chains with shunt resistances and resistances between the chain and the ground. Using a self-consistent harmonic approximation, we determine the phase diagram at zero temperature which exhibits a quantum phase transition between a long-range ordered phase, corresponding to the superconducting state, and a disordered phase, corresponding to the insulating state with localized superconducting charge. Interestingly, we find that the critical line separating the two phases has a non monotonic behavior as a function of the dissipative coupling strength. The non monotonic behavior is reflected also in the purity of the system that quantifies the degree of correlation between the system and the environment, and the logarithmic negativity as entanglement measure that encodes the internal quantum correlations in the chain.

[1] D. Maile, S. Andergassen, W. Belzig, G. Rastelli, arXiv:1711.11346

TT 88.6 Thu 12:45 H 3010

Emergent symmetry in quantum critical Dirac systems — •Lukas Janssen[1], Igor F. Herbut[2], and Michael M. Scherer[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [2]Department of Physics, Simon Fraser University, Burnaby, Canada — [3]Institut für Theoretische Physik, Universität Köln, Germany

Within the standard Landau-Ginzburg paradigm, $O(N)$ symmetry, when not present explicitly on the microscopic level, can emerge dynamically at some critical point only for small $N < 3$. We show that this classical conclusion becomes severely overturned in the presence of gapless fermion degrees of freedom. We study the quantum multicritical point in 2+1D Dirac systems between the semimetallic phase and two ordered phases that are characterized by anticommuting mass terms with $O(N_1)$ and $O(N_2)$ symmetry, respectively. Using ϵ expansion around the upper critical space-time dimension of four, we demonstrate that the multicritical point is characterized by an emergent $O(N_1 + N_2)$ symmetry for arbitrary values of N_1 and N_2 and fermion flavor numbers N_f, as long as the corresponding representation of the Clifford algebra exists. Put differently, small $O(N)$-breaking perturbations near the chiral $O(N)$ fixed point are irrelevant for all $N > 1$.

TT 89: Disordered Quantum Systems

Time: Thursday 11:30–12:45 Location: HFT-FT 131

TT 89.1 Thu 11:30 HFT-FT 131

Spin freezing and spin dynamics in the reentrant spin glass Fe_xCr_{1-x} — •Georg Benka[1], Steffen Säubert[1,2], Philipp Schmakat[2,3], Andreas Bauer[1], Stephen M. Shapiro[4], Peter Böni[3], and Christian Pfleiderer[1] — [1]Lehrstuhl für Topologie korrelierter Systeme, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Lehrstuhl für Neutronenstreuung, Technische Universität München, Garching, Germany — [4]Brookhaven National Laboratory, Department of Physics, Upton, USA

Fe_xCr_{100-x} shows reentrant spin glass behaviour below a concentration dependent freezing temperature T_f. In contrast to a classical spin glass, the ground state changes from antiferromagnetic to ferromagnetic order with increasing iron concentration x. For intermediate concentrations a coexistence of the spin glass and magnetic order is discussed [1, 2]. We present a comprehensive study of the Fe_xCr_{100-x} system over a wide range of concentrations by means of magnetisation measurements in combination with neutron depolarisation and neutron spin echo methods. This allows us to compare the relaxation process depending on the particular state at high temperatures. Our measurements provide an unprecedented combination of microscopic information on the spin dynamics and spin freezing on multiple length and time scales.

[1] S. K. Burke et al., J. Phys. F: Met. Phys. 13 (1983) 451
[2] S. M. Shapiro et al., Phys. Rev. B 24 (1981) 6661

TT 89.2 Thu 11:45 HFT-FT 131

Low Temperature Properties of Amorphous Polymers containing Nuclear Quadrupole Moments — •Benedikt Frey, Nicole Assmann, Patrick Schygulla, Annina Luck, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

The low temperature properties of amorphous solids are governed by atomic tunneling systems and can be described by the phenomenological standard tunneling model (STM). In recent years, two-pulse polarization echoes and dielectric measurements, have revealed the importance of nuclear electric quadrupole moments for the tunneling dynamics. Dielectric properties of the multicomponent glasses N-KZFS11 and HY-1, containing atoms with very large nuclear electric quadrupole moments, show significant deviations from the STM. This can be interpreted as a new quadrupole mediated relaxation process, which dominates the relaxation rate at low temperatures.

In order to further study this relaxation mechanism, we measured the low temperature dielectric properties of several amorphous polymers, which contain nuclear quadrupole moments with quadrupole splittings ranging from 30 MHz to 250 MHz. The well known chemical structure of these polymers and the large variety of chemically accessible compositions enables systematic investigations. We present first results from dielectric measurements of three different polymers at frequencies between 60 Hz and 140 MHz. In particular, the brominated samples show strong deviations from the STM at low temperatures and low frequencies.

TT 89.3 Thu 12:00 HFT-FT 131

Loschmidt amplitude in disordered spin systems — •Sebastian Paeckel[1], Francisco Simao[1], Timo Mutas[2], Thomas Köhler[1], Markus Schmitt[1], and Salvatore Manmana[1] — [1]Institut für Theoretische Physik, Georg August Universität Göttingen, Germany — [2]University of Copenhagen, Copenhagen, Denmark

Motivated by recent studies on systems exhibiting time translational symmetry breaking [1,2] we investigated the Loschmidt echo for disordered spins systems with special focus onto the transverse Ising model. Starting from the Z_2 symmetric limit ($h_z \equiv 0$) we analytically calculated the time-evolution for various short ranged correlated initial states. Our results enable us to draw an intuitive picture for the emergence of time translational symmetry breaking which also permits to generalize our findigs to the case of $h_z \neq 0$ and consider more elaborated systems breaking Z_n symmetry.

We acknowledge funding by DFG FOR 1807.

[1] D V. Else, B Bauer, Ch Nayak, Phys. Rev. Lett. 117, 090402
[2] K. Sacha, J. Zakrzewski, arXiv:1704.03735

TT 89.4 Thu 12:15 HFT-FT 131

Spectral densities of disordered quantum spin ladders — •Max Hörmann, Paul Wunderlich, and Kai Phillip Schmidt — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

We investigate the zero-temperature dynamic structure factor of a two-leg spin-1/2 Heisenberg ladder with quenched disorder relevant for inelastic neutron scattering. To this end we apply perturbative continuous unitary transformations about the limit of isolated rungs using a white-graph expansion [1] to derive the physical properties of the elementary triplon and two-triplon excitations of the disordered spin ladder in the thermodynamic limit. Here we study bimodal disorder on rungs and legs realizable in experiments by intential doping of existing spin-ladder compounds. The effect of disorder on the two-triplon properties is calculated with high precision in the weakly-coupled rung regime and with that the fate of the bound states is predicted. For the material class of $BPCB_xC_{1-x}$ one- and two-triplon neutron scattering responses are calculated in both symmetry sectors.

[1] K. Coester and K.P. Schmidt, Phys. Rev. E 92, 022118 (2015).

TT 89.5 Thu 12:30 HFT-FT 131

Corrections to the self-consistent Born approximation for Weyl fermions — •Andreas Sinner and Klaus Ziegler — Institut für Physik, Theorie II Universität Augsburg Universitätsstr. 1 D-86159, Augsburg, Germany

The average density of states of two- and three-dimensional Weyl fermions is studied in the self-consistent Born approximation (SCBA) and its corrections [1]. The latter have been organized in terms of a 1/N expansion. It turns out that an expansion in terms of the disorder strength is not applicable, as previously mentioned by other authors. Nevertheless, the 1/N expansion provides a justification of the SCBA as the large N limit of Weyl fermions.

[1] A. Sinner, K. Ziegler, Phys. Rev. B 96, 165140 (2017).

TT 90: Coherent Quantum Dynamics (joint session DY/TT)

Time: Thursday 12:00–12:45 Location: EB 107

TT 90.1 Thu 12:00 EB 107

Initial System-Environment Correlations via the Transfer Tensor Method — Maximilian Buser[1,2], •Javier Cerrillo[1], Gernot Schaller[1], and Jianshu Cao[2] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, German — [2]Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, Massachusetts 02139, USA

Open quantum systems exhibiting initial system-environment correlations are notoriously difficult to simulate. We point out that given a sufficiently long sample of the exact short-time evolution of the open system dynamics, one may employ transfer tensors for the further propagation of the reduced open system state. This approach is numerically advantageous and allows for the simulation of quantum correlation functions in hardly accessible regimes. We benchmark this approach against analytically exact solutions and exemplify it with the calculation of emission spectra of multichromophoric systems as well as for the reverse temperature estimation from simulated spectroscopic data. Finally, we employ our approach for the detection of spectral signatures of electromagnetically-induced transparency in open three-level systems.

TT 90.2 Thu 12:15 EB 107

Generation of subharmonic oscillations in driven quantum systems — •Onno Renke Diermann — Condensed Matter Theory, IfP Uni Oldenburg

We present an elementary model for the breaking of discrete time translational symmetry. We consider weakly anharmonic quantum oscillators and apply a time-periodic force which couples close-to-resonant energy levels. An appropriate version of the rotating wave approximation then is employed to derive an effective time-independent Hamiltonian describing a quasiparticle in a multi-well potential. The eigenstates of this potential, which extend over all wells, correspond to Floquet states which inherit the period of the driving force, whereas states localized in only one of the wells of the effective potential correspond to wave packets performing subharmonic motion.

TT 90.3 Thu 12:30 EB 107

Topological Qubit: Quantum States in the Sheaf/Scheme Framework — Antonina N. Fedorova and •Michael G. Zeitlin — Russia, 199178, St.Petersburg, V.O. Bolshoj pr., 61, IPME RAS, Mathematical Methods in Mechanics Group

We consider some generalization of the theory of quantum states, which is based on the analysis of long standing problems and unsatisfactory situation with existing interpretations of quantum mechanics. We demonstrate that the consideration of quantum states as sheaves can provide, in principle, more deep understanding of some well-known phenomena. The key ingredients of the proposed construction are the families of sections of sheaves with values in the proper category of the functional realizations of infinite-dimensional Hilbert spaces with special (multiscale) filtrations decomposed into the (entangled) orbits generated by actions/representations of internal hidden symmetries. In such a way, via proper categorification in a general scheme framework, we open a possibility for the exact description of a lot of phenomena like entanglement and measurement, wave function collapse, self-interference, instantaneous quantum interaction, many-worlds, hidden variables, etc. In the companion paper we consider the machinery needed for the generation of a zoo of the complex quantum patterns during Wigner-Weyl-Moyal evolution together with the constructive algebraic control.

TT 91: Correlated Electrons: Method Development

Time: Thursday 15:00–18:15 Location: H 0104

TT 91.1 Thu 15:00 H 0104

Changes in fRG critical scales due to frequency-dependence in a two-patch model — •Timo Reckling and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany

The frequency dependence of the running interactions has become an object of interest in various recent implementations of the functional Renormalization Group (fRG) for low-dimensional fermionic lattice models. In order to understand the main effects and to set up a simpler testbed for approximations, we study a two-patch g-ology model. We analyze the influence of the frequency dependence of the effective two-particle interaction on the critical scales of the flows to strong coupling. To this end the effective interaction which is generated in the fRG flow is parametrized by four interaction components $g_{1,2,3,4}$ each of which depend on three 3 fermionic Matsubara frequencies. Reducing this dependence on three frequencies defines various approximations, with the static approximation as the most drastic one. We can also switch the frequency dependence on and off in different channels which contain distinct loop contributions on the right hand side of the fRG flow equations. This allows us to gain constructive insight into how the frequency-(in)dependent multi-channel interplay determines the critical scales for ordering instabilities.

This work is supported by the DFG-RTG 1995 "Quantum many-body methods in condensed matter systems".

TT 91.2 Thu 15:15 H 0104

Full frequency and momentum parametrization of the two-particle vertex in functional RG for fermionic lattice models — •Cornelia Hille[1], Agnese Tagliavini[1,2], Alessandro Toschi[2], Sabine Andergassen[1], and Carsten Honerkamp[3] — [1]Universität Tübingen, Tübingen, Deutschland — [2]Technische Universität Wien, Wien, Österreich — [3]RWTH Aachen, Aachen, Deutschland

The functional renormalization group (fRG) provides an unbiased method to investigate competing instabilities in fermionic lattice models. So far fRG applications succeeded in describing the qualitative phase diagrams for the perturbative coupling regime of various classes of one-band and multi-band models. However, quantitative predictions, e.g. about energy scales or susceptibilities, were not truly controlled because the full parameter dependence of the two-particle vertex had to be simplified for the sake of numerical feasibility, mostly by disregarding the frequency dependence of the vertex which rendered the selfenergy hard to include. Here we show how combining the vertex parametrization guided by the high frequency asymptotics and the expansion of the momentum dependences in terms of form factors results in a significant improvement of the implementation. By including the selfenergy and the susceptibility flow, we can directly compute physical observables that stand the comparison with other methods. With our unbiased implementation, we can systematically investigate the corrections to previous fRG approximations in the 2D-Hubbard model.

TT 91.3 Thu 15:30 H 0104

Phase transitions with a fully consistent second order functional renormalization group scheme — •Lisa Markhof[1], Björn Sbierski[2], Volker Meden[1], and Christoph Karrasch[2] — [1]Inst. for Theory of Stat. Phys., RWTH Aachen, Germany — [2]Dept. of Phys., FU Berlin, Germany

The functional renormalization group (fRG) is a versatile tool to tackle interacting many-body systems [1]. Recently, starting from the generic flow equations, the "extended coupled-ladder approximation" (eCLA) for specific models has been developed which is exact up to second order in the interaction [2,3], while still being feasible from a computational point of view. We here employ this scheme to study phase transitions in models of spinless fermions. Using a channel decomposition and exploiting the structure of the bare interaction, all second order terms can be included while keeping the number of flow equations managable. In contrast to other fRG schemes used earlier to investigate phase transitions [1], the self-energy feedback is fully contained as well. It is furthermore possible to incorporate a feedback of the

vertex flow. In this approximation, the fRG captures phase transitions in one-dimensional tight-binding chains at half filling, which are inaccessible to a lowest order fRG scheme. We apply the eCLA to models in real space; a similar approach has been used in [4] in momentum space.

[1] W. Metzner et al., Rev. Mod. Phys. **84**, 299 (2012)
[2] F. Bauer et al., Phys. Rev. B **89**, 045128 (2014)
[3] L. Weidinger et al., Phys. Rev. B **95**, 035122 (2017)
[4] S. Sbierski and C. Karrasch, arXiv:1710.06373

TT 91.4 Thu 15:45 H 0104

Truncated unity functional renormalization group for multiband systems with spin-orbit coupling — •Giulio Schober[1], Jannis Ehrlich[1,2], Timo Reckling[1], and Carsten Honerkamp[1] — [1]RWTH Aachen University, Aachen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Although the functional renormalization group (fRG) is by now a well-established method for investigating correlated electron systems, it is still undergoing significant technical and conceptual improvements. In particular, the motivation to optimally exploit the parallelism of modern computing platforms has recently lead to the development of the "truncated unity" functional renormalization group (TU-fRG). Here, we review this fRG variant, and we provide its extension to multiband systems with spin-orbit coupling. Furthermore, we discuss some aspects of the implementation and outline opportunities and challenges ahead for predicting the ground state ordering and emergent energy scales for a wide class of quantum materials.

TT 91.5 Thu 16:00 H 0104

Charge dynamics of the antiferromagnetically ordered Mott insulator — •Xing-Jie Han[1], Yu Liu[2,3], Zhi-Yuan Liu[4], Xin Li[1], Jing Chen[1], Hai-Jun Liao[1], Zhi-Yuan Xie[5], B Normand[5], and Tao Xiang[1,6] — [1]Institute of Physics, Chinese Academy of Sciences — [2]LCP, Institute of Applied Physics and Computational Mathematics, Beijing — [3]Software Center for High Performance Numerical Simulation, Chinese Academy of Engineering Physics — [4]Institute of Theoretical Physics, Chinese Academy of Sciences — [5]Department of Physics, Renmin University of China — [6]Collaborative Innovation Center of Quantum Matter, Beijing

We introduce a slave-fermion formulation in which to study the charge dynamics of the half-filled Hubbard model on the square lattice. In this description, the charge degrees of freedom are represented by fermionic holons and doublons and the Mott-insulating characteristics of the ground state are the consequence of holon-doublon bound-state formation. The bosonic spin degrees of freedom are described by the antiferromagnetic Heisenberg model. Within this framework and in the self-consistent Born approximation, we perform systematic calculations of the average double occupancy, the electronic density of states, the spectral function and the optical conductivity. Qualitatively, our method reproduces the lower and upper Hubbard bands, the spectral-weight transfer into a coherent quasiparticle band at their lower edges and the renormalisation of the Mott gap, which is associated with holon-doublon binding, due to the interactions of both quasiparticle species with the magnons.

TT 91.6 Thu 16:15 H 0104

Efficient Bethe-Salpeter equations' inversion in dynamical mean-field theory — •Agnese Tagliavini[1,3], Stefan Hummel[2], Nils Wentzell[5], Sabine Andergassen[3], Alessandro Toschi[4], and Georg Rohringer[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [3]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [4]Russian Quantum Center, 143025 Skolkovo, Russia — [5]Institut de Physique Théorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France

Quantum many-body calculations of two-particle Greens' and vertex functions represent a very important, but also highly demanding task. Hence, a particular effort has been recently devoted to develop novel algorithmic procedures aimed at saving both memory and computational time. In this talk, we present two efficient and numerically stable asymptotic-based algorithms designed to correctly determine the local two-particle irreducible vertex in all scattering channels by means of the inversion of the corresponding Bethe-Salpeter equations. The latter operation is, in fact, a fundamental step in diagrammatic extensions of DMFT like the Dynamical Vertex Approximation (DΓA). The two algorithms have been tested, and critically compared, for the single-band 3D Hubbard model in the vicinity of the Mott transition, where the asymptotic structures of the vertex functions become dominant.

TT 91.7 Thu 16:30 H 0104

Fractional quantum Hall effect in the interacting Hofstadter model via tensor networks — Matthias Gerster[1], •Matteo Rizzi[2], Pietro Silvi[1,3], Marcello Dalmonte[4], and Simone Montangero[1,5,6] — [1]ICQS & IQST, Ulm University, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [3]Institute for Theoretical Physics, University of Innsbruck, Austria — [4]Abdus Salam ICTP, Trieste, Italy — [5]Theoretische Physik, Universität des Saarlandes, Saarbrücken, Germany — [6]Dipartimento di Fisica e Astronomia, Università di Padova, Italy

We show via tensor network methods that the Harper-Hofstadter Hamiltonian for hard-core bosons on a square geometry supports a topological phase realizing the $\nu - 1/2$ fractional quantum Hall (FQH) effect on the lattice. We address the robustness of the ground-state degeneracy and of the energy gap, measure the many-body Chern number, and characterize the system using Green functions, showing that they decay algebraically at the edges of open geometries, indicating the presence of gapless edge modes. Moreover, we estimate the topological entanglement entropy by taking a combination of lattice bipartitions that reproduces the topological structure of the original proposals by Kitaev and Preskill, and Levin and Wen. The numerical results show that the topological contribution is compatible with the expected value $\gamma = 1/2$. Our results provide extensive evidence that FQH states are within reach of state-of-the-art cold-atom experiments.

[1] Gerster *et al.*, Phys. Rev. B **96**, 195123 (2017)

15 min. break.

TT 91.8 Thu 17:00 H 0104

Identifying the pairing mechanism in strontium ruthenate via renormalization — •Mario Fink and Ronny Thomale — Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The superconducting state of strontium ruthenate Sr_2RuO_4 has mysteriously succeeded in defying any valid theory and the identification of its gap function for more than twenty years. Even the results of different experimental techniques seem to contradict each other when trying to pinpoint the order parameter. Former theories aiming at a description in terms of a time-reversal symmetry broken (chiral) state were experimentally disproven by the non-existence of edge currents. Our calculations are based on a more complete single-particle model that does not only incorporate the on-site spin-orbit interaction but also more extended non-local spin-orbit coupling terms which are evaluated in all d-orbitals. Using a combined weak-coupling and functional renormalization group approach we integrate out the high-energy degrees of freedom to identify the gap functions for a set of realistic interaction parameters. Motivated by recent experimental results showing a strong increase of the critical temperature under uniaxial pressure, we also explore the consequences of breaking the lattice symmetry D_{4h} down to D_{2h}.

TT 91.9 Thu 17:15 H 0104

Applications of time-dependent full configuration interaction quantum monte carlo — •Kai Guther[1], Werner Dobrautz[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Cambridge, Cambridge, United Kingdom

We employ the full configuration interaction quantum monte carlo [1] method to compute spectral functions of correlated electron systems by the means of complex time evolution [2] in combination with a Maximum Entropy Method [3] analytic continuation approach.

We discuss the dependence of the resulting spectral functions on the chosen complex time contour and simulation parameters and discuss the effect of the stochastic approximation. We study the effect of the chosen integrator for the time-evolution on a few examples and conclude that a second-order Runge-Kutta integrator is well-suited for our application. We discuss possible applications in a self-consistent DMFT scheme.

[1] G. H. Booth, A. J. W. Thom, and A. Alavi, The Journal of Chemical Physics 131, 054106 (2009)
[2] K. Guther, W. Dobrautz, O. Gunnarsson, A. Alavi,

arXiv:1709.00218
[3] M. Jarrell and J. Gubernatis, Phys. Rep. 269, 133 (1996)

TT 91.10 Thu 17:30 H 0104

Having Monte Carlo decide which part of the weight to calculate: eigenstates-sampling in CTQMC — •Alexander Kowalski[1], Andreas Hausoel[1], Patrik Gunacker[2], and Giorgio Sangiovanni[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

Continuous-time quantum Monte Carlo algorithms are numerically exact methods for the solution of the Anderson impurity model often employed in DMFT calculations for strongly correlated electron systems. In the hybridization expansion CT-QMC algorithm, the local part of the system is solved exactly, which usually takes up most of the calculation time due to the exponential scaling of the local Hilbert space with the number of orbitals. A commonly used improvement is the use of conserved quantities to block-diagonalize the local Hamiltonian. We investigated the possibility of additionally sampling outer states separately in the Monte Carlo simulation, either grouped by the blocks of the Hamiltonian or individually.

We describe the details of the new Monte Carlo procedure, such as the modified updates we use to ensure ergodic and efficient sampling, as well as the influence on the average sign.

Using our implementation, we performed multi-orbital calculations at low temperatures and discuss the performance of the new method compared to conventional sampling.

TT 91.11 Thu 17:45 H 0104

Hybrid quantum Monte Carlo simulations of the two dimensional half-filled Su-Schrieffer-Heeger (SSH) model — •Stefan Beyl, Martin Hohenadler, Florian Goth, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Su-Schrieffer-Heeger (SSH) model describes electrons interacting with quantum phonons via a bond coupling. While the model is understood in detail in one dimension, no systematic results are available in two dimensions. Here, we use the Hybrid Quantum Monte Carlo (HQMC) method to simulate the model on the square lattice without a sign problem. We determine the phase diagram and discuss the advantages and challenges of HQMC in the context of electron-phonon systems.

TT 91.12 Thu 18:00 H 0104

Functional renormalisation group for quantum critical metals in $d = 2$ — •Matthew Trott and Chris Hooley — SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9SS, United Kingdom

We present a novel functional renormalisation group calculation for quantum critical metals in two spatial dimensions. We utilise soft frequency regulators to stop the suppression of particle-hole excitations in an attempt to consistently describe Landau damping and non-Fermi liquid effects. Additionally we track bosonic interactions up to sextic coupling to elucidate the fixed point structure.

TT 92: Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions II (joint session MA/TT)

Time: Thursday 15:00–18:00 Location: H 1012

Invited Talk TT 92.1 Thu 15:00 H 1012

Spin orbit fields at the Fe/GaAs(001) interface — •Christian Back — Fakultät für Physik, Universität Regensburg — Physik-Department, TU München

Interfacial spin-orbit torques (SOTs) enable the manipulation of the magnetization through an in-plane charge current. Here, we study a particularly simple single crystalline interface, Fe/GaAs(001)[1], which we use to demonstrate various effects related to interfacial SOTs. We demonstrate crystalline anisotropic magneto-resistance showing C_{2v} symmetry [2], second we show anisotropic magneto-optic response [3]. Finally, we use ferromagnetic resonance based methods to investigate interfacial SOTs and report the observation of robust SOT occuring at a single crystalline Fe/GaAs (001) interface at room temperature [4]. We find that the magnitude of the interfacial SOT, caused by the reduced symmetry at the interface, is comparably strong as in ferromagnetic metal/non-magnetic metal systems. The large spin-orbit fields at the interface also enable the spin-to-charge current conversion at the interface, known as spin-galvanic effect [4]. The results suggest that single crystalline Fe/GaAs interfaces may enable efficient electrical magnetization manipulation.

[1] M. Gmitra et al., Phys. Rev. Lett. 111, 036603 (2013) [2] T. Hupfauer et al., Nat. Commun. 6, 7374 (2015) [3] M. Buchner et al., Phys. Rev. Lett. 117, 157202 (2016) [4] L. Chen et al. Nat. Commun. 7, 13802 (2016)

TT 92.2 Thu 15:30 H 1012

Spin-charge interconversion in single crystalline Bismuth films grown on Ge(111) — •minh tuan dau[1], carlo Zucchetti[2], federico bottegoni[2], céline vergnaud[1], thomas guillet[1], alain marty[1], cyrille beigné[1], andrea picone[2], alberto calloni[2], giovanni isella[2], franco ciccacci[2], pranab kumar das[3], jun fujii[3], ivana vobornik[3], marco finazzi[2], and matthieu jamet[1] — [1]INAC-Spintec, CEA/CNRS/Grenoble-INP and Université Grenoble Alpes, 38054 Grenoble, France — [2]LNESS-Dipartimento di Fisica, Politecnico di Milano, 20133 Milano, Italy — [3]CNR-IOM Laboratorio TASC, 34149 Trieste, Italy

In this study, we have grown a bismuth wedge (0-12 nm) on Ge(111) by molecular beam epitaxy. Using structural characterization (RHEED and x-ray diffraction), we found a critical thickness of ~ 4.5 nm below which Bi exhibits an allotropic pseudocubic phase. A careful angle-resolved and spin-resolved photoemission spectroscopy study using synchrotron radiation showed that the pseudocubic phase exhibits surface states with linear band dispersion and a characteristic helical spin texture. We have then investigated the spin-charge interconversion at these surface states using different techniques: magneto-optical Kerr effect to probe the spin Hall effect (SHE), inverse SHE using optical spin orientation in the Ge film beneath and finally spin pumping from a ferromagnetic layer grown on top of Bi separated by an Al spacer. We found a significant signature of the spin-charge interconversion in these surface states and a clear Bi-thickness dependence of the conversion signals.

TT 92.3 Thu 15:45 H 1012

Scattering of surface and interface states at skyrmionic quasi-particles interacting with defects. — •Imara L. Fernandes, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Magnetic skyrmions are promising candidates as bits of a future information technology. The precise manipulation and detection of such small magnetic nanostructures is a key ingredient for future applications in spintronics devices. Recently, we proposed the tunneling spin-mixing magnetoresistance (TXMR) to detect magnetic skyrmions by all-electrical means [1,2]. The TXMR effect originates from the non-alignment of magnetic moments and it is affected by the presence of spin-orbit interaction. We explore from a full *ab initio* approach the possibility of tuning the TXMR by inserting *3d* and *4d* transition metal defects at the vicinity of skyrmions generated in PdFe bilayer deposited on Ir(111). In the latter system, we identify surface and interface states leading to pronounced TXMR signals after scattering at skyrmionic quasi-particles. We extract the lifetimes of these confined states and draw conclusions concerning the impact of skyrmions and various atomic defects.

[1] D.M. Crum *et al.*, Nat. Commun. **6**, 8541 (2015).
[2] C. Hanneken *et al.*, Nat. Nanotech, **10**, 1039 (2015).
– Funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

TT 92.4 Thu 16:00 H 1012

Orbital fingerprints of skyrmions in ferro- and antiferromagnets — •Manuel dos Santos Dias and Samir Lounis —

Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

X-rays are a very powerful tool for investigating the magnetic properties of materials. The magnetic circular dichroism in ferromagnets can be combined with sum rules to separate the net spin and orbital magnetic moments, while compensated antiferromagnets have no circular dichroism. In this contribution, we explain why skyrmions in ferromagnets encode topological information in their orbital magnetic moment, that can in principle be extracted via sum-rule analysis [1]. This part of the orbital moment originates from magnetic noncoplanarity, as found in our original work and in a simple model description [2]. We then extend the analysis to a skyrmion lattice in an antiferromagnetic background. We investigate whether the topological orbital signature is present, and whether circular dichroism exists and can detect topological information.

This work was supported by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator Grant No. 681405-DYNASORE).

[1] M. dos Santos Dias *et al.*, Nat. Commun. **7**, 13613 (2016)
[2] M. dos Santos Dias and S. Lounis, Proc. SPIE **10357**, Spintronics X, 103572A (2017)

15 minutes break

TT 92.5 Thu 16:30 H 1012

Large perpendicular magnetic anisotropy and Dzyaloshinskii Moriya chiral interaction at room temperature in epitaxial graphene-based structures — Fernando Ajejas[1], Adrian Gudin[1], Ruben Guerrero[1], Leticia De Melo Costa[1], Jose Manuel Diez[1], Pablo Olleros[1], Alberto Anadon[1], Maria Varela[2], Manuel Valvidares[3], Pierluigi Gargiani[3], Jan Vogel[4], Stefania Pizzini[4], Julio Camarero[1], Rodolfo Miranda[1], and •Paolo Perna[1] — [1]IMDEA Nanociencia, Madrid, Spain — [2]ALBA SYNCHROTRON, Barcelona, Spain — [3]Universidad Complutense de Madrid, Madrid, Spain — [4]CNRS Institut Néel, Grenoble, France

A major challenge for future spintronics is to develop suitable spin transport channels with superior properties as long spin lifetime and propagation length. Graphene can meet these requirements, even at room temperature. On the other side, the use of fast motion of Néel-type chiral domain walls (and magnetic skyrmions) can satisfy the demands for high-density data storage, low power consumption and high processing speed. Here, by engineering the epitaxial growth of gr/Co/Pt(111) stacks on (111)-oriented oxide crystals, we achieve an enhanced perpendicular magnetic anisotropy (PMA), with Co thickness up to 4 nm, and left-handed Néel-type chiral domain walls (DWs) stabilized by a strong effective Dzyaloshinskii Moriya interaction (DMI).

TT 92.6 Thu 16:45 H 1012

Analysis of the Dzyaloshinskii-Moriya interaction and spin-orbit torques in Co-based trilayers — •Jan-Philipp Hanke, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Originating from the interplay of spin-orbit coupling and broken inversion symmetry, the Dzyaloshinskii-Moriya interaction (DMI) attracts ever-growing attention as it mediates the formation of chiral spin textures such as magnetic skyrmions. To predict the magnitude of this chiral interaction from *ab initio*, typically, one adopts either demanding computational frameworks or limiting approximations for the spin-orbit interaction. In contrast, we present an advanced Wannier interpolation scheme that evaluates DMI in its modern theory [1] based on the ferromagnetic ground state including spin-orbit coupling self-consistently. Utilizing this technique, we identify the microscopic origin of DMI and spin-orbit torques in the trilayers Ir_xPt_{1-x}/Co/Pt and Au_xPt_{1-x}/Co/Pt [2]. Tuning the composition x, we find that DMI changes sign, promoting the respective systems as promising candidates for detailed experimental studies. We examine also the consequences of the obtained anisotropy of the spin-orbit torques with the magnetization direction for the dynamical properties of skyrmions.

Funding from the DFG (Grant No. MO 1731/5-1) and from the EU Horizon 2020 via the FET-Open project MAGicSky is acknowledged.

[1] F. Freimuth *et al.*, J. Phys. Condens. Matter **26**, 104202 (2014).
[2] J.-P. Hanke *et al.*, arXiv:1711.02657.

TT 92.7 Thu 17:00 H 1012

Electrically and thermally-induced spin polarization in semiconductor heterostructures and at perovskite oxides interfaces — •Anna Dyrdał[1,2], Łukasz Karwacki[3], Józef Barnaś[2,3], Vitalii Dugaev[4], and Jamal Berakdar[1] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, Halle, Germany — [2]Faculty of Physics, A. Mickiewicz University, Poznan, Poland — [3]Institute of Molecular Physics, Polish Academy of Sciences, Poznan, Poland — [4]Department of Physics and Medical Engineering, Rzeszow University of Technology, Rzeszow, Poland

Spin-orbit interaction leads to a variety of spin and transport phenomena that enable control of single spins in a pure electrical manner. The physics that stands behind such effects is very rich and depends on the nature of spin-orbit coupling in the host material. We will discuss and summarize our recent results on electrically and thermally induced nonequilibrium spin polarization obtained within effective models describing 2DEG in semiconductor heterostructures and perovskite oxide interfaces [1-3]. In principle, we will focus on analytical and numerical results describing temperature dependences and show that impurities vertex correction plays important role in thermally-induced spin polarization. We will comment relations between spin polarization and Berry curvature. The influence of spin-orbit torque induced due to non-equilibrium spin-polarization in magnetic systems on spin dynamics will be also discussed.

[1] A. Dyrdał, et al., arXiv:1711.07707; [2] Ł. Karwacki, et al., arXiv:1711.07702; [3] A. Dyrdał, et al., PRB 95, 245302 (2017).

TT 92.8 Thu 17:15 H 1012

Engineering Chiral and Topological Orbital Magnetism of Domain Walls and Skyrmions — •Fabian R. Lux, Frank Freimuth, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the field of spin-orbitronics, the orbital physics of electrons plays a central role, with the orbital magnetization representing a key concept. While the orbital magnetism in ferromagnets is relatively well understood, very little is known about it for non-collinear structures such as magnetic skyrmions and domain walls. By employing a semiclassical Green's function formalism, we demonstrate how the orbital magnetization in extended chiral magnetic systems can be understood as the electronic response to emergent electromagnetic fields [1]. We discovered that in such systems the spin-orbit interaction can be used to a great advantage in that it promotes a complex interplay of real-space and k-space topology leading to enhanced orbital responses in interfacial chiral magnets. Besides discussing possible applications of the emergent orbital magnetism in chiral spin systems we also suggest new perspectives for the field of chiral orbitronics.

[1] F. R. Lux *et al.*, arXiv:1706.06068 (2017)

TT 92.9 Thu 17:30 H 1012

Current-induced remagnetization in epitaxial Au/Fe/MgO(001) heterostructures — •Pika Gospodaric[1], Ewa Mlynczak[1], Daniel E. Bürgler[1], Lukasz Plucinski[1], Yuriy Mokrousov[2], and Claus M. Schneider[1] — [1]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the emerging field of the spintronics devices the focus shifts towards the three-terminal cell structure. In this geometry, the magnetization of the recording magnetic layer is switched with an in-plane electric current. Presently, the spin-orbit torque is considered as one of the most promising ways of current-induced switching of ferromagnets and antiferromagnets. Here, we study an epitaxial Fe(001) ultra-thin film, with in-plane remanent magnetization, sandwiched between the MgO substrate and an epitaxal Au thin film. This system has well-defined interfaces between the layers and a good crystalline quality, which gives rise to the typical four-fold in-plane magneto-crystalline anisotropy of Fe(001) layers. In a Hall bar geometry we observed reproducible switching of the magnetization of the Fe(001) thin film after applying a current density beyond $2 \cdot 10^7$ A/cm^2. The magnetic state was read-out by measuring the planar Hall voltage in the transversal channel. By varying the current density we were able to induce intermediate magnetization states, which could be explained with changes in the magnetic domain structure. These results give the prospect to apply Fe/Au heterostructures in neuromorphic architectures.

TT 92.10 Thu 17:45 H 1012

Dynamics of interacting Skyrmions in densely populated Skyrmion lattices — •Martin Stier and Michael Thorwart — University of Hamburg, Hamburg, Germany

We address issues which may arise in densely populated Skyrmion lattices which are possibly used in future high-capacity memory devices. A manipulation of the information-carrying Skyrmions is typically achieved by electrical currents - either in terms of spin-transfer or spin-orbit torques. However, Skyrmions themselves distort these torques in their surrounding area. This can actually result in the creation of new Skyrmions under certain conditions. Furthermore, an interaction between Skyrmions in different layers, e.g. in an artificial antiferromagnet, will change the dynamics of the according Skyrmions. This can even have beneficial effects, such as the prevention of the drift due to the Skyrmion Hall effect and an increase of the velocity.

TT 93: Quantum Coherence and Quantum Information Systems (joint session TT/MA)

Time: Thursday 15:00–17:00 Location: H 2053

Invited Talk TT 93.1 Thu 15:00 H 2053

Non-Markovian Quantum Thermodynamics: Second Law and Fluctuation Theorems — •Robert S Whitney — Laboratoire de Physique et Modélisation des Milieux Condensés, Université Grenoble Alpes & CNRS, 25 avenue des Martyrs, BP166 38042 Grenoble, France

The thermodynamics of quantum systems which are strongly coupled to reservoirs is fraught with difficulties, such as non-factorizable initial conditions and non-Markovian system dynamics. However, there is huge practical interest in machines (heat engines, refrigerators, etc) in this strong coupling regime, because weak-coupling implies very small currents, and hence very small power outputs.

This work shows that a real-time diagrammatic technique is an equivalent of stochastic thermodynamics for strongly-coupled non-Markovian quantum machines. Symmetries are found between quantum trajectories and their time-reverses on the Keldysh contour, for any interacting quantum system coupled to ideal reservoirs of electrons, phonons or photons. These lead to quantum fluctuation theorems the same as the well-known classical ones (Jarzynski and Crooks equalities, non-equilibrium partition identity, etc), whether the system's dynamics are Markovian or not. Some of these also hold for non-factorized initial states. We identify a family of approximations, suitable for concrete calculations of a machine's power and efficiency, which respect the symmetries that ensure fluctuation theorems. In all cases, including non-factorized initial states, the second law of thermodynamics is proven to hold on average, with fluctuations violating it.

[1] arXiv:1611.00670

TT 93.2 Thu 15:30 H 2053

Nuclear spin decay in semiconductor quantum dots — •Nina Fröhling[1], Mikhail M. Glazov[2], and Frithjof B. Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund — [2]A. F. Ioffe Physico-Technical Institute, 26 Politechnicheskaya, 194021 St. Petersburg, Russia

We study bath spin auto-correlation functions of nuclear spin decay in an isolated semi-conductor quantum dot doped with an electron or an electron hole as described by the central spin model. The electronic central spin is coupled to a bath of nuclear spins via hyperfine interaction, which dominates the short time regime. We study the analytical solution of the nuclear spin decay with homogeneous hyperfine coupling, as well as other limiting cases. Furthermore, we describe the nuclear spin correlation fully quantum mechanically for up to N = 18 bath spins through time evolution via the Lanczos method and discuss the influence of quadrupolar interaction and nuclear Zeeman splitting on nuclear spin decay.

TT 93.3 Thu 15:45 H 2053

Magnetic field dependency of the electron spin revival amplitude in periodically pulsed quantum dots — •Iris Kleinjohann and Frithjof Anders — Lehrstuhl für Theoretische Physik II, Technische Universität Dortmund, 44227 Dortmund

When pump-probe experiments are performed on singly charged quantum dots, the spin dynamics synchronizes with the periodic pump pulses. In experiments an external magnetic field is applied in Voigt geometry and the synchronization of spin dynamics can be observed in the electron spin polarization along the optical axis. After a pump pulse the electron spin polarization shows a complete dephasing due to the hyperfine interaction. Directly before the impact of the next pump pulse a revival of polarization occurs indicating synchronization. We describe the spin dynamics in a periodically pulsed quantum dot within the central spin model. The time evolution is calculated by a Lindblad approach and shows a revival of electron spin polarization as well as an alignment of nuclear spins. The resonance condition favors an integer or a half-integer number of electron Larmor precession over one pulse interval. The non-monotonic revival amplitude as function of the external magnetic field is related to the nuclear Zeeman term.

TT 93.4 Thu 16:00 H 2053

Semiclassical simulation of weakly coupled semiconductor quantum dots — •Andreas Fischer and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

In two-color pump-probe experiments one can excite distinct subsets of singly charged quantum dots independently by laser pulses of different photon energies. The optically oriented electron spins precess in an external magnetic field applied in Voigt geometry. Phase shifts, changing dephasing times and amplitude modulations in the signal depending on the pump configuration indicate a coherent interaction between the quantum dots. The experimental signatures can be reproduced by comprising two central spin models augmented by a Heisenberg interaction between the two central spins. The time evolution is calculated using a semiclassical approximation (SCA). To include the trion state excited by the pump pulses and the subsequent decay we combine the SCA with the quantum mechanical Lindblad equation. Our approach can be extended to multi-color pump-probe experiments.

TT 93.5 Thu 16:15 H 2053

Mode locking in a periodically pulsed quantum dot — •Natalie Jäschke and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

In pump-probe experiments single electron charged semiconductor quantum dots are subjected to periodic optical excitation generating electron and nuclear spin polarization. In the short time regime the decoherence of the electron spin polarization is governed by the hyperfine interaction with the nuclear spins. We present a theory that combines the effect of the periodic laser pump pulses and the nuclear spin bath on the electron spin polarization.

While we treat the laser pumping quantum-mechanically, a classical simulation of the Overhauser field bridges the time between two laser pulses. We analyze the time dependence of the electron spin dynamics as well as the electron spin noise spectrum. Data for the non-equilibrium steady state spectral distributions of the Overhauser field are presented for the long time limit. Using a steady state Floquet condition the peak locations of the Overhauser field distribution parallel to the external magnetic field can be derived.

TT 93.6 Thu 16:30 H 2053

Holographic Flow Equation Calculation of Entanglement Entropies of Spin Chains — •Hannes Coners and Stefan Kehrein — University of Göttingen

The Holographic Flow Equation Approach was introduced in arxiv/1703.03925 and provides a new method for quantifying entanglement of quantum many-body systems. In this talk the method will be motivated and results for different spin chains (XY, XX and Ising model) are shown. These spin chains consist of two subsystems which are coupled by a weak link (coupling strength g). To benchmark the method, different sizes of the subsystems as well as different values of g are considered.

TT 93.7 Thu 16:45 H 2053

Quantum spin systems at the edge of a quantum memory — •Yevheniia Cheipesh, Lorenzo Cevolani, and Stefan Kehrein

— University of Göttingen

We consider the Kitaev Toric Code with open boundary conditions. This system has a highly degenerate ground state that lives on the boundary and can be described as a one dimensional system. The ground state is derived explicitly and its dimension scales exponentially with the size of the system. Based on this, the entanglement properties of the model are studied for two types of bipartition: the first, where the subsystem A is completely contained in B; and the second, where the boundary of the system is shared between A and B. In the former case the entanglement entropy is the same as for periodic boundary conditions, which means that the bulk is completely decoupled from the boundary on distances larger than the correlation length. In the latter, deviations from the torus configuration appear due to the edge states, and lead to the increase of the entropy. We also derive the dispersion relation of the boundary theory under the perturbation with an external magnetic field along the x-direction.

TT 94: Correlated Electrons: Other Theoretical Topics

Time: Thursday 15:00–18:30 Location: H 3010

TT 94.1 Thu 15:00 H 3010

Charge disproportionation, mixed valence, and Janus effect in multi-orbital systems: A tale of two insulators — •Aldo Isidori, Maja Berovic, Laura Fanfarillo, Michele Fabrizio, and Massimo Capone — International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

We propose an interpretation for the Janus effect in multi-orbital electron systems, suggested by the duality between Jahn-Teller and Hund's metals at commensurate fillings. The effect emerges from the competition between two distinct insulating states, namely a Mott and a charge disproportionation insulator, favored either by the Coulomb interaction or the exchange coupling, respectively, and characterized by a different ionic valence. This competition results in an asymptotic mixed-valence metallic state, at arbitrarily large interaction strength, along the line where the two parent insulators are degenerate. In this state, charge fluctuations arise from the presence of hopping processes that connect the two degenerate insulators. Experimental evidence for the mixed-valence state and the charge disproportionation insulator-to-metal transition can be found in the chromium perovskite system.

TT 94.2 Thu 15:15 H 3010

Lattice coordination vs. space dimension in 2nd order phase transitions: a dynamical vertex approximation study — •Andreas Hausoel[1], Georg Rohringer[2], Thomas Schäfer[3], Giorgio Sangiovanni[1], and Alessandro Toschi[4] — [1]University of Wuerzburg, Germany — [2]Russian Quantum Center, Moscow, Russia — [3]École Polytechnique and Collège de France, Paris, France — [4]Technical University of Vienna, Austria

The dynamical vertex approximation (DΓA) includes spatial correlations of all length scales beyond the dynamical mean-field theory (DMFT) description. The most relevant changes due to nonlocal fluctuations are a deviation from the mean-field critical behaviour and a sizeable reduction of magnetic ordering temperatures [1].

Here we extend the analysis to different lattice types; in particular, we compare DΓA calculations for the simple, the body-centered and face-centered cubic lattices to the corresponding DMFT ones.

On general grounds, one expects a overall reduction of the differences w.r.t. DMFT, the larger the coordination number of the lattice considered is. Our analysis will clarify the underlying aspects of this trend, investigating the difference between (i) an increase of the coordination number by changing the lattice type (i.e. keeping space dimension fixed), and (ii) an increase of coordination number by keeping the lattice type fixed and increasing the space dimension.

[1] G. Rohringer, A. Toschi, A. Katanin, K. Held, PRL **107**, 256402.

TT 94.3 Thu 15:30 H 3010

Breakdown of Traditional Many-Body Theories for Correlated Electrons — •Thomas Schäfer[1,2,3], Olle Gunnarsson[4], Georg Rohringer[5], Giorgio Sangiovanni[6], and Alessandro Toschi[1] — [1]TU Wien, Austria — [2]Collège de France, Paris, France — [3]CPHT École Polytechnique, Palaiseau, France — [4]MPI Stuttgart, Germany — [5]Russian Quantum Center, Moscow, Russia — [6]Uni Würzburg, Germany

Starting from the (Hubbard) model of an atom, we demonstrate that the uniqueness of the mapping from the interacting to the noninteracting Green function, $G \to G_0$, is strongly violated, by providing numerous explicit examples of different G_0 leading to the same physical G. We argue that there are indeed infinitely many such G_0, with numerous crossings with the physical solution. We show that this rich functional structure is directly related to the divergence of certain classes of (irreducible vertex) diagrams, with important consequences for traditional many-body physics based on diagrammatic expansions. Physically, we ascribe the onset of these highly nonperturbative manifestations to the progressive suppression of the charge susceptibility induced by the formation of local magnetic moments and/or resonating valence bond (RVB) states in strongly correlated electron systems.

TT 94.4 Thu 15:45 H 3010

Divergences of the irreducible vertex functions in correlated metallic systems: Insights from the Anderson Impurity Model — •Patrick Chalupa[1], Patrik Gunacker[1], Thomas Schäfer[1,2,3], Karsten Held[1], and Alessandro Toschi[1] — [1]Institute of Solid State Physics, Technische Universität Wien, 1040 Vienna, Austria — [2]Collége de France, 75005 Paris, France — [3]Centre de Physique Théorique, École Polytechnique, 91128 Palaiseau, France

We analyze in detail the occurrence of divergences in the irreducible vertex functions of the Anderson impurity model (AIM). These divergences — a surprising hallmark of the breakdown of many-electron perturbation theory — have been recently observed in several contexts, including the dynamical mean-field solution of the Hubbard model. Hitherto, however, a clarification of their origin could be obtained only in the limit of high temperatures and large interactions, where the underlying physics is greatly simplified by the absence of low-energy quasiparticle excitations. In this respect, our numerical calculations for the AIM, as well as their comparison with the corresponding results for the Hubbard model, allow us to clarify several open questions about the origin and the properties of vertex divergences occurring in a more interesting context, the correlated metallic regime at low- temperatures. In particular, our analysis (i) rules out a direct correspondence between the vertex divergences and the presence of a Mott metal-insulator transition, (ii) clarifies their relation with the underlying Kondo physics, and, eventually, (iii) individuates which divergences might also appear on the real frequency axis in the limit of zero temperature.

TT 94.5 Thu 16:00 H 3010

Signatures of non-Abelian anyons in the thermodynamics of a perturbed $\mathbf{SU(3)_{N_f}}$ WZNW model — •Daniel Borcherding and Holger Frahm — Institute for Theoretical Physics, Leibniz University Hannover

The contribution of anyonic degrees of freedom emerging in the non-Abelian spin sector of a one-dimensional system of interacting fermions carrying both $SU(3)$ and $SU(N_f)$ degrees of freedom to the thermodynamic properties of the latter is studied based on the exact solution of the model. For sufficiently small temperatures and fields the anyons appear as zero energy modes localized at the massive kink excitations. From their quantum dimension they are identified as $SU(3)_{N_f}$ anyons. The density of kinks (and anyons) can be controlled by external fields leading to the formation of collective states of these anyons described by various conformal embeddings of the $SU(3)_{N_f}$ WZNW model for large fields. Based on the numerical analysis of the thermodynamic Bethe ansatz equations we propose a phase diagram for the anyonic modes.

15 min. break.

Invited Talk TT 94.6 Thu 16:30 H 3010

Discrete Time Crystals — •Roderich Moessner — MPI-PKS, Dresden, Germany

Periodically driven ("Floquet") systems provide perhaps the simplest setting for studying quantum systems out of equilibrium. Their properties have turned out to be remarkably rich. In particular, the inter-

play of disorder and driving has given rise to an entirely new form of spatio-temporal ordering which has been given the name discrete time crystal.

This talk presents an introduction to the physics of Floquet systems and explains how non-equilibrium phases and their concomitant ordering arise.

This work was done in collaboration with Achilleas Lazarides, Arnab Das, Vedika Khemani, and Shivaji Sondhi. For an introductory review, see Nature Physics 13, 424-428 (2017).

TT 94.7 Thu 17:00 H 3010

Excitations of the square lattice Heisenberg model using tensor-network methods — •Ruben Verresen[1,2], Frank Pollmann[1], and Roderich Moessner[2] — [1]Technical University of Munich — [2]Max-Planck-Institute for the Physics of Complex Systems

The square lattice Heisenberg model is a paradigmatic example of spontaneous symmetry breaking. Despite the apparent simplicity of the model, spin wave theory fails to describe its excitations at certain momenta. Opposing descriptions —strongly-interacting magnons and emergent spinons— have been proposed. We use a time-dependent density matrix renormalization group (DMRG) method to obtain the dynamical structure factor. In particular, we investigate its features by continuously tracking the spectral function as a function of a tuning parameter around a simple soluble limit. This leads us to a simple picture which already at low order in perturbation theory accounts for the features beyond SWT in a semi-quantitative way.

TT 94.8 Thu 17:15 H 3010

Heisenberg-like model for correlated electrons and quantum spin fluctuations near magnetic instabilities — •Evgeny Stepanov — Radboud University, Institute for Molecules and Materials, 6525AJ Nijmegen, The Netherlands

Theory of magnetism and magnetic interactions is the one of the most attractive areas of physics nowadays. Nevertheless, a quantum nature of the exchange interaction that occurs between spins is not clear yet. Up to now, studies of magnetic interactions have been mostly limited to a classical description, which makes their generalization on the case of strongly correlated systems rather difficult.

Here we consider an extended Hubbard model for correlated electrons and derive a corresponding Heisenberg-like problem. Our approach is based on the Dual Boson theory, which allows to introduce quantum collective variables associated to bosonic excitations and separate charge and spin degrees of freedom. The obtained result for the exchange interaction accounts for important quantum fluctuations and improves Anderson's idea of the superexchange, which makes possible description of collective excitations in the most interesting physical regimes. Thus, the study of quantum spin fluctuations in paramagnetic (PM) phase near the PM to AFM phase transition allows to detect the antiferromagnetic "soft" mode and manifest the tendency of the system to the spin ordering before the actual transition to the ordered state happens. Importantly, the derived exchange interaction is expressed in terms of single-particle quantities, which can be efficiently used in realistic calculations of multiband systems.

TT 94.9 Thu 17:30 H 3010

Single-particle properties of the 2D Hubbard model within a four-pole approximation — •Andrea Di Ciolo and Adolfo Avella — Dipartimento di Fisica "E. R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy

We present a solution of the 2D Hubbard model in the framework of the Composite Operator Method (COM) [1-3] within a four-pole approximation (4p). First, we characterize the 2-site exact solution and identify the crucial role played by spin fluctuations. Then, we adopt a basis of fields given by the two Hubbard operators plus two fields describing the electronic transitions dressed by the nearest-neighbor spin fluctuations. As well as this approximate solution is in remarkable agreement with the 2-site exact one, the corresponding 2D solution performs very well once compared to advanced (semi-)numerical methods, being by far less computational-resource demanding. Moreover, this solution, featuring a well-developed momentum selectivity of the spectral properties, opens up the possibility to directly address the underdoped-cuprate puzzle. Therefore, we adopt this 4p approximation to study the single-particle properties of the 2D model in the strong coupling regime (intermediate-large interaction and small-intermediate doping), where the effects of spin-fluctuations, accurately treated in our approach, are more relevant and induce anomalous features in all analyzed properties.

[1] F. Mancini, and A. Avella, *Adv. Phys.* **53**, 537 (2004).
[2] A. Avella, *Eur. Phys. J. B*, **87**, 45 (2014).
[3] A. Avella, *Adv. Cond. Matt. Phys.* **2014**, 515698 (2014).

TT 94.10 Thu 17:45 H 3010

Sharp entanglement thresholds in the logarithmic negativity of disjoint blocks — •Younes Javanmard[1], Daniele Trapin[1], Soumya Bera[1,2], Jens. H Bardarson[1,3], and Markus Heyl[1] — [1]MPIpks, Dresden, Germany — [2]Indian Institute of Technology Bombay, Mumbai, India — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Entanglement has developed into an essential concept for the characterization of quantum many-body phases and phase transition in the ground state. However, the conventional approach using the entanglement entropy faces a challenge for thermal states where it loses its status as an entanglement measure. In this work, we study the entanglement properties of the transverse-field Ising chain using the logarithm negativity, which remains a valid entanglement measure also for mixed states. Specifically, we investigate the logarithm negativity for two disjoint blocks as a function of their separation. In this way, we obtain information on the spatial structure of entanglement. In particular, we find a sharp entanglement threshold as a function of the distance of the two blocks beyond which the logarithm negativity exactly vanishes, indicating that beyond this critical distance the two blocks become unentangled as measured by the logarithm negativity. We explore this feature as a function of temperature and size of the two blocks and thereby map out the spatial structure of entanglement in the transverse-field Ising chain.

TT 94.11 Thu 18:00 H 3010

Error estimates for extrapolations with matrix-product states — •Claudius Hubig[1,2], Jutho Haegeman[3], and Ulrich Schollwöck[1] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Department of Physics and Astronomy, Ghent University, Ghent, Belgium

We introduce a new error measure for matrix-product states (MPS) based on an approximation of the full variance $\langle\psi|(\hat{H}-E)^2|\psi\rangle$. When applied to a series of MPS at different bond dimensions obtained from a single-site density matrix renormalization group (1DMRG) calculation, it allows for the extrapolation of observables towards the zero-error case representing the exact ground state of the system.

The calculation of the error measure is split into a sequential part of cost equivalent to two calculations of $\langle\psi|\hat{H}|\psi\rangle$ and a trivially parallelized part scaling like a single operator application in two-site DMRG (2DMRG). The reliability of the new error measure is demonstrated at four examples and extrapolation in the new error measure is shown to be on-par with extrapolation in the 2DMRG truncation error or the full variance $\langle\psi|(\hat{H}-E)^2|\psi\rangle$ at a fraction of the computational effort.
[1] arxiv.org/abs/1711.01104

TT 94.12 Thu 18:15 H 3010

Conditions where RPA becomes exact in the high-density limit — •Klaus Morawetz[1,2,3], Vinod Ashokan[4], Renu Bala[5], and Kare Narain Pathak[4] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum if the relation between Fermi energy and Fermi momentum is $\epsilon_{\rm f} \sim p_{\rm f}^{\beta}$ and the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d<\beta+\alpha$ specifies systems where RPA is exact in the high-density limit. The one-dimensional structure factor is found to be the interaction-free one in the high-density limit. A cancellation of RPA and vertex corrections render this result alternatively valid up to second-order contact interaction. For finite-range potentials of cylindrical wires a large-scale cancellation appears and found to be independent of the width parameter. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.

TT 95: Cold Atomic Gases, Superfluids, Quantum Fluids and Solids

Time: Thursday 15:00–17:45 Location: HFT-FT 131

TT 95.1 Thu 15:00 HFT-FT 131

Vortex states in one- and two-band rotating Fermi gases in the BCS-BEC crossover — •Serghei Klimin[1], Jacques Tempere[1], and Milorad Milosevic[2] — [1]TQC, Universiteit Antwerpen, Antwerpen, Belgium — [2]Departement Fysica, Universiteit Antwerpen, Antwerpen, Belgium

Atomic Fermi superfluids can be described in terms of an effective field theory [1] for a macroscopic wave function representing the field of condensed pairs, analogous to the Ginzburg-Landau theory for superconductors. Rotation can stabilize vortices in atomic gases similarly to the magnetic field in superconductors, leading to the appearance of an effective vector potential. On the basis of the effective field theory, equilibrium vortex state diagrams are derived. They are in good agreement with available results of the Bogoliubov - de Gennes theory and with experimental data. We report also the equilibrium vortex phase diagram of a rotating two-band Fermi gas. This study is particularly focused on novel features due to interband interactions which can be experimentally resolved. We reveal the non-monotonic resonant dependence of the free energy for a two-band superfluid as a function of temperature, which is directly manifested in vortex phase diagrams, where areas of stability for both integer and fractional vortex states are found. The present investigation embraces the BCS-BEC crossover regime and the entire temperature range below the critical temperature.

[1] S. N. Klimin, J. Tempere, G. Lombardi, J. T. Devreese, EPJ B **88**, 122 (2015)

TT 95.2 Thu 15:15 HFT-FT 131

Bose-Einstein condensation of a non-ideal Bose gas of atoms with large spin — •Andrei Pavlov[1], Vladimir Babichenko[2], and Ilya Polishchuk[2,3] — [1]IFW Dresden, Dresden, Germany — [2]Kurchatov Institute, Moscow, Russia — [3]MIPT, Dolgoprudnii, Russia

A non-ideal diluted quantum Bose gas of atoms with spin-spin interaction of dipole type is described in the spin coherent states representation. Large values of spin can be treated quasi-classically up to exponentially small corrections, that allows to derive effective interaction between particles of the gas. A preferable ground state configuration of the system is determined by this effective interaction, the spin-spin coupling constant regulates whether the system takes ferromagnetic or antiferromagnetic ground state. The coupling constants of long-ranged spin-spin interaction and short-ranged scattering also define a condition when the system collapses, causing formation of molecules.

TT 95.3 Thu 15:30 HFT-FT 131

Dynamics and decay of dark solitons in superfluid Fermi gases — •Wout Van Alphen[1], Giovanni Lombardi[1], Serghei Klimin[1,2], and Jacques Tempere[1,3] — [1]Universiteit Antwerpen, B-2610 Antwerpen, Belgium — [2]State University of Moldova, 2009 Chisinau, Moldova — [3]Harvard University, Cambridge, MA 02138, USA

Dark solitons are localized solitary density dips that retain their shape while propagating at a constant velocity. In recent work, we have studied their properties and dynamics in superfluid Fermi gases by means of a recently developed effective field theory that is capable of describing fermionic superfluids across the BEC-BCS crossover regime in a wide temperature domain.

In superfluid gases, dark solitons are subject to an instability mechanism called the snake instability, which makes the soliton decay into vortices if the radial width of the atom cloud is too large. We have estimated the maximal radial size that the atomic cloud can have in order to preserve the soliton stability. An analysis of the effect of population imbalance on this critical size reveals a stabilization of the soliton with increasing imbalance.

We have also simulated the evolution of two counter-propagating solitons to investigate the properties of dark soliton collisions in different conditions of temperature and imbalance. The collisions are demonstrated to introduce a spatial shift into the soliton trajectories and become increasingly more inelastic when moving towards the unitarity regime of the interaction domain.

TT 95.4 Thu 15:45 HFT-FT 131

Manipulating the Mott lobes: optical lattice bosons coupled to atomic quantum dots — •Anna Posazhennikova[1] and Florian M. Dobler[2] — [1]Royal Holloway University of London, Egham, UK — [2]Universitaet Konstanz, Konstanz, Germany

We analyse quantum phase transitions in a system of optical lattice bosons coupled to an array of atomic quantum dots. The difference to Bose-Hubbard model is in that direct tunnelling between the lattice sites is prohibited and instead there is an assisted tunnelling via the quantum dots. We calculate the phase diagram of the combined system within the Gutzwiller-Ansatz. It turns out that the superfluid-Mott transition is still present in the system, however, the Mott lobes strongly depend on the system parameters. One can, for example, even reverse the usual hierarchy of the lobes with the first lobe becoming the smallest. We discuss the physics of the combined system in detail and overview possible applications of the model.

TT 95.5 Thu 16:00 HFT-FT 131

Noise correlations in the attractive Hubbard model — •Stephan Humeniuk — Institute for Theoretical Physics III, University of Stuttgart

In cold atom experiments, noise correlations, which can be obtained through the analysis of time of flight images, are an important probe of the quantum state inside the trap. Determinantal quantum Monte Carlo simulations of noise correlations are presented at low and experimentally relevant, high temperatures for the attractive Hubbard model, which was recently realized in optical lattices. At half filling, the Hubbard model possesses an enlarged symmetry which leads to the degeneracy of a charge density wave and superconductivity in the ground state, and both orders show characteristic peaks in the noise correlation signal. The presence of Cooper pairs with non-zero centre of mass momentum for large Hubbard attraction (in the BEC regime of strongly bound molecules) and the detectability of η-pairing are discussed.

TT 95.6 Thu 16:15 HFT-FT 131

Dynamics of the density of quantized vortices in counterflow turbulence — Emil Varga and •Ladislav Skrbek — Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Thermal counterflow of superfluid 4He represents the most extensively studied form of quantum turbulence, initiated by pioneering experiments of Vinen, who also introduced a phenomenological model for its description based on the concept of a random tangle of quantized vortices of vortex line density L. Recently the interest in thermal counterflow has been renewed and resulted in an intense theoretical debate about what form, if any, of the so-called Vinen equation accurately captures the dynamics of L. We address this problem experimentally, in a square channel equipped by three pairs of second sound sensors. Based on large statistics of experimental data in square-wave modulated thermally induced counterflow we investigate the phase portrait of general form of the governing dynamical Vinen-like equation and conclude that for sparse tangles all proposed forms of this equation provide equally adequate description of the growth of L while for dense tangles neither of them is satisfactory and cannot account for the significant slow-down in tangle growth rate as the steady state is approached. We claim, however, that agreement with theory is recovered if geometric parameter c2 introduced in numerical studies by Schwarz is allowed to vary with vortex line density which also greatly improves the prediction of the observed decay rate.

The support of the Czech Science Foundation under project GA17-03572S is acknowledged.

15 min. break.

TT 95.7 Thu 16:45 HFT-FT 131

Anisotropic superfluidity of two-dimensional excitons in a periodic potential — •Pavel A. Volkov[1], Igor L. Kurbakov[2], and Yurii E. Lozovik[2,3] — [1]Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Institute of Spectroscopy RAS, Moscow, Troitsk, Russia — [3]MIEM, National Research University Higher School of Economics, Moscow, Russia

Electrostatic potentials created with nanofabricated electrodes provide

a versatile tool to control and probe excitonic systems. As a particular case, we consider the emergence of anisotropy of superfluid properties in a two-dimensional system of dipolar excitons subject to an external periodic potential. We study anisotropies of helicity modulus, excitation spectrum, sound velocity and angle-resolved luminescence spectrum. We discuss possible experiments that could detect these effects and provide estimates of their magnitude for GaAs/AlGaAs heterostructures as well as MoS_2/hBN/MoS_2 and $MoSe_2$/hBN/WSe_2 transition metal dichalcogenide bilayers.

TT 95.8 Thu 17:00 HFT-FT 131

Non-local transport properties of an excitonic insulator — •Bogusz Bujnowski[1], Jerome Cayssol[2], and Dario Bercioux[1,3] — [1]Donostia International Physics Center (DIPC), Manuel de Lardizbal 4, E-20018 San Sebastian, Spain — [2]LOMA (UMR-5798), CNRS and University Bordeaux, F-33045 Talence, France — [3]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Basque Country, Spain

The availability of high-quality mono- and bilayer- graphene samples has motivated Coulomb drag experiments in electron/hole bilayer systems made of these materials. Such electron/hole bilayer systems have a rich and still not fully understood transport behavior and are also potential candidates to host indirect excitonic condensates. We study the ballistic transport properties within a Coulomb drag measurement set-up, assuming a coupling between sheets due to the formation of an excitonic condensate. This coupling allows a charge transfer between the sheets, which we investigate for various sheet types as a function of the distance between the contact compared to the typical coherence length of the excitonic condensate.

TT 95.9 Thu 17:15 HFT-FT 131

Out-of-bounds hydrodynamics in anisotropic Dirac fluids — Julia M. Link[1], Boris N. Narozhny[1,2], •Egor I. Kiselev[1], and Jörg Schmalian[1,3] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), Moscow, Russia — [3]Insitute for Solid State Physics, Karlsruhe Institute of Thechnology (KIT), Karlsruhe, Germany

We study the hydrodynamic transport in an interacting electronic system with an anisotropic dispersion, which is Dirac-like along one crystallographic direction and Newtonian-like along the other. Such a dispersion is realized in systems with merging Dirac points at charge neutrality and leads to highly anisotropic transport coefficients. The shear viscosity is a fourth-rank tensor whose distinct elements characterize the momentum flow in different directions and exhibit fundamentally different scalings with temperature. One of the viscosity coefficients violates the lower bound for the shear viscosity to entropy density ratio stemming from the AdS/CFT duality.

TT 95.10 Thu 17:30 HFT-FT 131

AC conductivity of a two-dimensional electronic fluid — Roderich Moessner, Piotr Surowka, and •Piotr Witkowski — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

Motivated by experiments on a hydrodynamic regime in electron transport, we study the effect of an oscillating electric field in such a setting. We consider a long two-dimensional channel of, whose geometrical simplicity allows an analytical study as well as hopefully permitting experimental realisation. We find two, distinctive regimes: a quasi-static flow, and a boundary layer type behaviour. The latter includes a splitting of the location of maximal flow velocity from the centre towards the edges of the boundary layer, an an increasingly reactive nature of the response, with the phase shift of the response varying across the channel. In which regime we are, depends on dimensionless combination of channel width, viscosity and forcing frequency, similar to the Reynolds number. The scaling of the total optical conductance with channel width differs between the two regimes, while its frequency dependence resembles a Drude form throughout, even in the complete absence of ohmic heating, against which, at the same time, our results are stable. Current estimates for transport coefficients in graphene and delafossites suggest that the boundary layer regime should be experimentally accessible.

TT 96: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France Paul R. Kent, Oak Ridge National Laboratory, USA Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Thursday 15:00–17:45 Location: HL 001

Invited Talk TT 96.1 Thu 15:00 HL 001

Recent developments in FCIQMC: real-time propagation and improved convergence with walker number — •Ali Alavi — Max Planck Institute for Solid State Research, Stuttgart, Germany

The Full Configuration Interaction QMC method samples Slater determinants using an imaginary-time propagation of walkers, and can yield essentially exact ground- and excited states energies and wavefunctions for Fermionic systems. Recently we have extended this methodology to real-time propagation, enabling the calculation of spectral functions along the real-frequency axis. This method will be described in the talk, together with representative examples from molecular and lattice models. We will also describe a second development in the FCIQMC methodology which substantially improves the rate of convergence of the ground-state technique with respect to the number of walkers. With the new method, we can compute essentially the exact ground state energy of the benzene molecule, correlating 30 electrons (the entire valence) in the full set of 108 orbitals of a VDZ basis. Perspectives of the new methods will be discussed.

TT 96.2 Thu 15:30 HL 001

Quasi-Continuous LDA+DMFT calculations for SrVO3. — •Evan Sheridan, Christopher Rhodes, Evgeny Plekhanov, and Cedric Weber — King's College London, Theory and Simulation of Condensed Matter (TSCM), The Strand, London, United Kingdom.

The Dynamical Mean Field Theory (DMFT) is an extremely powerful tool in the treatment of strongly correlated electron systems and many DMFT calculations suffer from a computational bottleneck when it attempts to solve the Anderson Impurity Model (AIM).

Common among the early Anderson Impurity solvers was the Auxiliary Field Quantum Monte Carlo (AF-QMC) approach which relies on a discretisation of the imaginary time grid. AF-QMC solvers suffer from the notorious Suzuki-Trotter error,as a result of this , that has largely been ignored in recent years with the advent of Continuous Time-QMC (CT-QMC) solvers.

Here, we present a systematic study of how this issue can be overcome for realistic material properties using LDA+DMFT. We find that our quasi-continuous time method compares well to the state-of-the-art CT-QMC calculations for SrVO3, with the added advantage of linear scaling in temperature. The theoretical framework proposed is quite general and can be extended to cluster DMFT calculations.

TT 96.3 Thu 15:45 HL 001

High temperature superconducting oxychlorides: a light element model for cuprates — •Matteo d'Astuto[1,2], Blair Lebert[2,3], Ikuya Yamada[4], and Masaki Azuma[5] — [1]Institut NEEL CNRS/UGA UPR2940 25 rue des Martyrs BP 166 38042 Grenoble cedex 9 FRANCE — [2]IMPMC, UMR7590 UPMC-Sorbonne Universités - CNRS, Paris, France — [3]Synchrotron SOLEIL, Gif-sur-Yvette, France — [4]Nanoscience and Nanotechnology Research Center (N2RC), Osaka, Japan — [5]Materials and Structures Laboratory, TITech, Yokohama, Japan

The copper oxychloride cuprate $Ca_2CuO_2Cl_2$ (CCOC) system, with vacancy or Na doping on the Ca site, is unique among the high temperature superconducting cuprates (HTSCs) since it: lacks high Z

atoms; has a simple I4/mmm 1-layer structure, typical of 214 (LSCO) cuprates, but which is stable at all doping and temperatures; and has a strong 2D character due to the replacement of apical oxygen with chlorine. It also shows a remarkable phase digram, with a superconducting T_C growing to the optimal doping without any minimum around 1/8 doping, despite the observation of charge modulations by near-field spectro-microscopy. Due to the reduced number of electrons, advanced calculations that incorporate correlation effects, such as quantum Monte Carlo are easier, but relatively little is known about CCOC (for a cuprate) from an experimental point of view. We are now filling this gap by a comprehensive experimental study covering the whole phase diagram, in particular of the (para)magnon and phonon dispersion..

TT 96.4 Thu 16:00 HL 001

Antiferromagnetic correlations in the metallic strongly correlated transition metal oxide $LaNiO_3$ — •Hanjie Guo[1], Zhiwei Li[1], Li Zhao[1], Zhiwei Hu[1], Chunfu Chang[1], Changyang Kuo[1], Wolfgang Schmidt[2], Andrea Piovano[2], Tunwen Pi[3], Oleg Sobolev[4], Daniel Khomskii[1], Liu Hao Tjeng[1], and Alexander Komarek[1] — [1]MPI CPfS, Dresden, Germany — [2]ILL, Grenoble, France — [3]NSRRC, Taiwan — [4]FRMII, Munich, Germany

The material class of rare earth nickelates with high Ni^{3+} oxidation state is generating continued interest due to the occurrence of a metal-insulator transition with charge order and the appearance of non-collinear magnetic phases within this insulating regime. The recent theoretical prediction for superconductivity in $LaNiO_3$ thin films has also triggered intensive research efforts. $LaNiO_3$ seems to be the only rare earth nickelate that stays metallic and paramagnetic down to lowest temperatures. So far, centimetre-sized impurity-free single crystal growth has not been reported for the rare earth nickelates material class since elevated oxygen pressures are required for their synthesis. Here, we report on the successful growth of centimetre-sized $LaNiO_3$ single crystals by the floating zone technique at oxygen pressures of up to 150 bar. Our crystals are essentially free from Ni^{2+} impurities and exhibit metallic properties together with an unexpected but clear antiferromagnetic transition.

TT 96.5 Thu 16:15 HL 001

First-principles quantum Monte Carlo study of correlated materials — •Huihuo Zheng — Argonne Leadership Computing Facility, Argonne National Laboratory, Lemont, USA

Strongly correlated electronic systems have become an important subject of condensed matter physics, because of many fascinating phenomena arising in these systems such as metal-insulator transition, high temperature superconductivity, etc. Accurate characterization of the electron-electron correlations in these systems from first principles is essential for us to understand how these phenomena emerge from microscopic interactions. I will present our efforts in modeling correlated materials using the first-principles quantum Monte Carlo (QMC) method by showing two representative *ab intio* studies (vanadium dioxide and graphene) and a density-matrix downfolding theory for constructing low energy effective models from *ab initio* simulations. Using QMC, we correctly characterized the electronic structure of vanadium dioxide and unveiled the electronic origin of the metal-insulator transition which has been a mystery for decades. For graphene, we computed the electron screening from σ bonding electrons and illustrated how the emergent physics from underlying Coulomb interactions results in the observed weakly correlated semimetal. On the other hand, the downfolding approach we developed provides a way to quantitatively identify important microscopic interactions relevant to the macroscopic physics.

TT 96.6 Thu 16:30 HL 001

Reduced Density Matrix Theory for Coupled Fermion-Boson Systems — •Florian Buchholz[1], Iris Theophilou[1], Michael Ruggenthaler[1], Heiko Appel[1], and Angel Rubio[1,2,3] — [1]MPSD, Hamburg, Germany — [2]CCQ, The Flatiron Institute, New York, United Sates — [3]Nano-bio Spectroscopy Group, San Sebastián, Spain

Reduced density matrix (RDM) theory proved to be successful in describing a wide range of many-body problems that are not easily accessible by the more common many-body perturbation theories or density functional theory. Especially as RDM theories are non-perturbative, they are advantageous in strong coupling scenarios.

However, RDM theory was to our knowledge never applied to systems with more than one active particle type. The focus of this talk is to analyze the possibilities and problems of an extension to coupled fermion-boson theories. Comparing a typical bilinear interaction term of the form $c_i^+ c_j (a_k^+ + a_k)$, where c^+/c and a^+/a indicate fermion and boson creation/annihilation operators, respectively and the fermionic 2-body interaction term $c_i^+ c_j^+ c_k c_l$, the former should have a considerably reduced definition space, which we hope to be exploitable. On the other hand, the bilinear interaction has a very different structure than the 2-body interaction and it is not clear at all, how to define a RDM that carries all information to compute experimental observables of a coupled fermion-boson system.

Specifically, I will illustrate some of the peculiarities of the fermion-boson interaction for simple model systems and present some ideas to deal with those.

TT 96.7 Thu 16:45 HL 001

Critical temperatures as function of magnetic anisotropy in two-dimensional systems from first-principles calculations — •Daniele Torelli — Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark

Recent observation of ferromagnetic out-of-plane order in monolayer CrI_3 highlights the importance of a microscopic understanding of anisotropy in ground state magnetic systems. Single-ion anisotropy accounts mainly for spin-orbit coupling interaction and, in particular for two-dimensional (2D) materials, it's crucial to escape the Mermin-Wagner theorem. Here we investigate the variation of critical temperatures as functions of anisotropy in Heisenberg model systems using Metropolis Monte Carlo simulations. Results for square, hexagonal and honeycomb lattices are compared with equivalent simulations in the Ising model, which is confirmed to represent the limit with infinite anisotropy. Based on a new developed computational 2D materials database, we predict a vast number of 2D structures with high critical temperatures. As testing system, relevant Heisenberg exchange couplings and magnetic anisotropy energy in CrI_3 monolayer are extracted from first principle calculations and energy mapping analysis, yielding to an estimation of Curie temperature in good agreement with experimental results.

TT 96.8 Thu 17:00 HL 001

Oxygen vacancy-induced absorption of visible light in SrNbO3 — •Marcello Turtulici, Steffen Backes, and Silke Biermann — Centre de Physique Théorique, Ecole Polytechnique, 91128 Palaiseau, France

SrNbO3 has recently attracted attention as a bright red photocatalyst. Several, mutually contradicting, models have been proposed in the literature in order to explain the strong absorption in the visible spectrum, and no consensus even on the basic nature of the mechanism has been reached. In this work we investigate the optical properties of this material by means of state-of-the-art Density Functional Theory and many-body perturbation theory techniques. We evidence a high sensitivity of the optical properties on deviations from the ideal crystal structure. In particular, the optical properties should strongly depend on the presence of oxygen vacancies, which give rise to additional absorption channels in the visible frequency range. Most notably, the experimentally observed red color is likely due to transitions between orbitals of dominant Nb-eg character, which are enhanced by the strong hybridization of the quite extended 4d-states of Nb with oxygen p-states.

TT 96.9 Thu 17:15 HL 001

Transient charge and energy flow in the wide-band limit — Fabio Covito, •Florian Eich, Riku Tuovinen, Michael Sentef, and Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Thanks to recent advances in ultra-fast pump-probe spectroscopies and nano-thermometry it is possible to study charge and energy flow at atomic time and length scales. In order to analyze the transient dynamics of nanoscale devices theoretically, the wide-band limit is a commonly used approximation. Here we investigate the applicability of the wide-band limit to the study of charge and heat transport through nanojunctions exposed to voltage biases and temperature gradients. We find that while this approximation faithfully describes the long-time steady-state charge and heat transport, it fails to characterize the short-time transient behavior of the junction. In particular, we find that the charge current flowing through the device shows a discontinuity when a temperature gradient is applied, while the energy flow is discontinuous when a voltage bias drives the dynamics and even diverges when the junction is exposed to both a temperature gradient

and a voltage bias. We discuss this pathological behavior and propose two possible solutions.

TT 96.10 Thu 17:30 HL 001

From DFT to Coupled Cluster Theory - Understanding Oxygen Activation on Coin Metal Nanoparticles — •Wilke Dononelli and Thorsten Klüner — Institut für Chemie, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

In this study we focus on one of the most fundamental catalytic model reactions, the oxidation of CO on a metal catalyst. We studied the activation of molecular oxygen via dissociation or direct reaction of CO and O_2 within density functional theory (DFT) and high level CCSD(T) calculations. Therefore we use Au_{13} and Au_{55} nanoparticles (NPs) and a periodic Au(321) surface as model systems and compare the catalytic activity of the gold substrates to Ag and Cu based, as well as bimetallic NP catalysts. Part of the DFT calculations were performed, using the well-established PBE functional as implemented in the Vienna ab initio simulation package (VASP). Hybrid and double hybrid DFT calculations on the NPs were performed in Gaussian09. CCSD(T) calculation were performed in Gaussian09 using conventional CCSD(T) for the M_{13} (M=Au,Ag,Cu) NPs and CCSD(T)/PBE in a QM/QM embedding scheme using the ONIOM approach for M_{55} NPs. For systems of 55 metal atoms PBE gives the same results as double hybrids or even CCSD(T). For smaller M_{13} NPs interaction energies differ between PBE and higher levels of theory, which might be explained by the molecule like character of these NPs.

TT 97: Spintronics (joint session HL/TT)

Time: Thursday 15:00–17:30 Location: EW 201

TT 97.1 Thu 15:00 EW 201

Anisotropic Spin Diffusion and Spin Helix Dynamics in a CdTe Quantum Well — •Felix Passmann[1], Sergiu Anghel[1], Alexander Valerievich Poshakinskiy[2], Sergey Anatolyevich Tarasenko[2], Alan Douglas Bristow[3], and Markus Betz[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, Otto-Hahn-Straße 4a, D-44227 Dortmund, Germany — [2]Ioffe Institute, St. Petersburg 194021, Russia — [3]Department of Physics and Astronomy, West Virginia University, Morgantown, WV 26506-6315, USA

In the recent past various experiments conducted on zinc-blende type III-V semiconductor quantum wells like GaAs have revealed the dynamics of persistent electron spin helices. However, similar investigations in a doped CdTe single quantum well remained unexplored. Here, we employ ultrafast two-color Kerr rotation spectroscopy to study the spatio-temporal evolution of a photo-excited spin distribution into a long living spin helix (SH). The evolution is governed by the spin-orbit interaction related to bulk and structural inversion asymmetries which manifests as an effective magnetic field. We directly extract the Dresselhaus and Rashba contributions via the coherent spin precession of the diffusing electrons. Further investigations of the SH evolution in the presence of in-plane magnetic fields reveal a so far unseen and theoretically unexpected behavior that we attribute to spatial and temporal gradients of the electron density. The experiments are well supported by corresponding theoretical simulations.

TT 97.2 Thu 15:15 EW 201

Magnetoconductance correction in zinc-blende semiconductor nanowires with spin-orbit coupling — •Michael Kammermeier[1], Paul Wenk[1], John Schliemann[1], Sebastian Heedt[2], Thomas Gerster[2], and Thomas Schäpers[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Peter Grünberg Institute (PGI-9) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

We study the effects of spin-orbit coupling on the magnetoconductivity in diffusive cylindrical semiconductor nanowires [1]. Following up on our former study on tubular semiconductor nanowires [2], we focus now on nanowire systems where no surface accumulation layer is formed but instead the electron wave function extends over the entire cross-section.The derived model is fitted to the data of magnetoconductance measurements of a heavily-doped back-gated InAs nanowire [3] and transport parameters are extracted. At last, we compare our results to previous theoretical and experimental studies and discuss the occurring discrepancies.

* * *

[1] M. Kammermeier *et al.*, arXiv:1709.02621 (2017).
[2] M. Kammermeier *et al.*, PRB **93**, 205306 (2016).
[3] S. Heedt *et al.*, Nanoscale **7**, 18188 (2015).

TT 97.3 Thu 15:30 EW 201

Measuring Anisotropic Spin Relaxation in Graphene — Sebastian Ringer, Stefan Hartl, Matthias Rosenauer, Tobias Völkl, Maximilian Kadur, Franz Hopperdietzel, Dieter Weiss, and •Jonathan Eroms — Institute of Experimental and Applied Physics, University of Regensburg, Germany

To measure the anisotropy of the spin-lifetime in graphene, the most notable experiments are out-of-plane rotation of the ferromagnetic electrodes and oblique spin precession. We present a third method which is a Hanle experiment where the electron spins precess around either a magnetic field perpendicular to the graphene plane or around an in plane field. In the latter case, electrons are subject to both in-plane and out-of-plane spin relaxation.

To fit the data, we use a numerical simulation that can calculate precession with anisotropies in the spin-lifetimes under magnetic fields in any direction. Our data show a small, but distinct anisotropy that can be explained by the combined action of isotropic mechanisms, such as relaxation by the contacts and resonant scattering by magnetic impurities, and an anisotropic Rashba spin-orbit based mechanism.

We also perform oblique spin precession on our sample and compare it to our experiment of in-plane/out-of-plane Hanle in terms of reliability and precision. We find a non-trivial magnetization in our contacts that was only detected in the in-plane/out-of-plane Hanle experiment but is essential for a correct analysis of the oblique spin precession data. We conclude that the in-plane/out-of-plane Hanle experiment is the most reliable and precise method to measure the anisotropy.

TT 97.4 Thu 15:45 EW 201

Magneto-Raman spectroscopy and theoretical modelling of spin-density excitations in (001)-grown GaAs-AlGaAs quantum wells — •Sven Gelfert[1], Christian Frankerl[1], Christian Reichl[2], Dieter Schuh[1], Werner Wegscheider[2], Dominque Bougeard[1], Tobias Korn[1], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Schweiz

We performed inelastic light scattering experiments on 12-nm-wide (001)-oriented GaAs-AlGaAs single quantum well samples in the presence of an external applied magnetic field. The investigated systems are Si doped to obtain a balanced Rashba and Dresselhaus SOI contribution (α=β). The resulting effective spin-orbit field is either parallel or antiparallel to the relevant in-plane crystal directions which leads to a highly anisotropic spin splitting of intrasubband transitions in the conduction band.

In order to get deailed insights on the behavior of the spin splitting we perform magnetic field series in different crystal directions. The intrinsic spin-orbit field strength and the electron g-factor can be deducted from our observations. We also provide theoretical considerations which quantitatively predict the modified spin splitting under these experimental conditions.

TT 97.5 Thu 16:00 EW 201

Spin valley coherent transport in Graphene — •Saber Rostamzadeh — Sabanci University, Orta Mahalle, Universite Caddesi No:27, 34956 Orhanli/Tuzla/Istanbul

Due to the advent of Spintronics, which attempts to perform calculations and store information using the spin instead of charge, there is a gradual increase in investigating methods to manipulate the spin degree of freedom of electrons in quantum confined structures to propose a surrogate for conventional electronic devices.

It has been shown that spin orbit coupling in Graphene plays a

major role in generating and manipulating of spin polarized currents which found useful in spintronics applications.

Extra degree of freedom such as valley index in Graphene always adds to the functionality of the system and in a sense enlarges the parameter space of the system and works as an additional control parameter without the effort to make one.

In this work we demonstrate the effect of Rashba spin orbit interaction in Graphene induced by adatoms and show that it produces spin-valley coupling. This feature is useful in manipulating spin degree of freedom via valley index and furthermore we illustrate and theoretically set up a formalism which suggest the extraction of spin current form a valley current.

15 min. break.

TT 97.6 Thu 16:30 EW 201

Calculation of Spin Diffusion Equations in Spin/Orbital Polarized Systems — •Vincent Sacksteder[1] and Yasufumi Araki[2] — [1]Royal Holloway University of London, UK — [2]Tohoku University, Japan

This talk is about how to derive coarse-grained spin diffusion equations suitable for modeling a spintronics device from realistic Hamiltonians describing spin and scattering at the atomic scale. The standard formalism for obtaining diffusion equations requires performing an average over the Fermi surface, weighted by the scattering time. In spin or orbital-polarized systems the scattering time depends on spin and/or the orbital index; we describe the consequences for spin diffusion. This is important for modeling new memory devices which combine spin-orbit interactions with magnetization.

TT 97.7 Thu 16:45 EW 201

Gate-controllable large magnetoresistance in a 2DES based spin valve device — •Franz Eberle, Martin Oltscher, Thomas Kuczmik, Andreas Bayer, Dieter Schuh, Dominique Bougeard, Mariusz Ciorga, and Dieter Weiss — Universität Regensburg, Regensburg, Germany

The realization of sFET like devices requires the presence of large local spin signals, which can be tuned by an electric field. In typical semiconductor structures, however, values of the magnetoresistance (MR) of only up to 1% have been observed. In this contribution we present the exceptionally large MR we observe in local two-terminal devices with the channel defined within a two-dimensional electron system (2DES) at an inverted GaAs/(Al,Ga)As interface.[1] Spin aligning source and drain contacts are based on a spin Esaki diode structure, consisting of ferromagnetic (Ga,Mn)As and n-doped GaAs. Depending on the applied bias, we observe MR ratios of up to 80%, which correspond to a signal height ΔR in the order of 1kΩ. We tune these large local signals by an electric gating scheme which, contrary to typical sFET proposals, is not based on the manipulation of spins due to the spin-orbit coupling. Instead, we use gates placed outside the current path to control confinement of spins in the region between the leads. With this method we can tune the MR in these devices by up to 14%.

The work was supported by the German Science Foundation through the project SFB 689.

[1] M. Oltscher et al., Nature Communications **8**, 1807 (2017)

TT 97.8 Thu 17:00 EW 201

Giant Bulk Rashba Splitting — •Louis Ponet and Sergey Artyukhin — Via Morega 30, 16163 Genova, Italy

Spintronics has been an exciting area in the last decades, due to a promise for devices that exploit the existence of spin-polarized states [1]. Important applications include storage media, where the use of spins to store data has been widespread since the earliest days of computing. An important challenge is the control of these states. Magnetic field control precludes further miniaturization. Possible solutions may include spin torques provided by spin-polarized currents. For use in electronic applications, there is a pressing need for electric control of the states, which was recently demonstrated in materials that showcase an anomalously large Rashba-effect [2]. Our research focused on quantitative description of the orbital Rashba-effect [3], an electrostatic effect that couples orbital angular momentum to the polarization. Due to its non-relativistic nature, the effect can be many orders of magnitude larger than would be expected from the spin Rashba-effect. We used model Hamiltonians and ab-initio calculations to examine the effect and outline the design principles for promising compounds.

References [1] S. D. Bader and S. S. P. Parkin, Spintronics Ann. Rev. Cond. Matt. Phys. 1, 71 (2010). [2] D. Di Sante, P. Barone, R. Bertacco, S. Picozzi, Advanced Materials, 25, 509 (2013). [3] Park J. H., Kim C. H., Rhim J. W., Han J. H., Phys. Rev. B 85, 195401 (2012).

TT 97.9 Thu 17:15 EW 201

Spin-transfer torques generated by strained 3D HgTe TI — •Graciely Santos, Simon Hartinger, Christian Jünger, Erwann Bocquillon, Charles Gould, and Laurens Molenkamp — Julius-Maximilians-Universität Würzburg, Würzburg - Germany

Strained bulk HgTe is a well known topological insulator (3D TI) showing the coexistence of an insulating bulk with metallic Dirac surface states presenting intrinsic spin-momentum locking. By applying an electric current through the surface states of a 3D TI, a spin-polarized current can be generated allowing transfer of angular momentum to an adjacent ferromagnetic layer. Preliminary spin-pumping ferromagnetic resonance (FMR) measurements on the HgTe 3D TI coupled to a ferromagnet island showed a background contribution in the measured voltages. In this work we report on spin-transfer torque ferromagnetic resonance (STT-FMR) measurements in order to better understand the previous results in this system.

TT 98: Poster Session: Superconductivity

Time: Thursday 15:00–19:00 Location: Poster B

TT 98.1 Thu 15:00 Poster B

A search for superconducting Heusler compounds without inversion symmetry in the AuPdTM set (T = Sc, Y and M = Al, Ga, In) — •Linus Kautzsch, Gerhard H. Fecher, Walter Schnelle, and Claudia Felser — Max Planck Institut CPFS, Dresden, Germany

Superconductivity is well-known in ternary centrosymmetric Heusler compounds like Pd_2YSn. One typical fingerprint in the band structure is a saddle point type van Hove singularity near by the Fermi energy ϵ_F, which leads to an enhanced density of states.

Furthermore, quaternary Heusler compounds with 1:1:1:1 stoichiometry show the Y-structure (LiMgPdSn, $F\bar{4}3m$ (216)) without inversion symmetry. The pairing state in superconductors with a lack of inversion symmetry should be a mixture of singlet and triplet Cooper pairs. Therefore, these compounds are of importance with respect to understanding superconducting pairing mechanisms. This work is dedicated to extend superconductivity to quaternary Heusler compounds and the experimental investigation of their properties. We identify new quaternary Heusler superconductors through prediction of the van Hove singularity in the band structure. Subsequently, samples of the AuPdTM set (T = Sc, Y and M = Al, Ga, In) were prepared by arc melting and their transport properties were characterized. As an example, AuPdScAl exhibits a transition into the superconducting state in the low temperature region (T_c = 3.0 K). Moreover, these findings enhance the understanding of superconductivity in the Heusler compounds.

TT 98.2 Thu 15:00 Poster B

Dielectric properties of thin Sn films near percolation probed with superconducting coplanar microwave resonators — •Nikolaj G Ebensperger, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

The two-dimensional limit of thin films at low temperatures opens up a plethora of interesting phenomena and physical processes. Here, knowledge of the dielectric properties at very low temperatures can be of vital help and can offer new insights into fundamental characteristics and interactions. However, the combination of thin films and very low temperatures often exceeds the limits of traditional experimental methods. We present a novel approach utilizing coplanar superconducting

microwave resonators, which overcomes these difficulties, allowing precise measurements of the dielectric constant in a temperature range up to 9 K and frequency range up to 30 GHz.

Granular films are known to show peculiar behaviour of the dielectric constant approaching the percolation transition. We apply our experimental approach to thin granular Sn films with thicknesses in the range 36 - 58 nm. We determine the dielectric constant and show that it has diverging behaviour approaching the percolation threshold, similar to behaviour found in other materials with percolation transitions. At low temperatures of about 4 K we find distinct features in our data, indicating a clear superconducting transition of the individual Sn grains.

TT 98.3 Thu 15:00 Poster B

Searching for novel low-dimensional materials with interesting electronic properties: New mixed-valent transition metal chalcogenides — •Mihai I. Sturza[1,2], Alexander J. E. Rettie[2], Daniel Bugaris[2], Fei Han[2], Duck Young Chung[2], Saicharan Askwartham[1], Mercouri Kanatzides[2,3], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden IFW, Institute for Solid State Research, 01069 Dresden, Germany — [2]Materials Science Division, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, Illinois 60439, United States — [3]Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, Illinois 60208, United States

The class of transition-metal chalcogenides that exhibits mixed valency has been of continuing interest for several decades. The emergence of superconductivity with a high superconducting transition temperature in mixed-valence $A_xFe_{2-y}Se_2$ (A = K, Rb, Cs, and Tl) phases has further increased interest in the chemistry and physics of complex ternary transition-metal chalcogenides. New results from the chemistry of the A/Cu/Q (A=Na, K, Ba, Q=S, Se) system will be reported. The synthesis, structure, and properties of new layered copper chalcogenide compounds, which are mixed-valent will be presented. Single crystals were grown by the reaction of Cu metal in a molten alkali/ alkaline-earth metal/polychalcogenides/flux. Electronic band structure calculations and physical property measurements reveal p-type metallic behavior, with moderately high electrical conductivity.

TT 98.4 Thu 15:00 Poster B

Transport properties of $In_xSn_{1-x}Te$ nanostructures — •Mengmeng Bai, Fan Yang, Zhiwei Wang, and Yoichi Ando — Institute of Physics II, Cologne, Germany

SnTe is a three-dimensional topological crystalline insulator. It is known that superconductivity can be induced in SnTe by indium doping, making $In_xSn_{1-x}Te$ a promising platform for searching for topological superconductivity. Here we present our study on superconducting $In_xSn_{1-x}Te$ nanostructures. $In_xSn_{1-x}Te$ nano-plates and nanowires were grown via vapor-transport method. After the growth, they were fabricated into devices and then measured in a cryostat. A sharp superconducting transition was observed in all devices. Point contact spectroscopy was also taken at low temperatures. The preliminary results are presented and discussed.

TT 98.5 Thu 15:00 Poster B

Growth and Characterizations of Superconducting $In_xSn_{1-x}Te$ Nanomaterials — •Zhiwei Wang, Felix Münning, Mengmeng Bai, Fan Yang, and Yoichi Ando — Institute of Physics II, University of Cologne, D-50937 Cologne, Germany

In recent years, possible existence of Majorana fermion (MF) in condensed matter has attracted extensive interest because of the potential application of MFs to the realization of topological quantum computation. So far, several strategies have been proposed to create and manipulate MFs based on nanowires of topological insulators (TI) and topological superconductors (TSC) [1-2]. In this contribution, we reported the nanomaterial growth and characterizations of one of the candidate TSCs, $In_xSn_{1-x}Te$ (IST). Nanowires and nanoflakes of IST are grown on SiO_2/Si wafer by using a vapour transport method in sealed quartz tubes with and without gold catalyst. Growth parameters such as the composition of source materials, source temperature, temperature gradient and growth time are optimized to obtain expected nanowires and nanoflakes. Scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDX) are used to investigate the morphology and composition of as-grown nanomaterials. For electronic transport characterization, devices based on nanowires and nanoflakes are fabricated by e-beam lithography and photo-lithography, respectively. Electronic transport properties are measured on helium-3 cryostat with the temperature down to 0.3 K.

[1] Liang Fu and C. L. Kane, Phys. Rev. Lett. 100, (2008) 096407
[2] Cook and M. Franz, Phys. Rev. B 84 (2011) 201105(R)

TT 98.6 Thu 15:00 Poster B

Superconducting properties of $[(SnSe)_{1+\delta}]_{m\in[1,9]}[NbSe_2]_{n=1}$ ferecrystals — •Theodor U. Griffin[1], Martina Trahms[1], Corinna Grosse[1], Danielle Hamann[2], Omar K. Hite[2], Matti B. Alemayehu[2], Olivio Chiatti[1], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Department of Chemistry, University of Oregon, Eugene, OR, 97401, USA

Ferecrystals are artificially layered materials that can be grown with atomically smooth layers in various sequences. Furthermore, as the layers are bound only through van der Waals interaction, strain due to lattice mismatch between layers is negligible and the material has turbostratic disorder. They can provide a model for naturally layered superconductors, including many high T_C superconductors. They also allow embedding interesting monolayers and thin films in buffer material, protecting them from external influences.

Here, we used ferecrystals composed of monolayers of the superconducting transition-metal dichalcogenide $NbSe_2$ and bilayers of the semiconductor SnSe. These layers are stacked in repeated sequences of a monolayer $NbSe_2$ with between one and nine bilayers of SnSe. We investigate the electrical transport properties near the superconducting transition. The aim is to ascertain at which, if any, ratio of $NbSe_2$ to SnSe the ferecrystals begin to show two-dimensional superconducting behaviour, using the angular dependence of the critical magnetic field. We hope to gain further insight into layered superconductors and 2D-superconductivity. For $m < 6$, 3D behaviour was observed.

TT 98.7 Thu 15:00 Poster B

Characterization of $Bi_2Sr_2CaCu_2O_8$ thin film and nanowire networks synthesized from sol-gel precursor — •XianLin Zeng[1], Fabian Laurent[1], Thomas Karwoth[1], Michael Koblischka[1], Crosby Chang[2], Thomas Hauet[2], and Uwe Hartmann[1] — [1]Institute of Experimental Physics, Saarland University, Campus C 6 3, D-66123 Saarbrücken, Germany — [2]Institut Jean Lamour, UMR CNRS-Université de Lorraine, 54506 Vandoevre-lès-Nancy, France

Thin films on $SrTiO_3$ substrates and substrate-free networks of superconducting $Bi_2Sr_2CaCu_2O_8$ (Bi-2212) were fabricated using the spin coating method and the electrospinning technique. To enable a comparison of the superconductivity of the two-dimensional and one-dimensional materials, both samples are prepared from the same sol-gel precursor. The morphologic characterization was done by scanning electron microscopy (SEM). The phases were confirmed by X-Ray diffraction (XRD). The magnetic properties characterized from SQUID measurements show that the nanowire samples have a lower T_c than the respective thin film samples. The electric properties reveal further differences. A double-step behavior in the $R(T)$ curves and an obvious residual resistance in the superconducting regime in the $U(I)$ curves were found for the nanowire samples. The hysteretic effect of the nanowire network sample is much weaker than in the thin film sample, and it vanishes at weak fields (0.6 T). This work is part of DFG-project Ko2323/8.

TT 98.8 Thu 15:00 Poster B

Magnetic and structural phase transition in $Fe_{(1+y)}Te$ — •Maik Barth, Kai Grube, Sebastian Kuntz, Thomas Wolf, Michael Merz, and Frank Weber — Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

To verify the established phase diagram of $Fe_{(1+y)}Te$ [1], we studied the temperature-dependent structural and magnetic properties on single crystals with an Fe content between 1.08 and 1.19. Independent of the excess Fe content, a magnetic transition from paramagnetic to antiferromagnetic is observed around $T_N \approx 60$ K. The lattice, on the other hand, undergoes a structural phase transition from tetragonal to monoclinic for Fe contents below 1.11 while a structural phase transition from tetragonal to orthorhombic is observed for Fe contents above 1.13; in the range between 1.11 and 1.13 a mixture of both phases appears. Moreover, the order of the structural phase transition changes continously from first to second order when going from 1.08 to 1.19. The structural characterization was done using x-ray diffraction, the magnetic measurements by utilizing a MPMS with a SQUID.

[1] Koz et al., Phys. Review B 88, 094509 (2013)

TT 98.9 Thu 15:00 Poster B

ω/T Scaling in Optimal Co-Doped $BaFe_2As_2$ — •Jakob Burgi[1], Florian Wasser[1], Chul-Ho Lee[2], Kunihiro Kihou[2], Jitae Park[3], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany — [2]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan — [3]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universitä München, Lichtenbergstr. 1, D-85748, Garching, Germany

The phase diagram of iron-based superconductors, in particular of $BaFe_2As_2$, indicates the existence of a quantum critical point (QCP) beneath the superconducting (SC) dome, where T_c is highest and the antiferromagnetic (AFM) phase terminates. Considering an AFM order parameter the associated susceptibility follows a simple scaling relation $\chi''(\boldsymbol{q}_{AFM}, \omega, T) = T^{-\alpha} f\left(\frac{\omega}{T^{-\alpha}}\right)$ within the Hertz-Millis scenario. In this regard, we performed inelastic neutron scattering experiments on 6 % Co doped $BaFe_2As_2$ ($T_c = 24$ K) and showed that magnetic fluctuations between 28 K and 400 K follow the scaling relation and thus indicate the presence of a QCP. Our observations are similar to the heavy fermion system $CeCu_{5.9}Au_{0.1}$ as the scaling function for both compounds seems well approximated by a simple mean-field approach. Moreover, the scaling law seems to be applicable over the nematic regime without any impact indicating that the nematic transition just follows the magnetic.

TT 98.10 Thu 15:00 Poster B

Mixed magnetic order and superconductivity in multiorbital Hubbard models — •Chris Koschenz and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, Germany

We extend a generalized Hartree-Fock theory that allows mixed phases [1] to multiorbital Hubbard models. Multiband and multiorbital physics are crucial for the understanding of superconductivity and magnetism and their possible coexistence in high-temperature superconductors. Handling that kind of system can be numerically expensive and is in general restricted to a limited number of ordering vectors in the standard Hartree-Fock approach. Applying a generalized Hartree-Fock theory including the minimization of the grand canonical potential allows to overcome these drawbacks and thereby permits extensive studies of phases of mixed magnetic order [1]. Furthermore, we have enhanced the usual tetrahedron integration method [2] by an adaptive refining algorithm at zero and finite temperatures. Using these methods, we are able to employ realistic multiorbital models to study the coexistence and competition of magnetic ordering or mixing and superconductivity. We elucidate the role played by orbital effects and compare with previous work [3]. Furthermore, we study the possibility of additional phase transitions in the coexistence regime. [1] E. Langmann and M. Wallin, J. Stat. Phys. **127**, 825 (2007)
[2] P. E. Blöchl et al., Phys. Rev. B **49**, 16223 (1994)
[3] J. Schmiedt et al., Phys. Rev. B **85**, 214425 (2012)

TT 98.11 Thu 15:00 Poster B

Evolution of the nematic susceptibility in a superconducting dome without structural transition — •Xiaochen Hong[1], Rhea Kappenberger[1], Federico Caglieris[1], Saicharan Aswartham[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW-Dresden, Dresden, Germany — [2]Institute of Solid State Physics, TU Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, Germany

The first step towards understanding the mechanism of the mysterious high-temperature superconductivity is to clarify the phase diagram of these compounds. The superconducting transition temperature of them always show dome-shaped dependence on tuning parameter(s). In the case of iron based superconductors (FeSC), a prevailing picture is that magnetic, structural and nematic transition are all entangled into the dome. Among these orders, the one which is "on the driver seat" should be most relevant to the formation of Cooper pairs.

Recently, an elegant technique based on piezoelectric apparatus was introduced to study the nematic susceptibility. Soon after, signatures of a nematic quantum critical point were found in many FeSCs by this technique. Here we present our study on cobalt doped LaOFeAs, which does not exhibit a structural transition inside its superconducting dome. We observe a divergent nematic susceptibility across the dome which peaks near the optimal doping. Our finding strongly suggest that the nematic fluctuation is intimately related to the superconductivity in FeSCs.

TT 98.12 Thu 15:00 Poster B

Quasiparticle Interference structure in the Spin Density Wave State of Iron Based Superconductors — •Dustin Altenfeld[1], Felix Ahn[1], Peter J. Hirschfeld[2], and Ilya Eremin[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics, University of Florida, Gainesville, Florida 32611, USA

Using 10-orbital model Hamiltonian we present quasiparticle interference (QPI) calculations in the spin density wave phase (SDW) of Fe-based superconductors (FeSc). We find that the QPI structure can be regarded as a robust way of studying the orbital driven effects on the magnetically ordered phase. In particular, we study the phase-relevant changes induced by the SDW order parameters with orbital structure starting from two-band model up to ab initio based band structure calculation using a realistic model Hamiltonian. We provide the detailed insight for the one dimensional QPI maps seen by STM experiment.

TT 98.13 Thu 15:00 Poster B

High field transport properties of 1111 parent compounds — •Martina Meinero[1,2], Federico Caglieris[3], Alessandro Leveratto[2], Ilaria Pallecchi[2], Gianrico Lamura[2], Fabio Bernardini[4], Alessia Provino[1,2], Pietro Manfrinetti[1,2], Maryam Shahrokhvand[5], Uli Zeitler[5], and Marina Putti[1,2] — [1]SPIN-CNR, C.so Perrone 24, 16152 Genova, Italy — [2]University of Genova, Via Dodecaneso, 16146 Genova, Italy — [3]IFW Dresden, 01069 Dresden, Germany — [4]CNR-IOM-Cagliari and University of Cagliari, 09042 Monserrato, Italy — [5]HFML-EMFL, Radboud University, Toernooiveld 7, 6525ED Nijmegen, Netherlands

The Fermi surface and the band structure of the 1111 family of Fe-based superconductors have been vastly theoretically investigated but a direct experimental insight is still lacking. We performed low-temperature transport measurements in high magnetic fields up to 30 T in several 1111 parent compounds. We detected Shubnikov de Haas oscillations in both the magnetoresistance of a single crystal of SmFeAsO and in the thermopower of a policrystalline sample of LaFeAsO. We also investigated the thermoelectric properties of polycrystalline CeFeAsO, PrFeAsO, NdFeAsO. Our results bring to the identification of a dominating cylindrical pocket, whose corresponding carrier density matches with the one obtained from Hall effect measurements. In addition we verified a good agreement with prediction of DFT calculations of the band structure.

TT 98.14 Thu 15:00 Poster B

Crystal growth of the iron pnictide superconductor $NdFeAsO_{1-x}F_x$ — •Marius Peters, Mahmoud Abdel-Hafiez, Abanoub Refat Hanna, and Cornelius Krellner — Goethe-Universität Frankfurt

The single crystal growth of the iron pnictide superconductor NdFeAsO in a NaCl/KCl-salt flux at ambient pressure has been improved optimizing growth temperature settings and profiles and developing a new growth geometry. Single crystaline samples of the 1111-system $NdFeAsO_{1-x}F_x$ were investigated with structural, magnetic and transport methods and are in overall agreement with the polycrystalline material [1,2]. For lower doping levels (up to about $x = 0.1$) the system shows a spin density wave transition (below $154\,K$), which is suppressed strongly with increased doping, and with higher doping levels yields unconventional superconductivity ($T_C = 50\,K$ for $x = 0.2$) [3]. We will present details of the optimization procedure of the crystal growth together with structural and magnetic characterization down to 2 K.
[1] A.Marcinkova et al., Chemistry of Materials **21**, 2967 (2009)
[2] G.Lamura et al., Phys.Rev.B **91**, 024513 (2015)
[3] A. Adamski et al., Phys. Rev. B **96**, 100503(R) (2017)

TT 98.15 Thu 15:00 Poster B

Electronic phase diagram of CeFeAsO as a function of hydrostatic pressure and As by P substitution — •Philipp Materne[1,2], Wenli Bi[2,3], Esen Ercan Alp[2], Jiyong Zhao[2], Michael Yu Hu[2], Dongzhou Zhang[2], Til Goltz[1], Anton Jesche[4], Christoph Geibel[4], Rhea Kappenberger[5], Saicharan Aswartham[5], Sabine Wurmehl[5,1], Bernd Büchner[5,1], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — [2]Argonne National Laboratory, Argonne, IL 60439, USA — [3]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA —

[4]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [5]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01069, Germany

We present a local probe study of the electronic properties of hydrostatic and chemical (due to As by P substitution) pressure in CeFeAsO by means of energy- and time-domain Mössbauer spectroscopy. The application of pressure results in a compression of the unit cell. We investigated the magnetic hyperfine field, the electric field gradient, and the electron density at the Fe nucleus. We found a distortion of the FeAs tetrahedra with increased P-substitution level while it remains unchanged in the case of hydrostatic pressure. We observed a nearly linear suppression of the magnetic hyperfine field to zero between 0 and 40 % P-substitution level while the field is reduced by 25 % between 0 and 4.5 GPa followed by an abrupt decrease to zero at 5.2 GPa.

TT 98.16 Thu 15:00 Poster B

Nernst effect of Rh-doped $BaFe_2As_2$: Evidence for superconductivity driven by nematic fluctuations — •Christoph Wuttke[1], Frank Steckel[1], Federico Caglieris[1], Steffen Sykora[1], Xiaochen Hong[1], Seunghyun Kim[1], Sabine Wurmehl[1], Sheng Ran[2], Paul C. Canfield[2], Bernd Büchner[1,3,4], and Christian Hess[1,4] — [1]Leibniz-Institute for Solid State and Materials Research, IFW-Dresden, 01069 Dresden, Germany — [2]Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA — [3]Institut für Festkörperphysik, TU Dresden, 01069 Dresden, Germany — [4]Center for Transport and Devices, Technische Universität Dresden, 01069 Dresden, Germany

The nematic phase of iron-based superconductors is a very debated topic since the role of nematic fluctuations in the appearance of high temperature superconductivity is still controversial. In this work we systematically investigate the phase diagram of $BaFe_2As_2$ as a function of Rh-doping through Nernst effect measurements. In particular we obtained an anomalously high Nernst coefficient in the tetragonal phase. Moreover, we observe, that upon doping its magnitude strikingly mimics the shape of the superconducting dome. Using a minimal orbital model for iron-based superconductors we show that the Nernst coefficient couples directly to the nematic fluctuations. Our experimental results therefore provide direct evidence for nematic fluctuations playing a crucial role for the mechanism of superconductivity in Rh-doped $BaFe_2As_2$. We discuss our findings using a comparison with the nematic susceptibility obtained from elastoresistance measurements.

TT 98.17 Thu 15:00 Poster B

Magnetic and electronic excitations in underdoped YBCO — •Ulrike Zweck, Mirko Riedl, Andreas Baum, Daniel Jost, Andreas Erb, and Rudolf Hackl — Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

The interrelation of magnetism, charge order and superconductivity is among the most complex open problems in the cuprates and possibly the key for understanding unconventional superconductivity. $YBa_2Cu_3O_{6+x}$ is a laboratory for systematic studies since single crystals with extremely high purity can be prepared. In addition, the most interesting doping range $0 \leq p \leq 0.18$ with p the number of holes per CuO_2 formula unit can be accessed by varying x between 0 and 1. For the intended Raman scattering experiments homogeneously doped and highly ordered crystals are crucial since impurities or residual strain compromise the results. In a first step crystals with oxygen contents of approximately $x = 0.56$ and $x = 0.67$ were prepared. For improving the order in the crystals the temperature and the oxygen partial pressure were reduced simultaneously after the initial annealing step at constant temperature in order to keep the oxygen concentration in the crystals constant. In this way the ordering was already substantially improved. After detwinning the crystals were equilibrated following the protocol of Liang *et al.* [Physica C **336**, 57 (2000)]. The resulting transition temperatures were 60 and 66 K. For $x = 0.56$ the two-magnon excitation in B_{1g} symmetry was found in the expected energy range as opposed to what was observed earlier in quenched samples.

TT 98.18 Thu 15:00 Poster B

Plaquette Valence Bond Theory of High-Temperature Superconductivity — •Malte Harland[1], Mikhail I. Katsnelson[2], and Alexander I. Lichtenstein[1] — [1]Universität Hamburg, Hamburg, Germany — [2]Radboud University Nijmegen, Nijmegen, The Netherlands

We present a strong-coupling theory of high-temperature superconductivity in the cuprates based on a quantum critical point of the two-by-two Hubbard Plaquette. This point is characterized by the crossing of the particle number sectors $N = 2, 3, 4$. The groundstates close to the quantum critical point are spin-doublets and spin-singlets supporting the idea of resonating valence bonds on the Plaquette. Embedding the Plaquette in an environment of other Plaquettes we find a $d_{x^2-y^2}$-wave superconducting order parameter where the electrons are on the border between itinerant and localized behavior and investigate its competition with other orders. The bottom-up approach enables us to investigate the superconductivity's dependence on microscopic parameters such as, e.g. the next-nearest-neighbour hopping. We provide finite-temperature results obtained by the Dynamical Mean-Field theory, that gives an exact solution of our model.

TT 98.19 Thu 15:00 Poster B

Higgs spectroscopy of superconductors in nonequilibrium — •Lukas Schwarz, Benedikt Fauseweh, and Dirk Manske — Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany

In superconductors, a fundamental collective excitation of Cooper pairs exists which arises due to the spontaneous U(1) symmetry breaking. This mode is called Higgs mode in analogy to high-energy physics. In recent years, Higgs oscillations in s-wave superconductors in nonequilibrium excited by short THz laser pulses were intensively studied. We show that such pump-probe experiments on unconventional superconductors with non-trivial gap symmetry can excite multiple different Higgs modes. As these modes can be classified by the underlying lattice point group, an identification of these modes allows to draw conclusions about the gap symmetry. Therefore, Higgs oscillations have a great potential to become a spectroscopic method for investigations of gap symmetries in superconductors.

TT 98.20 Thu 15:00 Poster B

Triplet superconducting correlations and spin imbalance in magnet-superconductor hybrid structures — •Kevin Marc Seja[1], Oleksii Shevtsov[2], and Tomas Löfwander[1] — [1]Chalmers University of Technology, Göteborg, Sweden — [2]Northwestern University, Evanston, IL, United States

We examine a superconductor that is in contact with a normal metal via a spin-active interface. Using quasiclassical theory of superconductivity, we study the system in equilibrium as well as in nonequilibrium induced by a voltage bias. Earlier investigations have shown that in equilibrium the interface gives rise to Andreev bound states that induce a spin magnetization in the superconductor. It was found that this equilibrium magnetization is related to non-trivial triplet superconducting correlations, a key feature of unconventional superconductivity. Out of equilibrium there is an additional contribution to spin imbalance related to spin-filtering and spin-mixing mechanisms. [1,2] However, in non-equilibrium the possible connection between magnetization and superconducting triplet correlations is not yet understood. The aim of this work is to examine this relation as well as the change in distribution and the spatial behavior of these correlations in non-equilibrium configurations.

[1] O. Shevtsov, T. Löfwander, *J. Phys Conf. Ser.* **568** 2 (2014)
[2] O. Shevtsov, T. Löfwander, *Phys. Rev. B.* **90** 085432 (2014)

TT 98.21 Thu 15:00 Poster B

Properties of self-consistent random matrices: Case study for the superconductor-insulator transition — •Matthias Stosiek and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg, Germany

Our general interest is in the properties of ensembles of random Hamiltonians that satisfy a self-consistency property. Such ensembles typically appear in mean-field treatments of interacting systems. The example we here consider is the Superconductor-Insulator Transition (SIT) where the superconducting gap is calculated self-consistently in the presence of short-range disorder. Our focus is on disordered films with conventional s-wave pairing that we study numerically employing the negative-U Hubbard model within the standard BogoliubovdeGennes approximation. The general question that we would like to address here concerns the auto-correlation function of the pairing amplitude: How does it decay in real space and in what way does it change across the SIT?

These correlations are typically neglected in analytical theories. Our research might have significant impact on the understanding of the SIT, if the correlations turn out sufficiently long-ranged, so that they influence properties of the critical point.

We present preliminary data that indicates the existence of very

long ranged (power-law) correlations that may indeed change the critical behavior in a significant way.

TT 98.22 Thu 15:00 Poster B

Delocalized Shiba bands in magnetic clusters at superconducting surfaces — •Simon Körber, Oleksiy Kashuba, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

If a number of magnetic atoms is placed sufficiently close to each other on the surface of a superconductor, their Shiba states hybridize and form a band structure inside the superconducting gap. We show that for particular cases a degenerate delocalized flat band emerges in the energy spectrum. We solve the problem analytically for arbitrary spin configuration and analyze both trivial and non-trivial solutions. The wave functions of the trivial solutions effectively decouple from the total magnetic moment of the cluster. This is the reason why they form flat bands. The energies of the dispersing bands corresponding by two non-trivial solutions can be characterized solely by the net magnetic moment of the cluster.

TT 98.23 Thu 15:00 Poster B

Non-uniform superconducting phases generated by spin-orbit interaction — •Julie Baumard[1,2], Jerome Cayssol[1], and Alexandre Buzdin[1] — [1]LOMA - UMR 5798, Bordeaux, France — [2]DIPC, Donostia-San Sebastián, Spain

Non-uniform superconducting states raise great interest in the scientific community. One of the most famous is the FFLO state, predicted in the 1960's. It is characterized by a higher critical field than the uniform superconducting state. The FFLO state appears at low critical temperature, which makes it difficult to observe experimentally. In this presentation, we will show that adding spin-orbit interaction allows the modulated phase to appear at high critical temperature.The system studied consists of a superconducting nanowire with Zeeman field and Rashba spin-orbit interaction.

TT 99: Poster Session: Transport

Time: Thursday 15:00–19:00 Location: Poster B

TT 99.1 Thu 15:00 Poster B

Interface coupling in magnetoconductance of Bi-films on Si(111) — •Doaa Abdelbarey[1], Philipp Kröger[1], Christoph Tegenkamp[1,2], and Herbert Pfnür[1] — [1]Inst. für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physik, TU Chemnitz

Bi ultrathin epitaxial films are governed by strongly spin-polarized bands that determine to a large extent their magnetotransport properties. Magneto conductance of films with a thickness of 20 to 60 bilayers on a Si(111) substrate was measured mostly at T = 11 K and in B-fields up to 4 T. The B-field orientation was varied from perpendicular to parallel to the surface. For the in-plane B-field orientation strong variations ofscattering properties between the interfaces were observed that depend both on the angle between B- and E-fields as well as on the film thickness. For the thinnest films, direct interaction between interfaces leads to strong spin depolarization and to a conductance almost independent of B. Thicker films exhibit a dominance of weak antilocalization, if B and E are parallel, but *weak localization* for both in plane, but perpendicular to each other. The latter contribution disappears at 100 K, where only WAL was seen. Since the potential gradients on both interfaces point in opposite directions normal to the surface, the spin directions in the same Rashba-split electronic bands are opposite (and in plane) for a given $\vec{k}_{\parallel}$. This means that only within the same layer backscattering is forbidden, since scattering from $+\vec{k}_{\parallel}\uparrow$ to $-\vec{k}_{\parallel}\downarrow$ requires spin Umklapp, but for scattering between the interfaces no Umklapp for the same process is necessary. Therefore, it is allowed.

TT 99.2 Thu 15:00 Poster B

Controlling conductivity by quantum well states: ultrathin Bi(111) films. — Philipp Kröger[1], Doaa Abdelbarey[1], •Marvin Detert[1], Herbert Pfnür[1], and Christoph Tegenkamp[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Physik, Technische Universität Chemnitz

Epitaxial Bi(111) films were subject to many and partly even controversial studies on the semimetal-semiconductor transition (SMSC) triggered by a robust quantum confinement. The remaining conductance was ascribed to conducting surface channels. We investigated ultra-thin crystalline Bi films on Si(111) as a function of film thickness between 20 and 100 bi-layers by means of electric transport measurements. Varying temperature and magnetic field, we disentangled essentially two transport channels. One remains indeed metallic at all thicknesses investigated with a slightly increasing conductance as a function of film thickness, d, whereas the second is activated with a d^{-1}-dependence of the activation energy, indicating a quasi-harmonic confining potential. Both channels reflect the properties of the whole quantized film and a strict separation into surface and bulk states, valid for electronic screening lengths much smaller than d, seems to be doubtful in these strongly quantum confined ultra-thin films. The metallic channel through the coupled edge states seems to be robust.

TT 99.3 Thu 15:00 Poster B

Transport spectroscopy of 3D Dirac materials — •Henry Legg and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, D-50937, Köln, Deutschland

Many materials that realise a 3D Dirac or Weyl dispersion contain multiple Dirac nodes within their Brillouin zone; examples include Cd_2As_2, Na_3Bi, and $Pb_{1-x}Sn_xSe$. In this work we propose a new transport mechanism to 'spectroscopically' map the bulk electronic structure of a 3D Dirac or Weyl semi-metal with multiple nodes within the Brillouin zone.

A positive magnetoresistance occurs when parallel magnetic and electric fields are orientated in a direction perpendicular to a vector connecting a pair of these Dirac nodes. In the presence of long ranged impurities this magnetoresistance becomes strongly dependent on angle. This angular dependence provides information about the position of Fermi-surfaces within the Brillouin zone, the Fermi-wave vector, and the extent of impurities within the material. Our results are compared to experiments on $Pb_{1-x}Sn_xSe$.

TT 99.4 Thu 15:00 Poster B

Shot noise of contacts to Fe atoms and FeH_n — •Michael Mohr, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The ballistic transport through contacts to pristine and hydrogenated Fe atoms on Au(111) surfaces is investigated with a 4 K scanning tunneling microscope. We observe a variation of the current shot noise measured from the two species suggesting an influence of hydrogen on the spin polarized transport.

This work was supported by SFB 677.

TT 99.5 Thu 15:00 Poster B

Extending the hierarchical quantum master equation approach to low temperatures and realistic band structures — •André Erpenbeck[1], Christian Hertlein[1], Christian Schinabeck[1], and Michael Thoss[1,2] — [1]Theoretische Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany

The hierarchical quantum master equation (HQME) approach, originally developed by Tanimura in the context of relaxation dynamics [1], has recently received renewed interest as an accurate method to describe quantum transport in interacting nanosystems [2-4]. Because the HQME approach relies on a decomposition of the bath correlation function in terms of exponentials, however, numerical complexity restricts its applicability to systems at higher temperatures coupled to leads with simple band structures. In this contribution, we outline an extension of the HQME approach, which uses a re-summation over poles and can be applied to calculate transient currents at a numerical cost that is independent of temperature and band structure of the leads. We demonstrate the performance of the extended HQME approach for noninteracting tight-binding model systems of increasing complexity as well as for the Anderson-Holstein model.

[1] Tanimura, J. Phys. Soc. Jpn. 75, 082001 (2006)
[2] Jin et al., JCP 128, 234703 (2008)
[3] Härtle et al., PRB 88, 235426 (2013)
[4] Schinabeck et al., PRB 94, 201407(R) (2016)

TT 99.6 Thu 15:00 Poster B

Molecular characterization in liquid and cryogenic environments — •Filip Kilibarda[1], Alexander Strobel[1], Mani Lokamani[1], Torsten Sendler[1], Michael Mortensen[2], Kurt Gothelf[2], and Artur Erbe[1] — [1]HZDR, 01328 Dresden, Germany — [2]Center for DNA Nanotechnology, 8000 Aarhus C, Denmark

Current industrial scaling processes are reaching limits. We see not only diminishing returns with further scaling attempts, but also physical limitations that come more and more into play. In our research we offer a novel approach, to use single molecules as electronic components. This approach offers not only size improvements, but also a reduction in power consumption and costs. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ). Here we present two different kinds of measurements. One is performed in liquid solution and under ambient conditions, and the other one in a cryogenic environment, under vacuum. As a test bed for these measurements we use salen and C_{60} molecules, respectively. In the case of salen molecules, we show, how chemical doping influences energy levels and affects electron transport through the molecule. The experimental results are supported by quantum chemical calculations. The C_{60} measurements demonstrate that we can remove the influence of the solvent by in situ molecular evaporation into the nanoscopic junction. Additionally, operation under vacuum allows us to use more reactive metals for the nano-junction, and thus vary metal-molecule orbital overlap, where in traditional approach contacts are made out of noble metals like gold.

TT 99.7 Thu 15:00 Poster B

Bias-dependent forces in single-molecule junctions — •Susanne Leitherer[1], Jonathan Brand[2], Nick P. Rübner[1], Nicolas Neel[2], Jörg Kröger[2], and Mads Brandbyge[1] — [1]Department of Micro- and Nanotechnology, Technical University of Denmark — [2]Institut für Physik, Technische Universität Ilmenau

We study the forces on single-molecule junctions formed by C_{60}-terminated Cu tips and C_{60} molecules adsorbed on Cu(111) employing first principles electronic structure and transport calculations based on density functional theory combined with non-equilibrium Greens functions (DFT-NEGF). The C_{60}-C_{60} bond force evaluated at different distances and voltages shows an asymmetric dependence on the bias polarity. This asymmetry can be related to bias-dependent electrostatic forces between the charge densities localized at the molecules, and also indicates the effect of current-induced forces. We discuss various ways to rationalize these forces in terms of transmission eigenchannels, charge redistribution, overlap populations and bond-currents. Our simulations support the results of scanning tunneling microscopy studies on the junctions using bias-dependent force spectroscopy, which cannot be explained without accounting for the non-equilibrium forces in single-molecule junctions.

TT 99.8 Thu 15:00 Poster B

Vibronic dephasing model for coherent-to-incoherent crossover in DNA — •Patrick Karasch, Dmitry A. Ryndyk, and Thomas Frauenheim — Bremen Center for Computational Materials Science, Universität Bremen, Germany

In this work we investigate the interplay between coherent and incoherent charge transport in cytosine-guanine (GC) rich DNA molecules. Our objective is to introduce physically grounded approach to dephasing in large molecules and to understand the length dependent charge transport characteristics and especially the crossover from coherent tunneling to incoherent hopping regime at different temperatures. Therefore, we apply a vibronic dephasing model and compare the results to the Büttiker probe model which is commonly used to describe decoherence effects in charge transport. Using the full ladder model and simplified 1D model of DNA, we consider molecular junctions with alternating and stacked GC sequences and compare our results to recent experimental measurements.

TT 99.9 Thu 15:00 Poster B

Electrical Characterization of Polyalanine Molecules — •Diana Slawig[1], Malte Böhsl[1], Herbert Pfnür[1], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany

A new promising and effective approach for spintronics has emerged using spin selectivity in electron transport through chiral molecules, named Chiral Induced Spin Selectivity (CISS) [1]. Recently, by utilizing this effect a proof of concept for a new type of chiral-based Si-compatible universal magnetic memory device was demonstrated [2]. Therefore the electrical transport through helical peptides is of high interest. Our study focuses on polyalanine molecules for their high conductivity over a long range [3] and their large intrinsic dipole [4]. The molecules were contacted using mechanically controlled break junctions made of gold, operating in high vacuums.
Systematic conduction measurements revealed different states, which in turn are split up. This indicates different configurations either of the thiole-gold bond or configuration of the molecules itself.
Current Voltage measurements show a large asymmetry in the curves, which can be traced back to the dipole of the molecule [5,6].
[1] R. Naaman et.al., J. Phys. Chem. Lett. 3 (2012)
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[3] Y. Arikuma et.al., Angew. Chem., Int. Ed.,**49** (2010)
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[5] S. Sek et al., J. Phys. Chem. B, 109 (2005).
[6] H. Uji, Phys. Chem. Chem. Phys. **757**, 15 (2013).

TT 99.10 Thu 15:00 Poster B

Charge transport in bottom-up synthesized graphene nanoribbon networks — •Zhou Zhou[1,2], Nils Richter[1,2], Alexander Tries[1,2,3], Kamal Asadi[3], Zongping Chen[3], Akimitsu Narita[3], Klaus Müllen[3,4], and Mathias Kläui[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, Mainz, Germany — [3]Max Planck Institute for Polymer Research, Mainz, Germany — [4]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Mainz, Germany

Graphene nanoribbons (GNRs) attract attention due to physical phenomena resulting from their geometrical confinement which also depend crucially on their width and edge morphology [1]. Using GNR field-effect transistors, we perform a systematic study on the electronic properties of chemically synthesized and atomically perfect armchair GNRs with a width of 5 and 9 carbon atoms (aGNR5 and aGNR9)[2,3]. Our measurements reveal nuclear tunneling-assisted charge carrier hopping [4] as the dominant charge transport mechanism allowing us to apply a universal scaling law valid for charge transport in networks of both GNR structures over a large range of driving voltages and temperatures from room temperature down to 4 K [5].
[1] Son et al., Phys.Rev.Lett.97, 216803 (2006).
[2] Z. Chen et al., J.Am.Chem.Soc., 139, 9483-9486 (2017).
[3] Z. Chen et al., J.Am.Chem.Soc., 139, 3635-3638 (2017).
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[5] N. Richter et al., (manuscript in preparation 2018)

TT 99.11 Thu 15:00 Poster B

Coupling suspended carbon nanotubes to superconducting resonators — •Stefan Blien, Alexander Albang, Patrick Steger, Simon Reinhardt, Thomas Huber, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

The dispersive coupling of nano-electromechanical systems (NEMS) to superconducting coplanar waveguide (CPW) resonators in the resolved sideband regime allows controlled energy transfer between the two systems and in particular the cooling of the vibration mode. Suspended carbon nanotubes as NEMS embody both single-electron tunneling devices as well as high quality mechanical resonators. They are already close to the mechanical quantum limit at cryogenic temperatures and single electron effects dominate the mechanical behaviour, making them an interesting testbed for novel optomechanical effects.

We show first results on clean carbon nanotubes that are pre-grown and successfully transferred to a niobium CPW resonator device. We have confirmed the high quality of the transferred nanotubes and the feasibility of transparent contacts by low-temperature transport measurements.

TT 99.12 Thu 15:00 Poster B

Clean $NbSe_2$-to-carbon nanotube contacts by all-dry transfer technique — •Christian Bäuml, Maria-Teresa Handschuh, Anh-Tuan Nguyen, Nicola Paradiso, and Christoph Strunk — University of Regensburg, Regensburg, Germany

The first demonstrations of devices sensitive to the presence of Majorana fermions (MFs) consisted of 1-dimensional semiconductors prox-

imitized by a superconductor (SC) in the presence of spin-orbit interaction and of perpendicular magnetic field. Recent proposals suggested that MFs exist in carbon nanotubes (CNTs) contacted with a thin SC which retains its superconducting gap in presence of large in-plane field [1]. We demonstrate an all-dry technique for contacting CNTs with few-layer-thick flakes of $NbSe_2$, as SC layered material of the family of the transition metal dichalcogenides (TMDCs). The choice of $NbSe_2$ is motivated by its large critical in-plane magnetic field. We show that the $NbSe_2$-to-CNT contact resistance is comparable to that observed for other methods. Moreover, we demonstrate that, owing to the spin-valley locking in $NbSe_2$, few-layer devices stay superconducting up to fields of 10 Tesla, with only minor change in T_c. Our results demonstrate the first building blocks for the practical implementation of CNT-based devices for MF physics.

[1] R. Egger *et al. Phys. Rev. B* **85**, 235462 (2012);
M. Marganska *et al.* arXiv: 1711.03616

TT 99.13 Thu 15:00 Poster B

Shaping a single electron in a nanotube with an axial magnetic field — Magdalena Marganska[1], Daniel R. Schmid[2], Peter L. Stiller[2], Alois Dirnaichner[2], Christoph Strunk[2], Milena Grifoni[1], and •Andreas K. Hüttel[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Institute for Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Transport measurements on single wall carbon nanotubes allow fascinating insights into the interplay of molecular structure and electronic wave functions. Here, we analyze the magnetic field behaviour of quantum states in the limit of a single electron strongly confined to a quantum dot. An axial magnetic field (in the experiment up to 17T) exposes a very distinct behaviour of the two valleys. K' valley states experience an increase of the tunnel coupling at low field, followed by subsequent decoupling. In contrast, K valley states decouple from the leads monotonically.

This phenomenon stems from the unique combination of cylindrical topology and honeycomb atomic lattice. Longitudinal and transversal momentum are coupled, allowing manipulation of the longitudinal electronic wave function via the Aharonov-Bohm phase. At zero field, the nanotube acts similar to a $\lambda/4$ resonator, where a wave function amplitude is finite near one of the contacts. A large magnetic field restores quantum box behaviour comparable to a $\lambda/2$ resonator, where the amplitude vanishes on both sides. This is directly reflected in the tunnel rates.

TT 99.14 Thu 15:00 Poster B

Light-Driven Dynamics in Finite Graphene Nanostructures — •Jan-Philip Joost, Niclas Schlünzen, and Michael Bonitz — CAU Kiel, Germany

The understanding of carrier multiplication effects in nanoscale graphene structures is essential for various applications including solar energy harvesting [1]. In this work, we observe impact excitation effects within a few femtoseconds after an optical laser pulse excitation. The finite graphene clusters, such as nanoribbons, are described using an extended Hubbard model that takes into account the overlap of adjacent orbitals and hopping between up to third nearest neighbors. The system dynamics is provided by a nonequilibrium Green functions [2] (NEGF) approach, that has been thoroughly tested against DMRG [3], combined with the second Born (SOA) and GW selfenergy to account for electron correlations. Our description allows to predict the correlated nonequilibrium dynamics of excited graphene nanostructures of arbitrary geometry containing up to 100 carbon atoms for up to 25 fs.

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TT 99.15 Thu 15:00 Poster B

Proximity induced superconductivity in edge connected ballistic normal metal-graphene-superconductor junctions — •Preeti Pandey[1], Romain Danneau[1], Ralph Krupke[1,2], and Detlef Beckmann[1] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University Darmstadt, Darmstadt, Germany

Here, we present an experimental study of proximity induced superconductivity in edge connected normal metal-graphene-superconductor (N-G-S) junctions. The monolayer graphene sheet was sandwiched between two hexagonal boron nitride (h-BN) crystals creating a van der Waals heterostructure. Conductance spectra for these junctions in the superconducting state were measured as a function of magnetic field and charge carrier density. Our experimental results have been analyzed and can be explained with a generalized BTK model. In addition, Fabry-Pérot interferences were observed in the normal state for hole as well as electron doping of the graphene sheet. It can be explained by the formation of different interfaces in the vicinity of the contacts designed with two different materials.

TT 99.16 Thu 15:00 Poster B

Currents in graphene and possible Cooper pair formation — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Based on the quantum kinetic equations for systems with SU(2) structure, regularization-free density and pseudospin currents are calculated in graphene realized as the infinite mass-limit of electrons with quadratic dispersion and a proper spin-orbit coupling. The currents possess no quasiparticle part but only anomalous parts. The intraband and interband conductivities are discussed with respect to magnetic fields and magnetic domain puddles. For large Zeeman fields the dynamical conductivities become independent of the density and are universal. The optical conductivity agrees well with the experimental values using screened impurity scattering and an effective Zeeman field. The universal value of Hall conductivity is shown to be modified due to the Zeeman field. The pseudospin current reveals an anomaly since a quasiparticle part appears though it vanishes for particle currents. The density and pseudospin response functions to an external electric field are calculated. A frequency and wave-vector range is identified where the dielectric function changes sign and the repulsive Coulomb potential becomes effectively attractive allowing Cooper pairing.

[1] Phys. Rev. B 94 (2016) 165415, Phys. Rev. B 92 (2015) 245425
[2] errata: Phys. Rev. B93 (2016) 239904(E), Phys. Rev. B 92 (2015) 245426

TT 99.17 Thu 15:00 Poster B

Dependence of structure factor and correlation energy on the width of electron wires — Vinod Ashokan[4], Renu Bala[5], •Klaus Morawetz[1,2,3], and Kare Narain Pathak[4] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

The structure factor and correlation energy of a quantum wire of thickness $b \ll a_B$ are studied in random phase approximation (RPA) and for the less investigated region $r_s < 1$. Using the single-loop approximation, analytical expressions of the structure factor are obtained. The exact expressions for the exchange energy are also derived for a cylindrical and harmonic wire. The correlation energy in RPA is found to be represented by $\epsilon_c(b, r_s) = \frac{\alpha(r_s)}{b} + \beta(r_s)\, ln(b) + \eta(r_s)$, for small b and high densities. For a pragmatic width of the wire, the correlation energy is in agreement with the quantum Monte Carlo simulation data.

[1] arXiv: 1708.06835

TT 99.18 Thu 15:00 Poster B

Universal short-time response and formation of collective mode — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck- Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The short-time response of two distinct systems, the pump and probe experiments with a semiconductor and the sudden quench of cold atoms in an optical lattice, are found to be described by the same universal function. This analytic formula at short time scales is derived from the quantum kinetic-theory approach observing that correlations need time to form. The influence of the finite-trapping potential is derived and discussed along with Singwi-Sjølander local-field corrections including the proof of sum rules. The quantum kinetic equation allows to understand how two-particle correlations are formed and how the

screening and collective modes are build up.
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[2] Phys. Rev. E 66 (2002) 022103
[3] Phys. Rev. E 63 (2001) 20102
[4] Phys. Lett. A 246 (1998) 311

TT 99.19 Thu 15:00 Poster B

Ultrafast collective response and possible photo-induced phase transition in the antiferromagnetic insulator Ca_2RuO_4 — •Parmida Shabestari[1,2], Hao Chu[1,2], Minjae Kim[1,2], Emily Huang[1,2], Maximilian Krautloher[1], Christopher Dietl[1], Joel Bertinshaw[1], Katrin Fürsich[1], Bernhard Keimer[1], and Stefan Kaiser[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Stuttgart, Germany

Among the diverse family of Ruthenates, the Antiferromagnetic Insulator Calcium Ruthenate, Ca_2RuO_4, has shown remarkable complexity in spin, orbital and phonons correlations. Raman Scattering [1] and Inelastic Neutron Scattering [2] experiments suggest strong spin-orbit coupling which manifests in the form of a complex Raman active Phonon, Magnon and collective Higgs mode responses. Utilizing ultrashort light pulses we are able to directly probe the interplay of these dynamics in time domain, disentangling the dynamics both in the ground state and possible light-induced metallic state, as a function of temperature and laser fluence.
[1] S. Souliou et al., Phys. Rev. Lett. 119, 067201 (2017)
[2] A. Jain et al., Nat. Phys. 13, 633 (2017).

TT 99.20 Thu 15:00 Poster B

Quantum correlation between two oscillators generated by non-local electron transport — •Felicitas Hellbach, Wolfgang Belzig, Fabian Pauly, and Gianluca Rastelli — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Since the realization of high quality superconducting microwave cavities one can envisage the possibility to investigate the coherent interaction of light and matter. We study two parallel quantum dots arranged in the geometry of an Aharonov-Bohm interferometer (ABI) with each dot linearly coupled to a local harmonic oscillator. We explore how quantum correlation and entanglement between the two oscillators is generated by the coherent transport of a single electron traveling in two different paths of the ABI. We calculate the covariance by use of a diagrammatic perturbative expansion (Keldysh Green's functions) to the fourth order in the dot-oscillator coupling constant, taking into account vertex corrections.

TT 99.21 Thu 15:00 Poster B

Readout sensitivity of mechanical motion in inductively coupled nano-electromechanical devices — •P. Schmidt[1,2,3], C. Utschick[1,2], D. Schwienbacher[1,2,3], L. Rosenzweig[1,2], N. Segercrantz[1,2], F. Deppe[1,2,3], A. Marx[1,2], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meißner-Institut, BAdW, Germany — [2]Physik-Department, TUM, Germany — [3]Nanosystems Initiative Munich, Germany

In recent years nano-electromechanics have demonstrated mechanical ground state cooling and the preparation of nonclassical states employing the linearized opto-mechanical interaction. However, the optomechanical coupling constant g_0 denoting the single photon - single phonon coupling rate has remained small compared to the cavity decay rate.

Here, we present an inductively coupled electromechanical system in contrast to the typically capactitively coupled mechanical elements. To this end, we place a dc-SQUID with a mechanical string resonator at the current anti-node of a superconducting microwave resonator. The electromechanical coupling is realized via the change of the SQUID loop area caused by the displacement of the string. Hereby, the coupling is increased as it is levered by the non-linear Josephson junctions of the dc-SQUID, approaching the resonator decay rate.

We focus on challenges related to the non-linearity of the microwave resonator. In particular, we compare the displacement noise of the thermal motion of the string resonator with the imprecision and the backaction noise imposed by the measurement.

TT 99.22 Thu 15:00 Poster B

Superconducting resonators for the study of Two-Level Systems — •Hartmut Schmidt[1], Alexander Bilmes[1], Jan Brehm[1], Shlomi Matityahu[2], Moshe Schechter[2], Alexander Shnirman[1], Georg Weiss[1], Alexey V. Ustinov[1,3], and Jürgen Lisenfeld[1] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Ben-Gurion University, Beer Sheva, Israel — [3]Russian Quantum Center, Moscow, Russia

Structural material defects, so called Two-Level Systems (TLS), received much recent interest due to their detrimental effect on various micro-structured quantum devices such as qubits, photon detectors and point contacts. In this work, we present superconducting lumped element resonators that enable one to resolve single TLS in deposited dielectric materials. We apply an electric field which, in addition to strain tuning by elastic chip deformation, permits us to manipulate the TLS' resonance frequency. This specific design allows us to study the TLS behavior under strain and external electric fields as well as to obtain the coupling-strength statistics of TLSs and their density. Especially, we study the resonator loss in presence of a TLS bath that is brought out of equilibrium via an electric-field sweep. We observe increased loss at intermediate sweep rates, which we explain by a theory based on Landau-Zener transitions.

TT 99.23 Thu 15:00 Poster B

Hybrid quantum circuits made of superconducting resonators and ferromagnetic magnons — •Tomislav Piskor[1], Marco Pfirrmann[1], Andre Schneider[1], Igor Golovchanskiy[2,3], and Martin Weides[1,4] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Moscow Institute of Physics and Technology, State University, 9 Institutskiy per., Dolgoprudny, Moscow Region, 141700, Russia — [3]National University of Science and Technology MISIS, 4 Leninsky prosp., Moscow, 119049, Russia — [4]Physikalisches Institut, Johannes Gutenberg University Mainz, Mainz, Germany

The field of Quantum Magnonics has evolved rapidly in the past few years. For example, for the growing field of quantum information, processing the coupling between natural spins and superconducting circuits is very promising for future implementations.

The aim of this work is to investigate the interaction between microwave photons in the GHz regime and magnetic spins. The coupling between superconducting resonators and ferromagnetic magnons will be investigated in order to study the hybrid system. Beside the Kittel mode showing the largest coupling strength, it is possible to observe weaker couplings, generated by magnetostatic spin waves. For periodic resonator structures, which is also the quantization condition, the spins can build up to propagating or standing spin waves. The coupling between the two systems is achieved by placing the ferromagnetic sample on top of the superconducting resonator structure.

TT 99.24 Thu 15:00 Poster B

Nonlocal thermoelectric effects in superconductor-ferromagnet hybrid structures — •Jonas Heidrich and Detlef Beckmann — Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

We report on our progress in experiments on nonlocal thermoelectric effects in superconductor-ferromagnet hybrid structures. In these samples thermoelectric effects are generated by the spin-dependent lifting of particle-hole symmetry. These latest efforts continue recent experiments [1].
[1] S. Kolenda *et al.*, Phys. Rev. Lett. **116**, 097001 (2016).

TT 99.25 Thu 15:00 Poster B

Electronic transport through quantum-dot spin valves - ISPI results — •Simon Mundinar, Stephan Weiss, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg

We study an interacting quantum dot coupled to ferromagnetic leads that introduce spin-dependent tunneling. We use a path integral approach to derive the tunneling current as functional derivative of the Keldysh partition function. The lead degrees of freedom are integrated out exactly and the on-dot interaction is decoupled via a Hubbard-Stratonovich transformation. The resulting Keldysh path sum is calculated using the technique of iterative summation of path integrals (ISPI) [1]. ISPI is based on the truncation of lead-induced correlations after a characteristic memory time. This method enables us to calculate the tunneling current through the system for different system parameters, such as gate/bias voltage, polarization, angle between the two leads' magnetizations and Coulomb interaction strength.
[1] S. Weiss, R. Hützen, D. Decker, J. Eckel, R. Egger, and M. Thorwart, Phys. Status Solidi B **250**, 2298 (2013)

TT 99.26 Thu 15:00 Poster B

Full counting statistics of electron transport through a negative-U Anderson impurity — •Eric Kleinherbers, Philipp Stegmann, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg

The process of electron tunneling through nanoscale systems (e.g. a metallic island or a quantum dot) is a stochastic process. Recent progress in nanotechnology has made it possible to monitor the transfer of individual electrons using sensitive electrometers (e.g. a quantum point contact). The resulting detector signal provides the full counting statistics (FCS) of the electron transport. A convenient tool to extract desired information out of the statistics are (generalized) factorial cumulants [1]. The sign of the cumulants reveals whether the transport of the electrons is statistically correlated or not.

Specifically, we focus on a single-level quantum dot with an *attractive* electron-electron interaction (negative -U Anderson impurity) subjected to a Zeeman field. Such a system has been observed in a recent experiment [2]. With FCS one can clearly differentiate between a repulsive and an attractive electron-electron interaction by analyzing the short-time limit [3] of the electron transport. Those differences are inaccessible by only measuring the net current or the current noise.

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[2] Cheng et al., Nature, 521, 196 (2015)
[3] P. Stegmann and J. König, Phys. Rev. B 94, 125433 (2016)

TT 99.27 Thu 15:00 Poster B

Probe independent mapping of electrostatic surface properties — Christian Wagner[1,2], •Niklas Friedrich[1,2,3], Pawel Chmielniak[4,5,2], Jeff Rawson[4,5,2], Taner Esat[1,2], Michael Maiworm[6], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich Aachen Reserach Alliance (JARA) - Fundamentals of Future Information Technology, Jülich, Germany — [3]CIC nanoGune, Donostia-San Sebastian, Spain — [4]Institute of Inorganic Chemestry, RWTH Aachen University, Germany — [5]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany — [6]Institut for Automation Engineering (IFAT), Otto-von-Guericke University Magdeburg, Germany

Mapping electrostatic surface properties with high spacial resolution, as well as high precision in the energy resolution is a desired goal in today's surface and interface physics. However, for many scanning probe techniques it remains unclear to which extend the probing mechanism itself influences the measurement. Here we demonstrate that scanning quantum dot microscopy (SQDM) [1,2] is a technique suited to overcome this problem. Using this technique we investigate a single PTCDA molecule on Ag(111). Independent of the tip-sample distance we measure its surface dipole moment to |p| = -624 ± 38 mD. Furthermore, we show that the imaging process does not depend on the LUMO energy of the molecule used as the quantum dot during SQDM imaging.

[1] C. Wagner et al. Phys. Rev. Lett. 115, 026101 (2015)
[2] M. Green et al. Japan. J. Appl. Phys. 55, 08NA04-7 (2016)

TT 99.28 Thu 15:00 Poster B

Finite-Frequency Noise of a Time-Dependently Driven and Interacting Quantum Dot — •Niklas Dittmann[1,2,3] and Janine Splettstoesser[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Germany — [2]Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [3]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Gothenburg, Sweden

We derive the current-noise spectrum stemming from a quantum dot weakly tunnel-coupled to a nearby electronic reservoir and driven by a time-dependent gate voltage. This experimentally relevant setup is frequently applied as an on-demand emitter of single electrons into a mesoscopic conductor. The presence of Coulomb interaction poses an additional challenge for a theoretical description. In this work, we extend a real-time diagrammatic technique to obtain the symmetric finite-frequency current noise. The derived noise spectrum reveals a rich interplay between different energy scales of this system, defined by the interaction strength, the tunnel-coupling strength, the temperature and the driving frequency. We discuss how the noise frequency probes features related to these energy scales.

TT 99.29 Thu 15:00 Poster B

Influence of the spin-polarized charge transport on the waiting time distribution in ferromagnet-quantum dot-superconductor systems — •Kacper Bocian and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

Based on the Markovian quantum master equation for the reduced density matrix we investigate the waiting time distribution of a single-level quantum dot (QD) system tunnel-coupled to the ferromagnetic (F) and/or superconducting (S) leads. Waiting times describe the delay times between the consecutive tunnelling events and carry the information about their dynamics. We compare the distributions of waiting times in different setups: F-QD-F, F-QD-S, and in the Cooper pair splitter geometry with two F and one S leads. By changing the spin-polarization of the ferromagnetic leads, the transition probabilities, and hence the waiting times, become modified. In the limiting case of the half-metallic leads all transitions can be blocked. We discuss the influence of presence of the superconductor on the waiting times and indicate the features of Cooper pair tunnelling. Furthermore, we analyze the impact of asymmetry of the couplings between the quantum dot and the external leads.

This work is supported by the National Science Centre in Poland as the Project No. DEC-2013/10/E/ST3/00213.

TT 99.30 Thu 15:00 Poster B

Non-spin-conserving effects in electronic transport through quantum dots — •Lucia Gonzalez[1,2], Jordi Pico[1], and Gloria Platero[1] — [1]Instituto de Ciencia de Materiales, CSIC, Cantoblanco, E-2 8049 Madrid, Spain — [2]Current affiliation: JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany

Pauli exclusion principle can lead to a spin dependant current blockade in a system of several quantum dots. This blockade is of great use for quantum manipulation and computation as it allows for spin-charge conversion, but non-spin-conserving processes can lift it by allowing the electrons to change its quantum numbers. Following previous research [1,2] on the effect in double quantum dots (DQD) of two of these processes, the hyperfine interaction and spin orbit coupling, we study theoretically their impact in transport in larger quantum dot systems.

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[2] N. Jouravlev, Yu. V. Nazarov, Phys. Rev. Lett. **96** (2006) 176804.

TT 99.31 Thu 15:00 Poster B

Correlation-induced refrigeration with superconducting single-electron transistors — •Rafael Sánchez — Universidad Autónoma de Madrid

The model of a superconducting tunnel junction is presented which refrigerates a nearby metallic island without any particle exchange. Heat extraction is mediated by charge fluctuations in the coupling capacitance of the two systems. The interplay of Coulomb interaction and the superconducting gap reduces the power consumption of the refrigerator. The island is predicted to be cooled down to temperatures close to 50 mK, for realistic parameters [1]. The results emphasize the role of non-equilibrium correlations in bipartite mesoscopic conductors. This mechanism can be applied to create local temperature gradients in tunnel junction arrays.

[1] R. Sánchez, Appl. Phys. Lett. 111, 223103 (2017).

TT 99.32 Thu 15:00 Poster B

Probing the interaction of single electron pumps using RF-SETs — •David Reifert[1], Niels Ubbelohde[1], Ralf Dolata[1], Vyacheslavs Kashcheyevs[2], Thomas Weimann[1], and Alexander Zorin[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig. Germany — [2]Faculty of Physics and Mathematics, University of Latvia, 25 Zellu street, LV-1002 Riga, Latvia

We utilize rf-driven semiconductor based quantum dots as single electron pumps (SEP). These SEPs transport a controlled number of n electrons per pump cycle and therefore create a precise quantized current $I = n \cdot e \cdot f$, where f is the pumping frequency. Since this current can achieve a high accuracy of 0.2 ppm, these SEPs can be utilized as a new primary standard for the unit ampere. To validate and improve the precision, we implemented an error counting scheme by operating several pumps in series and measuring the charge of the nodes in between them, with ultra-sensitive electrometers. For this purpose, we use semiconductor quantum dots, operating as single electron transistors (SET). To increase the measurement bandwidth, we applied rf-reflectometry, which allows us to read out the detector by analyzing the detuning of a LC-resonator due to the impedance change of the de-

tector. This measurement setup enables us to investigate the transfer probabilities of the pumps operated solo or in series, and lets us test for correlations and coupling between two pumps operated in series. This allows us to examine the mechanism of the coupling between several pumps which is necessary to further improve the precision.

TT 99.33 Thu 15:00 Poster B

Open system dynamics with energy-dependent tunnel couplings — •Jens Schulenborg[1], Maarten Wegewijs[2], and Janine Splettstoesser[1] — [1]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, Göteborg, Sweden — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany & JARA-FIT

A good theoretical understanding of the *dynamics* of tunnel-coupled electronic open nanosystems is crucial for the current strive towards controlled few-particle emission in the context of, e.g., metrology or quantum optics with electrons. However, while often experimentally relevant[1], most analytical studies on decay dynamics with strong local Coulomb interaction have so far neglected the energy structure of the tunnel barriers themselves, focussing only on the wideband limit.

Recently, we have shown the so-called *fermion-parity duality*[2] to be particularly insightful for such time-dependent problems. This work extends our approach to a general class of fermionic open systems with energy-dependent bare couplings in the Markovian, sequential tunneling limit. For the simplest relevant example of a spin-degenerate interacting single-level quantum dot, we show the duality to be similarly powerful as in the wideband limit. Even in an environment far away from equilibrium, it enables us to analyze the entire dot decay dynamics, including time-dependent particle- and energy current, in terms of simple-to-understand stationary equilibrium observables.

[1] J. D. Fletcher et al., Phys. Rev. Lett. **111**, 216807 (2013)
[2] J. Schulenborg et al., Phys. Rev. B **93**, 081411 (2016)

TT 99.34 Thu 15:00 Poster B

Investigation and application of propagating two-mode squeezed microwaves — •Minxing Xu[1,2], K. G. Fedorov[1,2], S. Pogorzalek[1,2], B. Ghaffari[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], E. Xie[1,2,3], A. Marx[1], F. Deppe[1,2,3], and R. Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

Josephson parametric amplifiers (JPAs) can be employed for the generation of itinerant quantum signals in the form of propagating two-mode squeezed (TMS) states, which are essential for quantum communication and sensing protocols with superconducting quantum circuits. In our work, we employ two flux-driven JPAs at the inputs of an entangling hybrid ring in order to generate two-mode squeezing between the hybrid ring outputs and investigate the resulting TMS states. In particular, we study the robustness of quantum entanglement and other nonclassical correlations, such as quantum discord, in the TMS states to external noise. Finally, we experimentally implement a remote state preparation protocol with an analog feed-forward using propagating squeezed states and determine detrimental effects of losses and noise on the protocol based on a theoretical model.

The authors acknowledge support from DFG through FE 1564/1-1.

TT 99.35 Thu 15:00 Poster B

Chains of nonlinear and tunable superconducting resonators — •M. Fischer[1,2,3], P. Eder[1,2,3], S. Pogorzalek[1,2], E. Xie[1,2,3], K. Fedorov[1,2], F. Deppe[1,2,3], A. Marx[1], and R. Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

We present theoretical predictions and characterization measurements of a quantum simulation system of the Bose-Hubbard-Hamiltonian in the driven dissipative regime in the realm of circuit QED. The system consists of series-connected, capacitively coupled, nonlinear and tunable superconducting resonators. The nonlinearity is achieved by galvanically coupled SQUIDs, placed in the current anti-node of each resonator and can be tuned by external coils and on-chip antennas.

The authors acknowledge support from the German Research Foundation through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, the IMPRS 'Quantum Science and Technology'.

TT 99.36 Thu 15:00 Poster B

Fabrication and Characterization of SQUID-Array Parametric Amplifiers — •Daniel Arweiler[1,2], Kirill G. Fedorov[1,2], Stefan Pogorzalek[1,2], Peter Eder[1,2,3], Michael Fischer[1,2,3], Edwar Xie[1,2,3], Achim Marx[1], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

In the rapidly evolving field of quantum information processing and circuit QED, Josephson parametric amplifiers (JPAs) have emerged as key building blocks. They consist of a coplanar waveguide resonator coupled to a dc superconducting quantum interference device (SQUID). The latter acts as flux-tunable nonlinearity enabling parametric effects, including quantum-limited amplification of weak signals and generation of squeezed microwave light.

In our work, we investigate advanced versions of JPAs with dc-SQUID arrays instead of a single dc-SQUID to enhance the dynamic range and 1-dB compression point. We employ the well-established technologies of electron-beam lithography and aluminium shadow evaporation to fabricate our samples. We characterize our JPAs at millikelvin temperatures using transmission microwave measurements with a network analyzer and conclude by comparing key properties such as gain and 1-dB compression point between various designs.

The authors acknowledge support from DFG through FE 1564/1-1.

TT 99.37 Thu 15:00 Poster B

Josephson vortex dynamics in nanoscale Josephson junction parallel arrays — •Micha Wildermuth[1], Amadeus Dieter[1], Yannick Schön[1], Martin Weides[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

One-dimensional parallel arrays of Josephson junctions are very interesting with respect to the rich dynamics inherent in this system. In quantum regime new physical phenomena are expected, which we aim to explore. The investigated system consists of several ultra-small Josephson junctions, which are arranged in parallel configuration forming an array of loops. We present preliminary measurements of such Josephson junction arrays, with novel I-V characteristics features.

TT 99.38 Thu 15:00 Poster B

Superconducting and insulating behaviour in granular aluminium oxide nano-wires — •Jan Nicolas Voss[1], Yannick Schön[1], Dominik Dorer[1], Micha Wildermuth[1], Sebastian T. Skacel[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

Granular aluminium oxide (AlOx) nano-wires are a promising alternative to Josephson tunnel junctions as a non-linear element in superconducting quantum circuits. Due to the internal structure, the sheet resistance of this material can be adjusted over a wide kOhm range [1]. Due to the high flexibility of this approach, we employ an electron beam lithography nano-fabrication process, with the intention of being used for highly coherent superconducting quantum circuits. The fabricated 20 nm wide nano-wires have a very clean interface to the sapphire substrate and no remaining fabrication residue in the vicinity of the circuit. Experimentally, we explore the phase transition from superconducting to insulating behavior in nano-wires with a length span between 50 nm and 1 μm.

[1] H. Rotzinger, S. T. Skacel, M. Pfirrmann, J. N. Voss, J. Müunzberg, S. Probst, P. Bushev, M. P. Weides, A. V. Ustinov and J. E. Mooij, Supercond. Sci. Technol. **30**, 025002 (2016)

TT 99.39 Thu 15:00 Poster B

Switching Current Distributions of Granular Aluminum micro-SQUIDs — •Felix Friedrich[1], Patrick Winkel[1], Hannes Seeger[1], Nataliya Maleeva[1], Christoph Sürgers[1], Ioan M. Pop[1], and Wolfgang Wernsdorfer[1,2,3] — [1]PHI, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]INT, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — [3]Institut Néel, CNRS, Grenoble, France

Granular aluminum (GrAl) is a strongly disordered superconductor consisting of nm-sized aluminum (Al) grains separated by aluminum oxide (AlO_x) tunnel barriers. The material shows both increased crit-

ical temperature and critical field compared to pure Al. Furthermore, its high kinetic inductance makes GrAl interesting for e.g. high inductance superconducting detectors or circuits [1]. In order to obtain a better understanding, we performed transport measurements in GrAl micro-SQUIDs and will present first results. We measure IV curves and analyze switching current distributions as a function of temperature, current sweep rate, as well as in- and out-of-plane magnetic field. Our micro-SQUIDs have loop areas in the order of 1 μm^2 and are interrupted by constrictions with a few 100 nm length and less than 100 nm width. We find strong deviation from the standard RCSJ-model that we try to relate to the granular nature of the junctions. As the grain size is much smaller than the junctions' dimensions, we expect Josephson junction arrays formed from the coupled Al/AlO_x grains to define the switching current modulation.
[1] H. Rotzinger, *et al.*, Supercond. Sci. Technol. 30, 025002 (2017)

TT 99.40 Thu 15:00 Poster B

Design considerations for a superconducting granular aluminum nano-wire qubit — •Yannick Schön[1], Jan Nicolas Voss[1], Sebastian T. Skacel[1], Alexander Stehli[1], Jochen Braumüller[1], Martin Weides[1], Hannes Rotzinger[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

At feature sizes of nano-meter scale, superconducting wires made from a material with a high normal conducting sheet resistance show a pronounced non-linear microwave response. If such a nano-wire is embedded in a self-resonating circuit, the non-linearity can be observed even at very low photon numbers. Unfortunately, these materials often show a rather high photon loss, which makes them unusable for long lived quantum circuits.

Granular aluminium is a new material for superconducting quantum circuits which features not only a very high kinetic inductance but also high quality factors. [1] To explore the potential of nanowires fabricated from granular aluminium, we propose a new type of superconducting qubit. Replacing the Josephson tunnel junction in a transmon qubit, the granular aluminium nano-wire is operated in a high-impedance Josephson weak-link regime. We present design considerations and preliminary measurements of first samples.
[1] H. Rotzinger, *et al.*, Supercond. Sci. Technol. **30**, 025002 (2016)

TT 99.41 Thu 15:00 Poster B

Fluxonium superconducting qubit using a granular aluminum superinductor — •Martin Spiecker[1], Lukas Grünhaupt[1], Nataliya Maleeva[1], Hannes Rotzinger[1], Alexey V. Ustinov[1,2], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

Superconducting quantum circuits have already shown several important milestones towards quantum information processing. An interesting subtype of superconducting qubits is the fluxonium. It consists of a Josephon junction shunted with a large 'super' inductance, which results in an offset charge insensitive qubit with an anharmonic level-structure. The superinductor is typically implemented using Josephson junction arrays. I will present an alternative path, based on the use of a high kinetic inductance material, namely granular aluminum.

TT 99.42 Thu 15:00 Poster B

Implementing an inductively shunted transmon qubit with tunable transverse and longitudinal coupling — •Sebastian T. Skacel[1], Nataliya Maleeva[1], Daria Gusenkova[1], Susanne Richer[2], David DiVincenzo[2], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We discuss some of the challenges in the physical implementation of an inductively shunted transmon qubit with flux-tunable transverse and longitudinal coupling to an embedded harmonic mode. The inductive shunt consists of a combination of compact, low-loss and linear inductances, in the range of several nH, and chains of Josephson junctions. The former could be realized by superconducting strips consisting of a high kinetic inductance material, granular aluminum, while the latter can be made from standard thin-film aluminum. The electrical connections between these different metallic layers could be realized using recently developed argon ion cleaning and contacting techniques which preserve the coherence of the circuit. The sample is enclosed in a 3D waveguide which offers the advantage of strong coupling for the resonator mode inside the designed pass band between 6 and 8 GHz, while the qubit mode can be efficiently decoupled from the microwave environment.

TT 99.43 Thu 15:00 Poster B

Investigation of a superconducting quantum metamaterial — •Jan David Brehm[1] and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Russian Quantum Center, National University of Science and Technology MISIS, Moscow 119049, Russia

Quantum metamaterials extend the idea of classical metamaterials to a regime where the quantum coherence of the meta-atoms exceeds the typical propagation time of an impinging wave through the medium. In recent works, it was proposed that this gives rise to various collective light-matter interaction effects such as selfinduced transparency, quasi-superradiant phase transitions and lasing. Superconducting qubits are strong candidates for an implementation of meta-atoms in the quantum regime because they feature well controllable properties, have subwavelength dimensions, and are known to have sufficiently long coherence times. First implementations of quantum metamaterials made of arrays of superconducting flux [1] and transmon [2] qubits were targeted at studying their collective interaction with a single mode of a microwave resonator. Here, we investigate a one-dimensional quantum material which consists of an array of transmon qubits coupled to a continuum of the light modes in a coplanar waveguide.
[1] P. Macha et al., Nature Commun. 5, 5146 (2014)
[2] K. V. Shulga et al., JETP Lett. 105, 47 (2017)

TT 99.44 Thu 15:00 Poster B

Local density of states in clean 2D SNS heterostructures — •Danilo Nikolic[1], Wolfgang Belzig[1], and Juan Carlos Cuevas[2] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain

The advent of 2D materials like graphene have reignited the interest in the study of the proximity effect in clean hybrid superconducting structures. Here, we present a systematic analysis of the local density of states in a clean 2D normal metal coupled to superconducting leads. By solving the Eilenberger equations in the framework of the quasiclassical theory of superconductivity, we are able to describe the impact in the Andreev bound state spectrum of these hybrid systems of, among others, a superconducting phase difference, a finite transmission of the interfaces or the presence of a weak magnetic field. Our results shed light on recent experiments on the Andreev bound states in graphene-based hybrid superconducting structures.
[1] L. Bretheau, J.I.J. Wang, R. Pisoni, K. Watanabe, T. Taniguchi, P. Jarillo-Herrero, Nature Physics, doi:10.1038/nphys4110 (2017)

TT 99.45 Thu 15:00 Poster B

Josephson junctions induced by strain in an individual few-layer $NbSe_2$ monocrystal — •Karl Enzo Kloss, Anh-Tuan Nguyen, Sofia Blanter, Paul Linsmaier, Christoph Strunk, and Nicola Paradiso — Institut für experimentelle und angewandte Physik, University of Regensburg

Superconducting transition metal dichalcogenides offer the opportunity to study superconductivity in the limit of clean 2D *monocrystals*. This opens the way to the study of phenomena that cannot be observed on bulk or disordered samples. One example is the impact of crystal distortions on the local superconducting order parameter. In this work we study the transport characteristics of few-layer $NbSe_2$ flakes with a crystal fold which divides them in two halves separated by a strained region. This latter may act as a weak link or as a strong barrier, depending on the crystal stress. The weak link corresponds to Josephson junction within the same monocrystal. This is confirmed by our finite-bias measurements in perpendicular field, which reveal a typical Fraunhofer pattern.

TT 99.46 Thu 15:00 Poster B

On unambigous quantum signatures in driven swept-bias Josephson junctions — •Harald Losert[1], Karl Vogel[1], and Wolfgang P. Schleich[1,2] — [1]Institut für Quantenphysik and Center for Integrated Quantum Science and Technology (IQ^{ST}), Universität Ulm, D-89069 Ulm — [2]Institute for Quantum Science and Engineering (IQSE), Department of Physics and Astronomy, Texas A&M University, College Station, TX 77843

Josephson junctions are one of the best examples for the observation of macroscopic quantum tunneling. In the case of a current-biased Josephson junction the phase difference behaves like the position of a particle in a tilted washboard potential. The escape of this phase-particle corresponds to the voltage switching of the associated junction. The escape from the potential can be explained by quantum tunneling from the ground state, or an excited state. However, it has been shown [1][2], that in the case of periodic driving the experimental data for quantum mechanical key features, e.g. Rabi oscillations or energy level quantization, can be reproduced by completely classical calculations.

Motivated by this discussion, we focus on the escape process in a swept-bias Josephson junction setup. We point out how a large or a small critical current of the junction affects the distinction between quantum and classical effects. In particular, we contrast the switching current distributions resulting from a quantum and a classical description of the time evolution in each case.

[1] Marchese*et al.*, *Eur. Phys. J. Special Topics* **147**, 333 (2007)
[2] Blackburn *et al.*, *Phys. Rev. B* **85**, 104501 (2012)

TT 99.47 Thu 15:00 Poster B

Reliability of different fabrication processes for window- and cross-type Nb/Al − AlO_x/Nb Josephson junctions — •F. Bauer, F. Zimmerer, A. Ferring, M. Wegner, S. Kempf, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Josephson tunnel junctions (JJs) are the basic element of many superconducting electronic devices such as SQUIDs or qubits. To allow for a successful and predictable operation of these devices, JJs having high quality and well-defined parameters are needed. The fabrication of window-type JJs is an often used approach to reliably produce such junctions. However, restrictions in alignment accuracy practically limits the junction size if not using advanced technologies such as e-beam lithography. Additionally, the overlap between the base electrode and the top wiring as well as the minimum junction size leads to constraints with respect to the junction capacitance and therefore to practical design parameters of SQUIDs and qubits. Both issues can be addressed by introducing a cross-type JJ fabrication process.

Within this context, we present different fabrication processes for Nb/Al − AlO_x/Nb based JJs. This includes not only our well-established, anodization-free fabrication process for window-type JJs but also different types of fabrication processes for cross-type JJs. We will compare all processes with each other by means of different figures of merit such as the ratio of subgap to normal resistance R_{sg}/R_n or the characteristic voltage $R_{sg}I_c$ and show that our JJs exhibit a very high quality.

TT 99.48 Thu 15:00 Poster B

Low frequency excess flux noise in dc-SQUIDs — •A. Ferring, S. Kempf, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Low frequency excess flux noise strongly impairs the performance of superconducting quantum devices (SQDs) such as SQUIDs and Qubits. It is, for example, the dominating mechanism causing decoherence in flux or phase Qubits and makes SQUID based measurements of low frequency signals rather challenging. But even though it has been extensively studied for many years, many open questions concerning its origin and properties remain. Recent experiments, for example, hint for surface adsorbates as a potential origin of noise contributions. It remains however unclear whether additional sources of low frequency excess flux noise exist. Therefore further investigations need to be done.

In this contribution, we first discuss a detailed study of low frequency excess flux noise in SQDs made of different materials like Nb, Al and PbIn, that hints for a material- and device-type dependence. We also show indications for a correlation between the $1/f$-noise amplitude of dc-SQUIDs and the dc-magnetization of the used insulating SiO_2 layer originating from magnetic contaminations introduced during the actual fabrication process. Finally, we present noise measurements on dc-SQUIDs having all Nb/Al-AlO_x/Nb Josephson Junctions but using washers made from different materials.

TT 99.49 Thu 15:00 Poster B

Optimal control pulses for a superconducting circuit with low anharmonicity — •Nicolas Wittler, Shai Machnes, and Frank Wilhelm-Mauch — Universität des Saarlandes, Saarbrücken, Deutschland

In order to perform specific operations on a superconducting quantum device with a desired fidelity, we investigate theoretical methods for shaping optimal control pulses of such systems. The 3D Transmon, a Josephson junction embedded in a microwave cavity, achieves a low sensitivity to charge noise, while retaining small, but sufficient anharmonicity, to allow for distinct transition frequencies. Because of this low anharmonicity, the difference in transition frequencies will be small, so that a pulse designed to drive a selected transition will also drive the neighboring transitions. Performing a desired quantum gate with a certain accuracy on the device requires driving pulses, that don't effect undesired transitions. With pulse shaping techniques such as **DRAG**[1] and **GOAT**[2], that engineer the frequency spectrum of a control pulse to suppress unwanted transitions, an increase in fidelity or shortening of the gate time can be achieved. The analytical method **DRAG** (**D**erivative **R**emoval by **A**diabatic **G**ate) presents an approach, where an initial pulse is shaped by adding its derivative with a suitable amplification factor to suppress certain transitions. **GOAT** (**G**radient **O**ptimization of **A**nalytic Con**T**rols) shapes pulses by numerically solving a differential equation for the control parameters, to find the optimial pulse.

[1] F. Motzoi *et al.*, Phys.Rev.Lett. 103 (2009) 110501,
[2] S. Machnes *et al.*, arXiv:1507.04261

TT 99.50 Thu 15:00 Poster B

Model Studies of High Fidelity Entangling Gates — •Joel Christin Pommerening and David DiVincenzo — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We study high-fidelity operations on two coupled superconducting qubits. We consider the cross-resonance gate, presenting a straightforward analytic derivation of its action based on the theory of Makhlin invariants.

Starting from an effective J coupling between the qubits, this derivation relies on a single rotating wave approximation to make the Hamiltonian time-independent in the frame that is rotating both qubits at the frequency of the cross-resonant drive. At that point no further frame or basis transformations are necessary, and the model can be solved exactly. A time evolution locally equivalent to a CNOT gate can then be found in multiple bases in the limit of small coupling strength J, and in one basis in particular for any J.

In practice the qubit basis is of course not arbitrary, but can be defined by the measurement basis or the basis in which single-qubit gates are applied. In this context we study how the (always-on) two-qubit coupling affects single-qubit measurements, and more specifically the measurement basis. In doing so we eventually seek to better understand the errors that arise from a possible mismatch between measurement and qubit basis.

TT 99.51 Thu 15:00 Poster B

Remote entanglement stabilization and distillation by quantum reservoir engineering — Didier Nicolas[2], •Jérémie Guillaud[1], Shyam Shankar[3], and Mazyar Mirrahimi[1] — [1]Inria Paris, Paris, France — [2]Rigetti Computing, Berkeley, USA — [3]Yale University, New Haven, USA

Quantum information processing protocols based on teleportation require highly entangled pairs of distant qubits as a primary resource. We present a new protocol that achieves an autonomous remote entanglement distillation using two-mode squeezed light as an imperfect source of entanglement. Two remote cavities are driven at distance using a three-wave mixing device that generates a two-mode squeezed light at resonance with the cavities. The autonomous distillation is performed through the local dispersive couplings of qubits to cavities and some additional local drives on the qubits. We will illustrate (numerically and analytically) how this protocol stabilizes a maximally entangled Bell state of the qubits regardless of the applied squeezing strength. We also study the robustness study of this reservoir engineering protocol in presence of various sources of imperfection and decoherence. This study is done through numerical simulations and systematic model reduction techniques such as adiabatic elimination of stable fast dynamics.

TT 99.52 Thu 15:00 Poster B

Effect of parasitic capacitances on Bloch oscillations measured via dual Shapiro steps — •Lisa Arndt, Fabian Hassler, and Ananda Roy — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Measurement of Bloch oscillations in a single Josephson junction in the

phase slip regime is a crucial element of metrology that links the current to the frequency standard. Bloch oscillations can be measured by applying a periodic drive to a DC-biased Josephson junction. Phase-locking between the two oscillations then gives rise to dual Shapiro steps. Unlike the normal Shapiro steps, a measurement of these dual Shapiro steps is impeded by parasitic capacitances. These parasitic capacitances can be screened by an on-chip superinductance. However, as the system is constantly driven, the energy has to be dissipated. To that end, we propose to add an additional large off-chip resistance. We investigate the resulting system by a set of analytical and numerical methods. We show that even in the presence of parasitic capacitances, it is possible to observe Bloch oscillations with realistic system parameters. In particular, we show that the leading effect of the parasitic capacitance is a reduction of the critical voltage of the phase slip junction by a factor of $\exp(-10\,\mathrm{k}\Omega/Z)$ where Z is the characteristic impedance formed by the parasitic capacitance and the superinductance.

TT 99.53 Thu 15:00 Poster B

Decoherence dynamics of the quantum Ising model in the strong coupling regime — •Hannes Weisbrich, Wolfgang Belzig, and Gianluca Rastelli — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

We study the decoherence dynamics of the 1D quantum Ising model within the framework of the Lindblad equation. We consider spins forming a 1D ring lattice uniformly coupled to a single bath via the spin component parallel to a transverse magnetic field. The system is analysed in the strong coupling regime in which the interaction strength is much larger than the transversal field, such that the spin chain has two degenerate ground states. We will focus on the dynamics between the ground states and the lowest excited states of the system. We find a decoherence free subspace as long as the dissipative coupling is parallel to the transverse magnetic field. Finally, we show that even if a more realistic model of non-uniform dissipative interaction is assumed, i.e. the local dissipation is uncorrelated with the rest of the ring, the decoherence free subspace is preserved due to parity conservation.

TT 100: Frustrated Magnets - Pyrochlore Oxides

Time: Thursday 15:30–18:00 Location: H 3005

TT 100.1 Thu 15:30 H 3005

Orientation Dependence of the Magnetic Phase Diagram of $Yb_2Ti_2O_7$ — •Steffen Säubert[1,2], Christopher Duvinage[1], Allen Scheie[3], Jonas Kindervater[3], Hitesh Changlani[3], Shu Zhang[3], Seyed Koohpayeh[3], Oleg Tchernyshyov[3], Collin Broholm[3,4,5], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, Germany — [3]Institute for Quantum Matter and Department of Physics and Astronomy, Johns Hopkins University, USA — [4]NIST Center for Neutron Research, National Institute of Standards and Technology, USA — [5]Department of Materials Science and Engineering, Johns Hopkins University, USA

The magnetic pyrochlore oxide $Yb_2Ti_2O_7$ received a lot of attention in recent years, as strong transverse quantum fluctuations significantly influence the system, and since the nature of its ground state is still under debate to host a spin liquid quantum state, i.e. quantum spin ice, at low temperatures. We report the orientation dependence of the magnetic phase diagram of $Yb_2Ti_2O_7$, inferred from magnetometry down to millikelvin temperatures, and further address the question of the ground state of $Yb_2Ti_2O_7$. The magnetic phase diagram for externally applied field shows an unusual field dependence of a first-order phase boundary, notably an applied field initially increases the ordering temperature when applied parallel to the crystalline $\langle 111\rangle$ or $\langle 110\rangle$ axes. This unusual field dependence is absent for field along $\langle 100\rangle$. The zero-field ground state was found to be of ferrimagnetic order, with spins slightly splayed away from one of the six $\langle 100\rangle$ directions.

TT 100.2 Thu 15:45 H 3005

The Magnetic Excitations in the Ground State of $Yb_2Ti_2O_7$ — •Viviane Peçanha-Antonio[1,2], Erxi Feng[1], Yixi Su[1], Franz Demmel[3], and Thomas Brückel[1,4] — [1]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstr. 1, D-85747 Garching, Germany — [2]Physik-Department, Technische Universität München, D-85747 Garching, Germany — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, United Kingdom — [4]Jülich Centre for Neutron Science (JCNS) and Peter Grünberg Institut (PGI), Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The nature of the zero-field ground state of $Yb_2Ti_2O_7$ remains an enigma within the pyrochlore titanate series. The disparate results are attributed to subtle changes in the sample stoichiometry, which seems to tune the magnetic order of different samples across a phase boundary. We report a study on the zero-field ground state of a powder sample of this pyrochlore. A sharp heat capacity anomaly at $T_c = 280$ mK is accompanied by a quasicollinear ferromagnetic order with a magnetic moment of $0.87(2)\mu_B$. Our high-resolution inelastic neutron scattering measurements show that, upon cooling, an inelastic continuum of excitations at ~ 0.6 is observed to persist from at least 2.5 K down to the lowest reached temperatures. Below T_c, the coexistence of sharp gapped low-energy magnetic excitations with a remnant quasielastic contribution evidences that spin fluctuations persist despite the long-range magnetic order.

TT 100.3 Thu 16:00 H 3005

Spin dynamics in the spin ice $Ho_2Ti_2O_7$ as measured by MIEZE spectroscopy — •Andreas Wendl[1], S. Säubert[1,2], C. Franz[2], P. Dharmalingam[3], A. Boothroyd[3], and C. Pfleiderer[1] — [1]Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [3]Clarendon Laboratory, University of Oxford, United Kingdom

In the cubic rare-earth pyrochlore $Ho_2Ti_2O_7$ the combination of a tetrahedral Ho-atom sub-lattice with strong local Ising anisotropies leads to a spin arrangement satisfying the spin ice rules at low temperatures [1]. At high temperatures the combination of crystal fields and phononic states creates rich physics: Thermally driven transitions of the ground state doublet deviate from an Arrhenius law [2] as phonon mediated spin-flipping becomes relevant[3]. Furthermore, crystal field transitions between excited states appear once these states are populated at sufficient temperatures [3,4]. We report a study of the high temperature spin flip excitations in $Ho_2Ti_2O_7$ employing the high-resolution neutron spin echo technique MIEZE. Our measurements provide unprecedented information on the spin dynamics measured over five magnitudes in time, thus allowing to close the gap between TAS [2,3] and NSE [2], and extending it towards lower momentum transfers. Our results agree with refs [2-4] and further confirm the single ion character of spin fluctuations.

[1] Gardner, Rev. Mod. Phys., **82**, 53 (2010)
[2] Ehlers, J Phys: Condens. Matter, **16**, S635 (2003)
[3] Ruminy, Phys. Rev. B, **95**(6), 60414 (2017)
[4] Ruminy, Phys. Rev. B, **94**(2), 24430 (2016)

TT 100.4 Thu 16:15 H 3005

Inverted hysteresis within the antiferromagnetic all-in-all-out state of the pyrochlore $Nd_2Hf_2O_7$ — •L. Opherden[1,2], T. Bilitewski[3], J. Hornung[1,2], T. Herrmannsdörfer[1], A. Samartzis[4,5], A. T. M. N. Islam[4], V. K. Anand[4], B. Lake[4,5], R. Moessner[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [4]Abteilung Quantenphänomene in neuen Materialien, HZB, Berlin, Germany — [5]Institut für Festkörperphysik, TU Berlin, Germany

We report the observation of an anisotropic and inverted hysteresis loop in the antiferromagnetic all-in-all-out ordered phase of $Nd_2Hf_2O_7$ having a negative remnant magnetization. The hysteresis emerges once exceeding a characteristic magnetic-field strength $H^\star(T)$ below the Neél temperature. The very unusual appearance of a negative remnant magnetization is observed for a field parallel to the [111] and [110] direction. However, for field parallel to [001] no hysteresis can be seen. For this orientation the projection of the field onto all four

local spin directions is equal and, hence, both realizations of the all-in-all-out state gaining equal Zeeman energy through a canting of their spins. We show further, that the underlying all-in-all-out phase is established in $Nd_2Hf_2O_7$ for temperatures below $T_N = 0.48$ K and persists up to fields of 0.27 T. We account for the inverted hysteresis in terms of a theory of uncompensated domain-wall spins of spherical domains forming inside a fully polarized single-domain state.

TT 100.5 Thu 16:30 H 3005

Spin dynamics of the ordered dipolar-octupolar pseudospin pyrochlore $Nd_2Hf_2O_7$ — •Alexandros Samartzis[1,2], Jianhui Xu[1], Vivek K. Anand[1], Nazmul A.T.M. Islam[1], Jacques Ollivier[3], and Bella Bella[1,2] — [1]Helmholtz-Zentrum Berlin — [2]Technical University Berlin — [3]Institut Laue-Langevin, Grenoble, France

The rare earth pyrochlore magnets have been extensively studied during the last decades due to their quintessential lattice for frustration which leads to exotic ground states with strong anisotropy. From this lattice the competition of crystal field, super-exchange and dipolar interactions can result in novel states, such as spin liquid, spin ice etc. The Nd^{3+} ion, on such a lattice has a Kramers doublet ground state with a 'dipolar-octupolar' wavefunction leading to a fascinating phase diagram. Here we report first results of inelastic scattering on a new Nd-based pyrochlore, $Nd_2Hf_2O_7$. Recent macroscopic measurements have revealed an ordered all-in - all-out AFM ground state with slow spin dynamics and a strongly reduced magnetic moment due to local fluctuations. Motivated by these interesting results, we performed low energy Inelastic Neutron scattering on a large single crystal grown by the floating zone technique. The results reveal a long range magnetic order below T=600mK. The excitations form a gapped flat band at energy DE 0.1meV reflecting the pinch-point pattern of a Coulombic phase. Above the flat band, collective dispersive excitations emerge from the pinch points. Linear spin-wave theory was used to determine the exchange parameters (Ja) applied in an appropriate Hamiltonian.

15 min. break.

TT 100.6 Thu 17:00 H 3005

Spin freezing in disordered pyrochlore magnets probed by NMR — Rajib Sarkar[1], •Felix Brückner[1], Jason W. Krizan[2], Robert J. Cava[2], and Hans-Henning Klauss[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, Germany — [2]Department of Chemistry, Princeton University, USA

The frustrated pyrochlore magnets $NaACo_2F_7$ ($A = Ca^{2+}, Sr^{2+}$) exhibit a mixed A-site with a random distribution of Na^+ and Ca^{2+}/Sr^{2+}. To investigate the effect of the resulting bond-disorder, we performed ^{23}Na and ^{19}F NMR experiments. While the Curie-Weiss temperature is ∼140 K (A = Ca) respective ∼ 130 K (Sr), the spin freezes at around 3 K, which gives high frustration indices of around 45. In fact, the ^{23}Na and ^{19}F broaden substantially below 3.6 K accompanied by a considerable reduction of the NMR signal intensity. A progressive slow-down of spin fluctuations is observed as per a BPP-like curvature of the ^{19}F spin-lattice relaxation rate. Eventually this ends up in a spin frozen state below 3.6 K in $NaCaCo_2F_7$. The hyperfine coupling to the magnetic moments increases significantly in this region. In addition to that, we present a simulation of ^{23}Na NMR spectra and compare it to results of a DFT calculation.

[1] Phys. Rev. B 89, 214401 (2014)
[2] Phys. Rev. B 95, 144414 (2017)
[3] R. Sarkar et al. (accepted in PRB)

TT 100.7 Thu 17:15 H 3005

Features of quantum spin ice in pyrochlore $Nd_2Zr_2O_7$ — •Jianhui Xu[1,2], A. T. M. Nazmul Islam[1], Owen Benton[3], Georg Ehlers[4], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan — [4]Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Magnetic pyrochlore oxides are intensively studied in the field of frustrated magnetism and the pyrochlores with Ising-anisotropic light rare earth are candidates for quantum spin ice. The recent studies on $Nd_2Zr_2O_7$ show that the single-ion ground state of Nd^{3+} is a well-isolated Kramers doublet with Ising anisotropy and the collective ground state is an antiferromagnetic order. Inelastic neutron scattering shows magnetic excitations containing a flat gapped ice-like mode and dispersive branches. The analyses based on spin wave theory indicate quantum moment fragmentation and yield a pseudospin-1/2 Hamiltonian which suggests quantum spin ice state above the ordering temperature (0.4K). Here we show that the extracted spin Hamiltonian gives a qualitative description of the macroscopic properties of $Nd_2Zr_2O_7$ based on mean-field and Monte Carlo simulations. We also present single-crystal inelastic neutron scattering data above T_N at 450mK and compare with the calculated spinon scattering.

TT 100.8 Thu 17:30 H 3005

Frozen state and persistent spin dynamics of new kagome compound $Fe_4Si_2Sn_7O_{16}$: A μSR and AC-susceptibility study — •S. Dengre[1], R. Sarkar[1], J.-C. Orian[2], C. Baines[2], L. Opherden[3], M. Uhlarz[3], T. Herrmannsdörfer[3], T. Söhnel[4], M.C. Allison[5], C.D. Ling[5], J. Gardner[6], and H.-H. Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01062 Dresden, Germany — [2]Laboratory for Muon-Spin Spectroscopy, PSI, 5232 Villigen PSI, Switzerland — [3]Dresden High Magnetic Field Laboratory, HZDR, D-01328 Dresden, Germany — [4]School of Chemical Sciences, UOA, Auckland 1142, New Zealand — [5]School of Chemistry, USYD Sydney 2006, Australia — [6]Australian Centre for Neutron Scattering, ANSTO, Menai 2234, Australia

We present the results of a new kagome compound $Fe_4Si_2Sn_7O_{16}$ as probed by bulk AC-susceptibility and μSR experiments. Zero field (ZF) μSR spectra shows the presence of two relaxation channels with faster and slower relaxation rates (λ_1, λ_2) respectively. A peak in both λ_1, λ_2 is observed in the temperature range of 2-3 K associated with the static magnetism. λ_1 exhibits a constant value below 1.5 K down to 270 mK indicating the presence of dynamic magnetism in the system. In AC-susceptibility, we observe a frequency dependent broad maximum which shifts from 3.5 K to 6 K (1.1 KHz). At low temperature below 0.15 K an upturn in the AC-susceptibility is evidenced. The combination of AC-susceptibility and μSR data suggests the presence of two relevant energy scales in $Fe_4Si_2Sn_7O_{16}$.

TT 100.9 Thu 17:45 H 3005

Magnetic semimetallic state in pyrochlore ruthenate $Cd_2Ru_2O_7$ — •Marian Blankenhorn[1], Tomohiro Takayama[2], Jürgen Nuss[2], Robert Dinnebier[2], Alexander Yaresko[2], and Hidenori Takagi[1,2] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

In pyrochlore oxides with the chemical composition $A_2B_2O_7$ strong geometrical frustration gives rise to interesting phenomena such as spin-ice behavior. Metallic pyrochlore oxides also show a variety of electronic phases including superconductivity in $Cd_2Re_2O_7$ and a metal-insulator transition (MIT) in $Tl_2Ru_2O_7$. While many Ru^{4+} pyrochlores have been intensively studied, only three Ru^{5+} pyrochlores, $A_2Ru_2O_7$ (A=Hg, Ca, Cd), are known so far. While $Ca_2Ru_2O_7$ remains metallic at low temperatures showing spin-glass behavior, $Hg_2Ru_2O_7$ undergoes a MIT at around 100 K. For $Cd_2Ru_2O_7$ the formation of a SDW was proposed based on a drop of magnetic susceptibility and an anomaly in resistivity but no detailed information is available. We obtained single crystals of $Cd_2Ru_2O_7$ by high pressure synthesis. Both magnetic susceptibility and resistivity exhibit a sharp drop at around 105 K. This transition accompanies a loss of carriers, indicating a low-carrier metallic state at low temperatures. The LDA + U band calculation suggests an antiferromagnetic semimetallic ground state with possibly all-in all-out magnetic order. We argue that $Cd_2Ru_2O_7$ displays a unique transition where magnetic order induces a coherent semimetallic state out of an incoherent paramagnetic bad-metal.

TT 101: Correlated Electrons: Other Materials

Time: Thursday 15:30–18:15 Location: HFT-FT 101

TT 101.1 Thu 15:30 HFT-FT 101

Proximity-induced spin-valley polarization in silicene or germanene on F-doped WS_2 — •Udo Schwingenschlögl, Shahid Sattar, and Nirpendra Singh — King Abdullah University of Science and Technology (KAUST), Physical Science and Engineering Division (PSE), Thuwal 23955-6900, Saudi Arabia

Silicene and germanene are key materials for the field of valleytronics. However, interaction with the substrate, which is necessary to support the electronically active medium, becomes a major obstacle. In the present work, we propose a substrate (F-doped WS_2) that avoids detrimental effects and at the same time induces the required valley polarization, so that no further steps are needed for this purpose[1]. The behavior is explained by proximity effects on silicene or germanene, as demonstrated by first-principles calculations. Broken inversion symmetry due to the presence of WS_2 opens a substantial band gap in silicene or germanene. F doping of WS_2 results in spin polarization, which, in conjunction with proximity-enhanced spin-orbit coupling, creates sizable spin-valley polarization.
[1] Phys. Rev. B **94**, 205415 (2016).

TT 101.2 Thu 15:45 HFT-FT 101

An optical study of the electrically driven insulator-metal transition in V_2O_3 — •Matthias Lange[1], Dennis Schwebius[1], Stefan Guénon[1], Yoav Kalcheim[2], Ilya Valmianski[2], Marcelo Rozenberg[2], Ivan K. Schuller[2], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut - Experimentalphysik II and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, D-72076 Tübingen — [2]Department of Physics and Center for Advanced Nanoscience, University of California - San Diego La Jolla, CA 92093, USA

The strongly correlated oxide V_2O_3 undergoes an insulator-metal transition (IMT) from a low-temperature antiferromagnetic insulating phase to a paramagnetic metallic phase at around 160 K, resulting in a several orders-of-magnitude change in resistivity. We investigated the electrical breakdown of a V_2O_3 thin film, grown by rf-sputtering on a r-cut sapphire substrate, by concomitantly measuring the electrical properties as well as the spatially resolved optical reflectivity. At temperatures near the IMT, the current voltage characteristics show jumps to lower voltages, indicating electrical breakdown of the insulating phase. Whether this electrically driven IMT is electric-field induced or caused by the creation of electro-thermal domains through Joule heating is in focus of recent research. The reflectivity measurement reveals that the breakdown is accompanied by a change in reflectivity, which can be attributed to the formation of spatially confined metallic filaments.

Work at UCSD supported by an MRPI and AFOSR grants.

TT 101.3 Thu 16:00 HFT-FT 101

Thermodynamics and transport properties of oxygen-deficient $EuTiO_3$ — •Johannes Engelmayer[1], Christoph Grams[1], Xiao Lin[1], Kamran Behnia[1,2], Joachim Hemberger[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Laboratoire Physique et Etude de Matériaux, PSL Research University, 75005 Paris, France

Various perovskite titanates $ATiO_3$ are known to undergo ferroelectric phase transitions, e.g., for $A = \mathrm{Ba, Pb, Cd}$. In contrast, $SrTiO_3$ shows quantum paraelectric behavior, that is, ferroelectric long-range order is suppressed by quantum fluctuations. A partial substitution of Sr with Ca ($Sr_{1-x}Ca_xTiO_3$) induces ferroelectricity. On the other hand, the insulating $SrTiO_3$ becomes metallic upon electron doping via oxygen deficiencies ($SrTiO_{3-\delta}$) and furthermore shows superconductivity for certain carrier concentrations. If both—Ca and electron doping—is combined ($Sr_{1-x}Ca_xTiO_{3-\delta}$), even a coexistence of ferroelectricity and superconductivity seems to be possible [1]. $EuTiO_3$ is a promising candidate for comparable phenomena, since Eu^{2+} and Sr^{2+} have the same ionic radii, which results in identical structural characteristics. However, Eu^{2+} has a large magnetic moment of $7\mu_B$, in contrast to nonmagnetic Sr^{2+}. Here, we present a detailed investigation of $EuTiO_{3-\delta}$ with $|\delta| \leq 10^{-2}$ based on thermodynamic and transport measurements.
[1] C. W. Rischau et al., *Nat. Phys.* **13**, 643 (2017)

TT 101.4 Thu 16:15 HFT-FT 101

The c-axis dimer and its electronic break-up: the insulator-to-metal transition in Ti_2O_3 — •chun-fu chang[1], thomas c. koethe[2], zhiwei hu[1], jonas weinen[1], stefano agrestini[1], jan gegner[2], holger ott[2], giancarlo panaccione[3], hua wu[4], maurits w. haverkort[5], holger roth[2], alexander c. komarek[1], francesco offi[6], giulio monaco[7], yen-fa liao[8], ku-ding tsuei[8], hong-ji lin[8], chien-te chen[8], arata tanaka[9], and liu hao tjeng[1] — [1]MPI CPfS, Dresden, Germany — [2]IOP II, Cologne, Germany — [3]TASC Laboratory, Trieste, Italy — [4]DOP, Shanghai, P.R. China — [5]Institute for Theoretical Physics, Heidelberg, Germany — [6]CNISM and DOS, Rome, Italy — [7]ESRF, Grenoble, France — [8]NSRRC, Hsinchu, Taiwan — [9]DOQM, ADSM, Hiroshima, Japan

We report on our investigation of the electronic structure of Ti_2O_3 using (hard) x-ray photoelectron and soft x-ray absorption spectroscopy. From the distinct satellite structures in the spectra we have been able to establish unambiguously that the Ti-Ti c-axis dimer in the corundum crystal structure is electronically present and forms an $(a_{1g})(a_{1g})$ molecular singlet in the low temperature insulating phase. Upon heating we observed a considerable spectral weight transfer to lower energies with orbital reconstruction. The insulator-metal transition may be viewed as a transition from a solid of isolated Ti-Ti molecules into a solid of electronically partially broken dimers where the Ti ions acquire additional hopping in the a-b plane via the e_g^π channel, the opening of which requires the consideration of the multiplet structure of the on-site Coulomb interaction.

TT 101.5 Thu 16:30 HFT-FT 101

Spin-polarized ballistic conduction through correlated Au-NiMnSb-Au heterostructures — Cristian Morari[3], •Wilhelm Appelt[1,4], Andreas Östlin[2], Ulrich Eckern[1], and Liviu Chioncel[2] — [1]Theoretical Physics II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]National Institute for Research and Development of Isotopic and Molecular Technologies, Cluj-Napoca, Romania. — [4]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We examine the ballistic conduction through Au-NiMnSb-Au heterostructures consisting of up to four units of the half-metallic NiMnSb in the scattering region, using density functional theory (DFT) in combination with dynamical mean-field theory (DMFT). For a single NiMnSb unit the transmission function displays a spin polarization of around 50% in a window of 1 eV centered around the Fermi level. By increasing the number of layers, an almost complete spin polarization of the transmission is obtained in this energy range. Supplementing the DFT calculations with local electronic interactions, of Hubbard-type on the Mn sites, leads to a hybridization between the interface and many-body states. The significant reduction of the spin polarization seen in the density of states is not apparent in the conduction electron transmission, which suggests that the hybridized interface and many-body induced states are localized.

15 min. break.

TT 101.6 Thu 17:00 HFT-FT 101

Orbital disproportionation of electronic density is a universal feature of alkali-doped fullerides — •Naoya Iwahara and Liviu Chibotaru — Theory of Nanomaterials Group, University of Leuven, Leuven, Belgium

Alkali-doped fullerides A_nC_{60} show a remarkably wide range of electronic phases in function of A = Li, Na, K, Rb, Cs and the degree of doping, n = 1-5. While the presence of strong electron correlations is well established, recent investigations give also evidence for dynamical Jahn-Teller instability in the insulating and the metallic phase of A_3C_{60} [1, 2]. To reveal the interplay of these interactions in fullerides with even n, we address the electronic phase of A_4C_{60} with accurate many-body calculations within a realistic electronic model including all basic interactions extracted from first principles [3]. We find that the Jahn-Teller instability is always realized in these materials too. More remarkably, in sharp contrast to strongly correlated A_3C_{60}, A_4C_{60} displays uncorrelated band-insulating state despite pretty similar in-

teractions present in both fullerides. Our results show that the Jahn-Teller instability and the accompanying orbital disproportionation of electronic density in the degenerate LUMO band is a universal feature of fullerides.

TT 101.7 Thu 17:15 HFT-FT 101

Doping and magnetic field induced spin gaps in spin chains explored by NMR — •Hans-Joachim Grafe[1], Yannic Utz[1], Franziska Hammerath[1,2], Lena Spillecke[1], Margarita Iakovleva[1], Evgeniya Vavilova[1], Vladislav Kataev[1], Tobias Ritschel[2], Jochen Geck[2], Chritian Hess[1], Livio Hozoi[1], Satoshi Nishimoto[1], Stefan-Ludwig Drechsler[1], and Bernd Büchner[1,2] — [1]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany

We present NMR measurements on the Heisenberg spin chain $SrCuO_2$ doped with Pd and Ni impurities [1], and on the frustrated edge-sharing $S = 1/2$ chain $LiCuSbO_4$ [2]. In $SrCuO_2$, the dopants cut the chains into segments which leads to strongly decaying spin lattice relaxation rates T_1^{-1} at low temperatures, indicating the opening of a spin gap. Thereby, it turned out that Ni is in a $S = 0$ state instead of a $S = 1$ state, which has been confirmed by x-ray absorption spectroscopy and quantum chemistry calculations. In $LiCuSbO_4$, we observe a strongly field dependent spin lattice relaxation rate at low temperatures: at magnetic fields below 13T, T_1^{-1} is dominated by a power-law increase, whereas above 13T, we observe a field induced spin gap-like decrease of T_1^{-1}. The former behavior is ascribed to diverging longitudinal spin correlations typical for a multipolar spin density wave liquid, whereas the latter is due to gapped transverse spin correlations characteristic for a spin-nematic liquid.

[1] Y. Utz et al., Phys. Rev. B 96, 115135 (2017)
[2] H.-J. Grafe et al., Scientific Reports 7, 6720 (2017)

TT 101.8 Thu 17:30 HFT-FT 101

Magnetic Properties and Spin Dynamics of Defects in Organic Spin Chain Systems as Probed by ESR Spectroscopy — •Julian Zeisner[1,2], Sylvain Bertaina[3], Olivier Pilone[3], Hervé Vezin[4], Olivier Jeannin[5], Marc Fourmigué[5], Bernd Büchner[1,2], and Vladislav Kataev[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]IFMP, TU Dresden, D-01069 Dresden, Germany — [3]Aix-Marseille Université, CNRS, IM2NP UMR7334, F-13397 Marseille, France — [4]LASIR, UMR-CNRS 8516, Université de Lille 1, F-59655 Villeneuve d Ascq, France — [5]ISCR, Université de Rennes 1, UMR-CNRS 6226, F-35042 Rennes, France

Defects in 1D spin systems continue to be an active field of solid state research as they are able to alter magnetic properties of the hosting materials drastically. In this work we studied the spin dynamics of defects in the spin chain compounds $(o\text{-DMTTF})_2X$ (X = Br, Cl) by means of ESR spectroscopy. Both materials exhibit spin-Peierls transitions at temperatures around 60 K, which allow a separation of the properties of defects inside the chains from the magnetic response of the spin chains. Temperature dependent CW ESR measurements evidence the evolution of spin dynamics from being governed by the spins in the chains at elevated temperatures to a low-temperature regime which is dominated by defects within the chains. Moreover, details of spin dynamics deep in the spin-Peierls phase were investigated by pulse ESR experiments which revealed Rabi-oscillations as well as anisotropic relaxation behaviour of the spins. We discuss the obtained results in terms of solitons localized at the defect sites.

TT 101.9 Thu 17:45 HFT-FT 101

Magnetic phase diagram and magneto-structural effects in tetra-$LiCoPO_4$ — •Changhyun Koo[1], Waldemar Hergett[1], Christoph Neef[1], Georg Bothmann[2], Anton Jesche[2], Alexander Tsirlin[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany. — [2]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

The magnetic phase diagram of a new $LiCoPO_4$ polymorph with tetrahedrally coordinated Co^{2+}-ions and $Pn2_1a$ symmetry is built-up based on magnetisation, thermal expansion, specific heat and muon spin rotation data. The system evolves long-range antiferromagnetic order at $T_N = 7$ K. The magnetic phase diagram shows a variety of competing antiferromagnetic phases. While the Weiss temperature is low, $\Theta \approx T_N$, our data imply large magnetostriction and anomalous contributions to the specific heat up ∼160 K. The presence of spin fluctuations up to $20T_N$ is further confirmed by μSR- and previously published NMR data. The nature of the complex magnetic phase diagram and of the spin fluctuation up to high temperatures will be discussed.

TT 101.10 Thu 18:00 HFT-FT 101

Competing phases in the model of Pr-based cobaltites — •Andrii Sotnikov and Jan Kuneš — Institute of Solid State Physics, TU Wien, Austria

Motivated by the physics of Pr-based cobaltites, we study the effect of the external magnetic field in the hole-doped two-band Hubbard model close to instabilities towards the excitonic condensation and ferromagnetic ordering. Using the dynamical mean-field theory we observe a field-driven suppression of the excitonic condensate. The onset of magnetically-ordered phase at the fixed chemical potential is accompanied by a sizable change of the electron density. This leads us to predict that Pr^{3+} abundance increases on the high-field side of the transition.

TT 102: Topology: Majorana Fermions

Time: Thursday 16:00–18:30 Location: A 053

TT 102.1 Thu 16:00 A 053

Structure and dynamics of Majorana states in hybrid superconducting nanowires — •Ivan Khaymovich[1,2], Alexander Kopasov[2], Jukka Pekola[3], and Alexander Mel'nikov[2,4] — [1]Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany — [2]Institute for Physics of Microstructures, Russian Academy of Sciences, 603950 Nizhny Novgorod, GSP-105, Russia — [3]Low Temperature Laboratory, Department of Applied Physics, Aalto University School of Science, P.O. Box 13500, FI-00076 Aalto, Finland — [4]Lobachevsky State University of Nizhny Novgorod, 23 Gagarina, 603950 Nizhny Novgorod, Russia

We perform a microscopic analysis of the inverse proximity effect in superconducting hybrid structures hosting Majorana bound states (MBS) as well as of the dynamic response of MBS in such systems. the critical temperature of the semiconducting nanowires with large g-factor and spin-orbit interaction, covered by a superconducting film and placed in a magnetic field H, is shown to be significantly reduced due to the presence of van Hove singularities in the wire and have a non-monotonic H-dependence attributed to the topological regime. Nonlocal AC response of a pair of MBS in a system with effective p-wave gap parameter is studied using a time-dependent Bogolubov-de Gennes equations. The time-dependent perturbations of transport excite finite period beating of the wave function between the MBS. We propose an experimental test to measure the characteristic time scales of quasiparticle transport through the pair of MBS defining, thus, quantitative characteristics of nonlocality attributed to MBS.

TT 102.2 Thu 16:15 A 053

Charge-response of the Majorana toric code — •Fabian Hassler and Ananda Roy — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

At zero temperature, a two dimensional lattice of Majorana zero modes on mesoscopic superconducting islands has a topologically ordered toric code phase. Recently, a Landau field theory has been proposed for the system that captures its different phases and the associated phase-transitions. It was shown that with the increase of Josephson tunneling between the islands, a continuous symmetry-breaking 3D-XY transition gets transformed into a discrete symmetry-breaking 3D-Ising transition through a couple of tricritical points and first order transitions. Using the proposed field theory, we analyze the charge-response of the system at the different continuous phase-transitions. We calculate the universal conductivity at the 3D-XY transitions and the change in the superconducting density at the Ising transition using 1/N expansion.

TT 102.3 Thu 16:30 A 053

Decaying spectral oscillations in a Majorana wire with finite coherence length — •Christoph Fleckenstein, Fernando Dominguez, Niccolo Traverso Ziani, and Björn Trauzettel — Institut für theoretische Physik, Universität Würzburg, Deutschland

Motivated by recent experiments, we investigate the excitation energy of a proximitized Rashba wire in the presence of a position dependent pairing. In particular, we focus on the spectroscopic pattern produced by the overlap between two Majorana bound states that appear for values of the Zeeman field smaller than the value necessary for reaching the bulk topological superconducting phase. The two Majorana bound states can arise because locally the wire is in the topological regime. We find three parameter ranges with different spectral properties: crossings, anticrossings and asymptotic reduction of the energy as a function of the applied Zeeman field. Interestingly, all these cases have already been observed experimentally. Moreover, since an increment of the magnetic field implies the increase of the distance between the Majorana bound states, the amplitude of the energy oscillations, when present, gets reduced. The existence of the different Majorana scenarios crucially relies on the fact that the two Majorana bound states have distinct k-space structures. We develop analytical models that clearly explain the microscopic origin of the predicted behavior.

TT 102.4 Thu 16:45 A 053

Majorana bound states in semiconducting carbon nanotubes - Part I (numerics) — •Magdalena Marganska[1], Lars Milz[1], Wataru Izumida[1,2], Christoph Strunk[3], and Milena Grifoni[1] — [1]Institute of Theoretical Physics, University of Regensburg, 93 053 Regensburg, Germany — [2]Department of Physics, Tohoku University, Sendai 980 8578, Japan — [3]Institute of Experimental and Applied Physics, University of Regensburg, 93 053 Regensburg, Germany

Considering the eminent usefulness which the Majorana states have for the field of quantum computing, their practical realization is eagerly awaited. The two best solid state candidates for Majorana hosts are the proximitized iron chains and proximitized semiconducting nanowires with spin-orbit coupling. The system which we investigate is a proximitized carbon nanotube, where the Majorana bound states arise through a physical mechanism similar as in the nanowire. The nanotube has however several advantages. First, it can be grown with minimal disorder. Second, due to its small size, it can be simulated numerically at the microscopic level. Finally, its tiny diameter reduces the number of relevant transverse modes to exactly one, with spin and valley degeneracy. We present here the results of numerical simulations of a proximitized nanotube, capturing the topological phase transition and the formation of Majorana states at the nanotube ends. We construct an effective analytical four-band model which allows us to analyze the system's symmetries and calculate a topological phase diagram, predicting the parameter ranges of chemical potential and magnetic field which hold the greatest promise for planned experiments.

TT 102.5 Thu 17:00 A 053

Majorana bound states in semiconducting carbon nanotubes - Part II (analytics) — •Lars Milz[1], Magdalena Marganska[1], Wataru Izumida[1,2], Christoph Strunk[3], and Milena Grifoni[1] — [1]Institut of Theoretical Physics, University of Regensburg, 93 035 Regensburg, Germany — [2]Department of Physics, Tohoku University, Sendai 980 8578, Japan — [3]Institute of Experimental and Applied Physics, University of Regensburg, 93 053 Regensburg, Germany

In this talk we present an effective two-band model Hamiltonian for superconducting carbon nanotubes, valid in the limit of small magnetic fields, which can be solved fully analytically. We will show the corresponding quasiparticle energy spectrum and the topological phase diagram for the bulk system. In the semi-infinite geometry we will demonstrate the presence of Majorana bound states in the topological non-trivial regions. The longitudinal component of the corresponding Majorana wave function has three contributions, one from the Γ-point and from each Fermi point. In order to obtain the full Majorana wave function we also include its transverse profile. Finally, we compare it with the wave function obtained by a numerical, real space tight-binding calculation.

15 min. break.

TT 102.6 Thu 17:30 A 053

Synthetic spin orbit interaction for Majorana devices — •Lauriane Contamin[1], Matthieu Desjardins[1], Matthieu Dartiailh[1], Laure Bruhat[1], Tino Cubaynes[1], Jeremie Viennot[2], François Mallet[1], Stanislas Rohart[3], André Thiaville[3], Audrey Cottet[1], and Takis Kontos[1] — [1]Laboratoire Pierre Aigrain, Ecole Normale Supérieure-PSL Research University, CNRS, Université Pierre et Marie Curie-Sorbonne Universités, Université Paris Diderot-Sorbonne Paris Cité, Paris, France — [2]JILA and Department of Physics, University of Colorado, Boulder, Colorado, USA — [3]3Laboratoire de Physique des Solides, Université Paris-Sud et CNRS, Orsay, France

The engineering of Majorana modes in condensed matter systems could allow one to study excitations with particle/antiparticle duality and non-abelian statistics. Most of the experimental setups with nanoscale circuits use nanowires with strong spin-orbit interaction connected to superconductors. Theoretical proposals have suggested inducing a spin-orbit coupling through a magnetic texture. In this work, we demonstrate experimentally such a platform using a single wall carbon nanotube as a conductor, which naturally exhibit few conduction channels. It is stamped over a magnetic gate and coupled to two superconducting electrodes. We observe subgap states in the conductance. A detailed study of their magnetic field evolution reveals a large synthetic spin-orbit energy. Furthermore, a robust zero energy state, the hallmark of localized Majorana modes, emerges at zero magnetic field.

TT 102.7 Thu 17:45 A 053

The influence of the non-locality of Majorana bound states on thesupercurrent — •Alexander Schuray[1], Alfredo Levy-Yeyati[2], and Patrik Recher[1,3] — [1]Institut für Mathematische Physik, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Departamento de Física Teórica de la Materia Condensada C-V, Condensed Matter Physics Center and Instituto Nicolás Cabrera, UAM, E-28049 Madrid, Spain — [3]LENA Braunschweig, D-38106 Braunschweig, Germany

The transport signatures of Majorana bound states (MBS), which emerge at the boundaries of one dimensional p-wave superconductors, have been in the center of many research activities. One of these proposed signatures is that the supercurrent in an s-wave-p-wave Josephson junction is blocked [1], if the considered superconductors are semi-infinite. However, recent experiments [2] and theoretical works [3,4] suggest that finite size effects need to be taken into account and that the second MBS can not always be neglected. We show analytically that the second MBS lifts the blockade of the supercurrent and that the resulting current carries information about the spin canting angle of the two MBS. We verify our analytical effective model numerically by using a tight-binding approximation for a spin orbit coupled nanowire in a magnetic field with proximity induced superconductivity.

[1] A. Zazunov and R. Egger, Phys. Rev. B **85**, 104514 (2012)
[2] M.T. Deng et al., Science **354**, 1557 (2016)
[3] A. Schuray et al., Phys. Rev. B **96**, 085417 (2017)
[4] E. Prada et al., Phys. Rev. B **96**, 085418 (2017)

TT 102.8 Thu 18:00 A 053

Transport properties of Coulomb blockaded T-junctions hosting Majorana bound states — •Johan Ekström[1], Patrik Recher[2], and Thomas Schmidt[1] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany

We study electron transport through a T-shaped nanowire junction hosting Majorana bound states (MBS). When the T-junction is in the topologically nontrivial regime it hosts three MBS at the ends of the wires and one MBS localized at the crossing point of the junction. For finite wire length, the MBS localized at the ends overlap with the MBS at the crossing point. It was found previously that such a setup can give rise to exotic transport processes such as double crossed Andreev reflections. In this work, we investigate the effect of Coulomb blockade and study the different transport processes due to the coupling between the MBS using a master equation in the sequential tunneling regime.

TT 102.9 Thu 18:15 A 053

Friedel-oscillations in inhomogeneous topological superconductors — •Lars Lauke[1,2], Mathias Scheurer[1,3], Andreas Poenicke[1,4], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Deutschland — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Deutschland — [3]Department of Physics, Harvard University, Cambridge MA 02138,

USA — [4]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe, Deutschland

In order to investigate Majorana bound states in p-wave superconductors and to reveal the precise influence of boundaries and inhomogeneities on the local structure of competing superconducting order parameters, we solve inhomogeneous Bogoliubov-de Gennes equations. Going beyond the quasi-classical approach we examine in particular the role of Friedel-oscillations due to inhomogeneities and the surface of the superconductor and analyse the distinct behaviour of the p-wave and the surface induced s-wave pairing amplitudes. We further discuss the observability of the local structure of the s-wave order parameter and the Majorana zero modes via scanning tunnelling microscopy.

TT 103: Superconductivity: Cryogenic Particle Detectors

Time: Thursday 17:15–18:30 Location: H 2053

Invited Talk TT 103.1 Thu 17:15 H 2053

From Fundamental Principles to Applications: Cryogenic Micro-Calorimeters — •Christian Enss, Sebastian Kempf, Loredana Gastaldo, and Andreas Fleischmann — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

Magnetic micro-calorimeters (MMCs) are state of the art cryogenic particle detectors which belong to the most sensitive devices to measure the energy of single quanta. They are composed of an absorber suited for the particles to be detected which is in close thermal contact with a paramagnetic temperature sensor. Together the two are coupled to a thermal bath through a weak thermal link. Fundamentally the energy resolution of such a detector is limited by thermal fluctuations between the absorber/sensor system and the thermal bath. Their universal applicability for particles and radiation as well as their high resolving power, broad bandwidth and linear response make them today a popular choice in many different experiments. Applications include X-ray spectroscopy, neutrino physics, material analysis, mass spectrometry and nuclear forensic. Currently, MMCs are used in several international projects like AMoRE, ECHo and SPARC. We will discuss the operating principle, the basic material science research behind their realization, the status of development and various recent applications.

TT 103.2 Thu 17:45 H 2053

Optimization of metallic magnetic calorimeter arrays with embedded ^{163}Ho for the ECHo experiment — •Federica Mantegazzini and the ECHo collaboration — Kirchhoff-Institute for Physics, Heidelberg University, Germany.

The ECHo experiment aims to determine the electron neutrino mass via the analysis of the calorimetrically measured electron capture spectrum of ^{163}Ho. The detector technology is based on metallic magnetic calorimeters (MMC) and the implantation of ^{163}Ho has been selected as method to enclose the source in the detectors, showing already good performances for activity values up to 1 Bq. Since the sensitivity of the ECHo experiment strongly depends on the total acquired statistics, the activity per pixel needs to be increased, taking into account two constraints: the resulting unresolved pile-up events fraction and the supplementary heat capacity due to the implanted ions. We have developed a novel experimental technique for the determination of the specific heat per ^{163}Ho ion, based on the simultaneous measurement of two MMC pixels with identical geometry which differ only because of the ^{163}Ho ions implanted in one of the two. At an operational temperature of 20 mK for an activity of about 1 Bq, the heat capacity increases of less than 3%. Therefore, a total activity of the order of 10 Bq per pixel - as required in order to keep the unresolved pile-up fraction under control - can be implanted without strongly affecting the detector performance. In this contribution, the development and the characterisation of the new microfabricated detector arrays is presented.

TT 103.3 Thu 18:00 H 2053

Microwave SQUID multiplexing of metallic magnetic calorimeters — •M. Wegner, D. Richter, F. Ahrens, L. Gastaldo, A. Fleischmann, S. Kempf, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

The most promising readout technique for large arrays of metallic magnetic calorimeters (MMCs) is microwave SQUID multiplexing (μMUXing), in particular since MMCs require a large bandwidth per channel. Each channel of a μMUX consists of a non-hysteretic rf-SQUID which is inductively coupled to a superconducting microwave $\lambda/4$ resonator. Due to the mutual inductance between SQUID and resonator and the flux dependence of the SQUID inductance, a signal in the MMC is transduced into a resonance frequency shift which can be detected by continuously monitoring the resonator transmission. By coupling many readout channels, each having a unique resonance frequency, to a common feedline, this technique allows for a simultaneous readout of hundreds of detectors.

In this contribution we present a full characterization of our state-of-the-art μMUX having 32 readout channels. By providing sufficient bandwidth per channel, we are able to resolve the fast intrinsic signal rise time of MMCs. The measured energy resolution is $\Delta E_{\mathrm{FWHM}} = 11\,\mathrm{eV}$. Based on the results of our comprehensive device characterization, we developed and fabricated a next-generation multiplexer chip. We will discuss our latest multiplexer design and will show our most recent experimental results.

TT 103.4 Thu 18:15 H 2053

On the interplay between kinetic inductance fraction and Kerr non-linearities in superconducting resonators for millimeter wave detection — •Francesco Valenti[1], Fábio Henriques[1], Nataliya Maleeva[1], Uwe Von Lüpke[1], Lukas Grünhaupt[1], Patrick Winkel[1], Sebastian T. Skacel[1], Alexander Bilmes[1], Alexey V. Ustinov[1,3], Florence Lévy-Bertrand[2], Alessandro Monfardini[2], and Ioan M. Pop[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institut Néel, CNRS and Université Grenoble Alpes, Grenoble, France — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

Following their proof-of-concept paper published in 2003, in the span of ten years Microwave Kinetic Inductance Detectors (MKIDs) found both widespread scientific interest in the superconducting electronics community and in technological applications as particle detectors. We explore the possibility of using Granular Aluminum (GrAl) with the goal of decreasing the Noise Equivalent Power (NEP) of the resulting MKIDS. One of the most attractive features of GrAl films is the wide-range tunability of the sheet resistance, which is in turn directly linked to the kinetic inductance. To exploit this resource we propose a theoretical model for the dependence of the NEP with the kinetic inductance fraction of the detector. We quantify the interplay between kinetic inductance fraction and non-linearities and we determine the kinetic inductance fraction value that gives the lowest NEP.

TT 104: Annual General Meeting of the Low Temperature Physics Division

Time: Thursday 18:45–20:00 Location: H 3005

TT 105: Focus Session: Mesoscopic Superconductivity and Quantum Circuits

The ongoing second wave of the quantum revolution has led to significant advances in complex quantum circuits. These circuits have not only demonstrated the basic building blocks for quantum information processing, but have also led to beautiful quantum optics experiments in the microwave frequency domain and atomic physics experiments using superconducting qubits as artificial atoms. This session covers the central advances by experimentalists and theorists working in the area of superconducting quantum circuits.

Organization: Gianluigi Catelani, Forschungszentrum Jülich; Denis Vion, CEA-Saclay; Martin Weides, Karlsruhe Institute of Technology

Time: Friday 9:30–13:05 Location: H 0104

Invited Talk TT 105.1 Fri 9:30 H 0104
New Hardware Components for Scalable Quantum Computers — •David DiVincenzo — Forschungszentrum Jülich

I introduce some new constructions for the optimal scaling of superconducting quantum processors.

Invited Talk TT 105.2 Fri 10:00 H 0104
Quantum Communcation with Propagating Microwaves — •Frank Deppe — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — Physik-Department, TU München, 85748 Garching, Germany — Nanosystems Initiative Munich (NIM), 80799 München, Germany

Due to the advent of superconducting architectures for quantum information processing, microwave frequencies have become a promising option for quantum communication and illumination. One prominent branch in the resulting line of research are continuous-variable propagating quantum microwaves. As opposed to discrete-variable (quantum-bit) based approaches, quantum information is encoded in a continuous degree of freedom such as space or momentum here. In this talk, I first introduce the fundamental concept of continuous-variable quantum systems in the context of superconducting circuits. Next,I summarize important milestones reached in the last years: generation and detection schemes, entanglement generation, displacement gate and finite-time correlations on single-mode squeezed and two-mode squeezed entangled microwave radiation. Finally, I discuss recent progress on the remote preparation of a squeezed microwave state.

Support is acknowledged from the German Research Foundation through FE 1564/1-1, the doctorate program ExQM of the Elite Network of Bavaria, the IMPRS 'Quantum Science and Technology'.

Invited Talk TT 105.3 Fri 10:30 H 0104
Dynamics of a Qubit While Simultaneously Monitoring its Relaxation and Dephasing — Quentin Ficheux[1,2], Sebastien Jezouin[2], Zaki Leghtas[2], and •Benjamin Huard[1,2] — [1]Ecole Normale Superieure de Lyon, France — [2]Ecole Normale Superieure, Paris, France

Measuring a spin-1/2 along one direction projectively maximally randomizes the outcome of a following measurement along a perpendicular direction. Here, using either projective or weak measurements, we explore the dynamics of a superconducting qubit for which we measure simultaneously the three components x, y and z of the Bloch vector.

The x and y components are obtained by measuring the two quadratures of the fluorescence field emitted by the qubit. Conversely the z component is accessed by probing an off-resonant cavity dispersively coupled to the qubit. The frequency of the cavity depends on the energy of the qubit and the strength of this last measurement can be tuned from weak to strong in situ by varying the power of the probe.

In this experiment, the tracked system state diffuses inside the Bloch sphere and performs a random walk whose steps obey specific rules revealing the backaction of incompatible quantum measurements. The associated quantum trajectories follow a variety of dynamics ranging from diffusion to Zeno blockade. Their peculiar dynamics highlight the non trivial interplay between the backaction of the two aforementioned incompatible measurements.

15 min. break.

Invited Talk TT 105.4 Fri 11:15 H 0104
Estimating the Error of an Analog Quantum Simulator by Additional Measurements — •Michael Marthaler — Theoretische Physik, Universität des Saarlandes — Institut für die Theorie der Kondensierten Materie, Karlsruher Institut für Technologie

We study an analog quantum simulator coupled to a reservoir with a known spectral density. The reservoir perturbs the quantum simulation by causing decoherence. The simulator is used to measure an operator average, which cannot be calculated using any classical means. Since we cannot predict the result, it is difficult to estimate the effect of the environment. Especially, it is difficult to resolve whether the perturbation is small or if the actual result of the simulation is in fact very different from the ideal system we intend to study. Here, we show that in specific systems a measurement of additional correlators can be used to verify the reliability of the quantum simulation. The procedure only requires additional measurements on the quantum simulator itself. We demonstrate the method theoretically in the case of a single spin connected to a bosonic environment.

Invited Talk TT 105.5 Fri 11:45 H 0104
On-demand distribution of quantum information between superconducting cavity quantum memories — •Wolfgang Pfaff — Department of Applied Physics, Yale University, USA — Microsoft Station Q, TU Delft, Netherlands

Superconducting cavities can store microwave fields for several milliseconds, naturally making them a promising system for realizing memories for superconducting circuits. In this talk, I will present our approach for using cavities for modular, distributed quantum computing.

Microwave cavities coupled to Josephson qubits can serve as long-lived quantum memories. In particular, 3D cavities made from bulk superconductors can store quantum states on millisecond time scales. Further, these systems are capable of processing and protecting quantum information encoded in complex multiphoton states stored in the cavity.

It is an ongoing challenge to scale up to large quantum computing architectures from individual cavity systems. We aim to realize a modular architecture in which individual nodes exchange quantum information through propagating photons in transmission lines. We show that we can, rapidly and on-demand, convert quantum states from a cavity memory into propagating channels. This enables us to realize deterministic quantum state transfer and entanglement between remote cavities. Our cavity system can thus serve as the backbone in a microwave quantum network. It can be used to realize error-protected distribution of quantum information and provides a route towards a modular quantum computer.

Invited Talk TT 105.6 Fri 12:15 H 0104
Quantum Simulation of Light-Matter Interaction — •Jochen Braumüller[1], Michael Marthaler[2], Andre Schneider[1], Alexander Stehli[1], Hannes Rotzinger[1], Martin Weides[1], and Alexey V. Ustinov[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

The quantum Rabi model describes the fundamental mechanism of light-matter interaction. It consists of a two-level atom or qubit coupled to a quantized harmonic oscillator mode via a transversal interaction. In the small coupling regime, it reduces to the well-known Jaynes-Cummings model by applying a rotating wave approximation (RWA). In the ultra-strong coupling (USC) regime, where the effective coupling strength is comparable to the subsystem energies, the RWA breaks down and remarkable features in the system dynamics are revealed. We demonstrate an analog quantum simulation of an effective quantum Rabi model in the ultra-strong coupling regime, achieving

a relative coupling ratio of up to 0.6. The quantum hardware of the simulator is a superconducting circuit. We observe fast and periodic quantum state collapses and revivals of the initial qubit state as one of the hallmark signatures of USC dynamics. As an outlook, we demonstrate first experimental efforts in implementing the spin boson model.
[1] Braumüller *et al.*, Nat. Commun. 8, 779 (2017)

TT 105.7 Fri 12:35 H 0104

Quantum Chemistry with Superconducting Qubits — •Nikolaj Moll[1], Stefan Filipp[1], Andreas Fuhrer[1], Jay M. Gambetta[2], Antonio Mezzacapo[2], and Kristan Temme[2] — [1]IBM Research – Zurich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland — [2]IBM T.J. Watson Research Center, Yorktown Heights, NY 10598, USA

Recent advances in the field of quantum computing have boosted the hope that one day we might be able to solve complex problems using quantum computers. Already smaller quantum processors with a couple of hundred physical qubits with no error correction will be available soon. Solving problems in quantum chemistry could benefit from such processors: Chemical systems could then be simulated and their properties, including correlation functions and reaction rates calculated. To calculate the ground states of chemical systems the quantum optimization based on the variational principle is especially suited. In this method, part of the computational load is transferred to the classical computer, while the complex trial wavefunctions are generated using entangling gates and single qubit rotations on the quantum processor. The advantage is that the calculation of the total energy can now be done efficiently using trial function of short depth and ideally run in much shorter time than the coherence time of the quantum processor.

TT 105.8 Fri 12:50 H 0104

Quantum microwaves with a DC-biased Josephson junction — •Fabien Portier, Ambroise Peugeot, Iouri Moukharski, Phillipe Joyez, Denis Vion, Daniel Estève, Patrice Roche, Carles Altimiras, Marc Westig, Max Hofheinz, and Olivier Parlavecchio — NanoElectronics and Quantronics groups, SPEC, CEA, CNRS, Université Paris-Saclay, CEA-Saclay, 91191 Gif-sur-Yvette Cedex, France

Tunneling of a Cooper pair through a dc-biased Josephson junction is possible if collective excitations (photons) are produced in the rest of the circuit to conserve the energy. The probability of tunneling and photon creation, well described by the theory of dynamical Coulomb blockade, increases with the coupling strength between the tunneling charge and the circuit mode, which scales as the mode impedance. Using very simple circuits with only one or two high impedance series resonators, we first show the equality between Cooper pair tunneling rate and photon production rate [1]. Then we demonstrate a blockade regime for which the presence of a single photon blocks the next tunneling event and the creation of a second photon. Finally, using two resonator with different frequencies, we demonstrate photon pair production [2], two-mode squeezing, and entanglement between the two modes leaking out of the resonators.
[1] M. Hofheinz et al., Phys. Rev. Lett. 106, 217005 (2011)
[2] M. Westig et al., arXiv:1703.05009 (2017)

TT 106: Complex Oxides: Bulk Properties, Surfaces and Interfaces (joint session TT/MA/KFM)

Time: Friday 9:30–13:00 Location: H 0110

TT 106.1 Fri 9:30 H 0110

Superconductivity in strontium titanate within the dielectric function method — •Serghei Klimin[1], Jacques Tempere[1], Jozef Devreese[1], Cesare Franchini[2], and Georg Kresse[2] — [1]TQC, Universiteit Antwerpen, Antwerpen, Belgium — [2]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria

Strontium titanate exhibits unique features which are not encountered in conventional polar crystals at the same conditions. It becomes a superconductor at unusually low carrier densities. $SrTiO_3$ is probably the only substance where superconductivity and optical absorption can be convincingly attributed to the Fröhlich-like electron-phonon interaction and polarons. In the present talk, we report on our theoretical studies of superconductivity in strontium titanate with a comparative discussion of different theoretical interpretations of superconductivity in $SrTiO_3$. It is demonstrated that the dielectric function method used in our works [1] adequately describes the superconducting phase transition using only parameters available from experiments and microscopic calculatuions. We are particularly focused on unusual isotope effect in $SrTiO_3$. It is shown that renormalization of optical-phonon frequencies following from the isotope substitution leads to an increase of the critical temperature within the dielectric function method.
[1] S. N. Klimin, J. Tempere, J. T. Devreese, and D. van der Marel, Phys. Rev. B **89**, 184514 (2014); J. Sup. Nov. Magn. **30**, 757 (2017).

TT 106.2 Fri 9:45 H 0110

Anisotropic Rashba-type spin-orbit coupling of the two-dimensional electron system in (110) $SrTiO_3$-based heterostructures — •Karsten Wolff, Roland Schäfer, Robert Eder, Matthieu le Tacon, and Dirk Fuchs — Karlsruhe Institute of Technology, Institute for Solid State Physics

The two-dimensional electron system in (110) $Al_2O_{3-d}/SrTiO_3$ heterostructures displays anisotropic electronic transport. Structured microbridges allow to probe 4-point resistivity along different crystallographic orientations, i.e. [001] and [1-10]. The conductivity and electron mobility along the [001] direction is largest, while differences in sheet carrier concentration are only minor. The measurements show anisotropic normal magnetotransport for $T < 30\,K$ which is correlated to the anisotropic mobility. For temperatures below 5 K transport is dominated by Rashba-type spin orbit interaction (SOI) which displays anisotropic behavior, too. SOI is found largest along the [001] direction.

TT 106.3 Fri 10:00 H 0110

Thermoelectric properties of $(SrXO_3)_1(SrTiO_3)_m$(001) superlattices, X=V, Mn and Ru — •Manish Verma, Benjamin Geisler, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

The thermoelectric properties of $SrTiO_3$ have been widely studied, primarily concerning the role of homogeneous bulk doping. However, the confinement realized in oxide superlattices may have a favorable effect on the thermoelectric properties. To this end we have investigated the electronic and thermoelectric properties of superlattices containing a monolayer of $SrXO_3$ (X=V, Mn and Ru) sandwiched between m=1,3 spacer layer(s) of $SrTiO_3$ (001) using a combination of density functional theory with an on-site Hubbard term and semi-classical Boltzmann theory. In all cases structural distortions containing octahedral tilts are energetically favored over tetragonal distortions and we explore their influence on the electronic and thermoelectric properties. Comparing the in-plane and out-of-plane transport properties we find no significant dependence on m for the in-plane transport properties. In turn on reduction of the $SrTiO_3$ thickness from m=3 to 1 enhances the dispersion along Γ-Z and thereby improves the out-of-plane thermoelectric properties. Funded by the DFG, CRC/TRR80 project G8.

TT 106.4 Fri 10:15 H 0110

Thermoelectricity close to a metal-insulator transition in ultrathin $LaNiO_3/LaAlO_3$(001) superlattices — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany

Transition metal oxides are a promising materials class for thermoelectric applications due to their chemical and thermal stability and environmental friendliness. Their thermoelectric response can be further improved by nanostructuring and reduced dimensionality. Here we explore the thermoelectric properties of $(LaNiO_3)_1/(LaAlO_3)_1$(001) superlattices near the confinement-induced metal-insulator transition by combining *ab initio* simulations including on-site Coulomb repulsion and Boltzmann theory. We find that the short-period vertical design strongly enhances the in-plane thermoelectricity owing to the Ni-site disproportionation, which is stabilized considerably by tensile epitaxial strain and octahedral tilting. The sensitivity of the system

to epitaxial strain provides an additional parameter to optimize the thermoelectric performance. For a $SrTiO_3(001)$ substrate, we predict room-temperature Seebeck coefficients and power factors that can compete with those of other oxide systems of current interest such as layered cobaltates. Comparison of the ultrathin superlattices with the metallic longer-period $(LaNiO_3)_3/(LaAlO_3)_3(001)$ case establishes the metal-insulator transition as a crucial mechanism to obtain a high thermoelectric response.

Funding by the DFG within TRR 80 (G3 and G8) is acknowledged.

TT 106.5 Fri 10:30 H 0110

Confinement-driven electronic and topological phases in corundum-derived oxide honeycomb superlattices — •Okan Koeksal and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg

On the basis of density functional theory calculations plus the Hubbard U interaction, we investigate electronic, magnetic and possibly topologically non-trivial phases in X_2O_3 honeycomb layers confined in the corundum structure α-Al_2O_3 (0001). Our results predict that the ground states for most of the systems of $X = 3d$ cations are trivial antiferromagnetic Mott insulators. If the symmetry of the two sublattices is imposed, the ferromagnetic phases of Ti, Mn, Co and Ni exhibit a characteristic set of four bands associated with the single occupation of e'_g (Ti) and e_g (Mn, Co, Ni) states. Moreover, the Dirac point can be tuned to the Fermi level by strain and a significant anomalous Hall conductivity arises when spin-orbit coupling (SOC) is switched on. A particularly strong SOC effect is identified for $X =$ Ti at $a_{Al2O3} = 4.81$ Å accompanied by an unusually high orbital moment of -0.88 μ_B nearly quenching the spin moment of 1.01 μ_B. The emergence of this orbital magnetism makes the realization of Haldane's model of spinless fermions possible. The extension of this work to the $4d$ and $5d$ series led to the identification of cases of high orbital moment (Os) or candidates for Chern insulators (CI), i.e. $X =$ Tc and Pt with C=-2 and -1, depending on the Coulomb repulsion strength. Support by the DFG within CRC/TRR80, project G3 is gratefully acknowledged.

TT 106.6 Fri 10:45 H 0110

Metal-Insulator Transition in Thin Films and Multilayers of Early Transition Metal Oxides from DFT+DMFT — •Sophie D. Beck and Claude Ederer — Materials Theory, ETH Zürich, Zurich, Switzerland

The wide variety of interesting phenomena and functionalities of complex oxide thin films and heterostructures is generally determined by a number of different factors, such as substrate-induced epitaxial strain, dimensional confinement, interface-related effects, or defects. Here, we systematically study the interplay between these effects in thin films and multilayers composed of materials such as correlated metals, Mott insulators and band insulators, using a combination of density functional theory (DFT) and dynamical mean-field theory (DMFT). In particular, we investigate the evolution of octahedral rotations across interfaces between two materials with different rotation angles and/or tilt systems, and how this affects the range of electronic reconstruction in the interfacial region. We then show that these effecs can give rise to phenomena such as metallic interfaces in multilayers of two Mott insulators $LaVO_3$ and $LaTiO_3$ up to a metal-insulator transition in the correlated metal $CaVO_3$, for which we find that both tensile strain or reduced film thickness can lead to a strong quasiparticle renormalization.

TT 106.7 Fri 11:00 H 0110

Dimensionality-driven metal-insulator transition in spin-oribt coupled $SrIrO_3$ — •Philipp Schütz[1], Domenico Di Sante[1], Lenart Dudy[1], Judith Gabel[1], Martin Stübinger[1], Martin Kamp[1], Yingkai Huang[2], Massimo Capone[3], Marius-Adrian Husanu[4], Vladimir Strocov[4], Giorgio Sangiovanni[1], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Röntgen Center for Complex Material Systems (RCCM), Universität Würzburg, Germany — [2]Van der Waals - Zeeman Institute, University of Amsterdam, Netherlands — [3]CNR-IOM-Democritos National Simulation Center and International School for Advanced Studies (SISSA), Italy — [4]Swiss Light Source, Paul Scherrer Institut, Switzerland

Upon reduction of the film thickness we observe a metal-insulator transition in epitaxially stabilized, spin-orbit coupled $SrIrO_3$ ultrathin films. By comparison of the experimental electronic dispersions with density functional theory at various levels of complexity we identify the leading microscopic mechanisms, i.e., a dimensionality-induced re-adjustment of octahedral rotations, magnetism, and electronic correlations. The astonishing resemblance of the band structure in the two-dimensional limit to that of bulk Sr_2IrO_4 opens new avenues to unconventional superconductivity by "clean" electron doping through electric field gating.

15 min. break.

TT 106.8 Fri 11:30 H 0110

Intrinsic defects effects to the electronic structure of Sr_2IrO_4 probed by scanning tunneling microscopy — •Zhixiang Sun[1], Jose M. Guevara[1], Ekaterina M. Pärschke[1], Steffen Sykora[1], Kaustuv Manna[1,2], Johannes Schoop[1], Andrey Malyuk[1], Sabine Wurmehl[1,3], Jeroen van den Brink[1], Bernd Büchner[1,3], and Christian Hess[1] — [1]IFW-Dresden, 01069 Dresden — [2]MPI-CPfS, 01187 Dresden — [3]Institute for Solid State Physics, TU Dresden

Due to its similarity to cuprates, there is tremendous interest on the possible superconducting ground-state in doped Sr_2IrO_4 (Ir214). Nevertheless, it has been found that doping of Ir214 is difficult. The mechanism of dopant induced insulator to metal transition (IMT) has not been fully clarified. We have carried out low temperature scanning tunneling microscopy/spectroscopy experiments on Ir214 crystals. Several different types of intrinsic defects have been identified and their effects to the local electronic structure have been probed. We noticed that for the apical oxygen site defects, their effects are spatially very localized (< 2 nm). Also on the spectra taken on top of these defects, in gap states with a charge transfer like behavior are observed. With a local defect model we simulated the spectra, which gives good a match with the results. Our results provide important observations on the effects of individual defects on the local electronic properties. This is crucial for further tailoring the electronic structure of Ir214. Furthermore, they can also facilitate the understanding of the general mechanism of IMT in Mott insulators.

TT 106.9 Fri 11:45 H 0110

Novel insights into the impurity-selective metal-insulator transition of paramagnetic V_2O_3 — •Frank Lechermann[1], Noam Bernstein[2], Igor Mazin[2], and Roser Valenti[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstr. 9, D-20355 Hamburg, Germany — [2]Code 6393, Naval Research Laboratory, Washington, DC 20375, USA — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

The phase diagram of V_2O_3 with temperature and concentration of different dopants (e.g. Cr and Ti), still poses a formidable problem in condensed matter physics. By means of the charge self-consistent combination of density functional theory with dynamical mean-field theory, i.e. the DFT+DMFT approach, we provide new clues to the delicate interplay between electronic and lattice degrees of freedom. The impact of the defect chemistry is highlighted beyond the sole lattice expansion/contraction affect usually associated with impurity doping in this system. Local symmetry breakings are identified as one key feature to understand the tight competition between metal and insulator in vanadium sesquioxide.

TT 106.10 Fri 12:00 H 0110

Growth and characterization of *Pmnb*-Li_2FeSiO_4 single crystals — •Waldemar Hergett[1], Christoph Neef[1], Hubert Wadepohl[2], Hans-Peter Meyer[3], Mahmoud Abdel-Hafiez[4], and Rüdiger Klingeler[1,5] — [1]Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany — [2]Institute of Inorganic Chemistry, Heidelberg University, Heidelberg, Germany — [3]Institute of Earth Sciences, Heidelberg University, Heidelberg, Germany — [4]Institute of Physics, Goethe University, Frankfurt, Germany — [5]Center for Advanced Materials, Heidelberg University, Heidelberg, Germany.

Li_2FeSiO_4 single crystals featuring the high temperature *Pmnb* phase were grown by the high-pressure optical floating zone method. The resulting single crystals have been characterized by means of polarised-light and electron microscopy, EDX, powder and single crystal X-ray diffraction. The impact of the growth parameters and of the applied pressure on the crystal quality was investigated. The single crystal structure of the *Pmnb*-polymorph was solved for the first time. It exhibits layers of corner-sharing FeO_4- and SiO_4-tetrahedra in the crystallographic *ac*-planes which alternate with layers of LiO_4-tetrahedra.

Magnetisation and specific heat studies confirm the high quality of the crystals and show a sharp λ-like anomaly associated with the onset of long-range antiferromagnetic order at $T_N = 17\,K$.

TT 106.11 Fri 12:15 H 0110

Excitonic dispersion of intermediate-spin state in $LaCoO_3$ revealed by resonant inelastic X-ray scattering — •Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1], Federica Frati[2], Jun Okamoto[3], Hsiao-Yu Huang[3], Amol Singh[3], Di-Jing Huang[3], Keisuke Tomiyasu[4], Chao-Hung Du[5], Frenk M. F de Groot[1], and Jan Kuneš[2] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]Inorganic Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, The Netherlands — [3]Condensed Matter Physics Group, National Synchrotron Radiatiation Research Center, Taiwan, — [4]Department of Physics, Tohoku University, Sendai, Japan — [5]Department of Physics, Tamkang University, New Taipei City, Taiwan,

We perform Co L-edge resonant inelastic X-ray scattering of $LaCoO_3$ at 20 K. We observe a dispersive state with an energy shift from 480 to 290 meV as a function of momentum from $\boldsymbol{q}$ = (0, 0, 0.26π) to $\boldsymbol{q}$ = (0, 0, 0.90π). This dispersion is attributed to the mobility of the intermediate-spin (IS) state, which is viewed as an exciton. A theoretical calculation considering the excitonic dispersion of the IS state on the background of the low-spin (LS) state supports the interpretation. The present result suggests that the mobility pushes the IS state into play to the thermal spin-state transition of $LaCoO_3$ in addition to the (immobile) high-spin and LS states with lower atomic-multiplet energies, as suggested by recent theoretical studies [1].

[1] A. Sotnikov and J. Kuneš, Sci. Rep. 6, 30510 (2016).

TT 106.12 Fri 12:30 H 0110

Electronic signature of the vacancy ordering in NbO (Nb_3O_3) — Anna K. Efimenko[1], Nils Hollmann[1], Katharina Hoefer[1], Jonas Weinen[1], Daisuke Takegami[1], Klaus K. Wolff[1], Simone G. Altendorf[1], Zhiwei Hu[1], A. Diana Rata[1], Alexander C. Komarek[1], Agustinus Nugroho[2], Yen-Fa Liao[3], Ku-Ding Tsuei[3], H. H. Hsieh[4], H. -J. Lin[3], C. T. Chen[3], Liu Hao Tjeng[1], and •Deepa Kasinathan[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Insitiut Teknologi Bandung, Bandung, Indonesia — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Chung Cheng Institute of Technology, Taoyuan, Taiwan

We investigated the electronic structure of the vacancy-ordered 4d-transition metal monoxide NbO (Nb_3O_3) using angle-integrated soft- and hard-x-ray photoelectron spectroscopies as well as ultra-violet angle resolved photoelectron spectroscopy. We found that density-functional-based band structure calculations can describe the spectral features accurately provided that self-interaction effects are taken into account. In the angle-resolved spectra we were able to identify the so-called vacancy band that characterizes the ordering of the vacancies. This together with the band structure results indicates the important role of the very large inter-Nb-4d hybridization for the formation of the ordered vacancies and the high thermal stability of the ordered structure of niobium monoxide.

TT 106.13 Fri 12:45 H 0110

Ultrahigh-resolution Resonant Inelastic X-ray Scattering from rare-earth nickelates: magnetic and dd-excitations — •Katrin Fürsich[1], Yi Lu[1], Davide Betto[2], Georg Christiani[1], Giniyat Khaliullin[1], Maurits W. Haverkort[3], Eva Benckiser[1], Matteo Minola[1], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]European Synchrotron Radiation Facility, Grenoble — [3]Institut für Theoretische Physik, Universität Heidelberg

Rare-earth nickelates ($RNiO_3$) have been subject to intense investigation, mostly because of the rich phase diagram comprising a sharp temperature-driven metal-to-insulator transition, an unusual antiferromagnetic ground state, and the prospect of mimicking the physics of high-T_c superconducting cuprates in orbitally engineered heterostructures. We have studied $RNiO_3$ thin-films and superlattices using ultrahigh-resolution resonant inelastic x-ray scattering (RIXS) at the Ni L_3 edge. Below the magnetic ordering temperature, we observe well-defined collective magnon excitations. Our experimental observation provides for the first time a solid basis for the theoretical description of the magnetism in $RNiO_3$. In addition to magnetic excitations, we investigated the electronic excitations of $RNiO_3$ as a function of temperature and tolerance factor, i.e. rare-earth radius. A sophisticated analysis based on an advanced double-cluster model gives intriguing insight into the microscopic and electronic structure of $RNiO_3$. Our study reveals that RIXS is an excellent technique to quantitatively characterize different ordering phenomena within one material.

TT 107: Focus Session: Spinorbitronics - From Efficient Charge/Spin Conversion Based on Spin-Orbit Coupling to Chiral Magnetic Skyrmions III (joint session MA/TT)

Time: Friday 9:30–12:45 Location: H 1012

Invited Talk TT 107.1 Fri 9:30 H 1012

Manipulation of interface-induced Skyrmions studied with STM — •Kirsten von Bergmann — University of Hamburg, Germany

Isolated magnetic skyrmions are envisioned as the basis for future spintronic devices. They can be stabilized by a favorable interplay of magnetic exchange, Dzyaloshinskii-Moriya interaction (DMI), anisotropy and Zeeman energy. The Fe/Ir(111) interface is known to exhibit strong DMI [1] and serves as an ideal basis to build up materials that host single skyrmions on the nanometer length scale. Such small magnetic objects can be imaged, characterized and manipulated using (spin-resolved) scanning tunneling microscopy (STM) [2].

Building upon the Fe/Ir(111)-interface a fine-tuning of the relevant magnetic energies is performed by adding metallic overlayers, by adsorption of hydrogen, or by a variation of the strain within the magnetic film. Magnetic field dependent STM measurements can be used to obtain the specific material parameters [3]. In addition, spectroscopy using a non-magnetic tip electrode reveales the correlation between the local magnetoresistance and the non-collinearity of the spin texture [4]. Such a read-out of the local magnetic state could be combined with the demonstated reversible switching between skyrmion and ferromagnet by local electric fields [5].

[1] Heinze et al., Nature Phys. 7, 718 (2011). [2] von Bergmann et al., J. Phys.: Condens. Matter 26, 394002 (2014). [3] Romming et al., Phys. Rev. Lett. 114, 177203 (2015). [4] Hanneken et al., Nature Nanotech. 10, 1039 (2015). [5] Hsu et al., Nature Nanotech. 12, 123 (2017).

TT 107.2 Fri 10:00 H 1012

anisotropic DMI and micromagnetics of antiskyrmions — •Lorenzo Camosi[1], Olivier Fruchart[2], Stefania Pizzini[1], Stanislas Rohar[3], and Jan Vogel[1] — [1]Institut Néel , CNRS , Grenoble, France — [2]INAC-SPINTEC, CNRS, CEA, Grenoble, France — [3]LPS , CNRS , Orsay , France

A review of our pioneer works for understanding the Antiskyrmions physics in ultrathin magnetic layers is presented. They are topological chiral solitons that may be stabilized when the circular symmetry of the spin configuration is broken due to the inversion of the chirality between perpendicular directions.

In the first part of the talk we explain the relationship between crystal and Dzyaloshinskii-Moriya interaction (DMI)symmetry. Moreover the particular case of anisotropic dmi in ultrathin epitaxial Au/Co/W(110) is presented.

In the second part we show a combined analytical and numerical micromagnetic study of the equilibrium energy, size and shape of antiskyrmionic magnetic configurations. Anti-skyrmions and skyrmions are compared in systems with the same strength of magnetic interactions. We show that in the presence of dipolar interaction energy of the anti-skyrmion is strongly reduced and its equilibrium size increased with respect to the skyrmion.

TT 107.3 Fri 10:15 H 1012

Skyrmions like it Hot - Temperature Dependence of the Skyrmion Hall Effect — •Kai Litzius[1,2,3], Pedram Bassirian[1], Jonathan Leliaert[4], Sascha Kromin[1], Jakub Zazvorka[1], Ivan

Lemesh[5], Nico Kerber[1,2], Alexandra Churikova[5], Daniel Heinze[1], Niklas Keil[1], Markus Weigand[3], Gisela Schütz[3], Geoffrey S. D. Beach[5], and Mathias Klaeui[1,2] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [2]Graduate School of Excellence Materials Science in Mainz, 55128 Mainz, Germany — [3]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [4]Department of Solid State Sciences, Ghent University, Krijgslaan 281-S1, B-9000 Ghent, Belgium — [5]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA

Magnetic skyrmions are topologically stabilized nanoscale spin structures that show promise for future spintronic devices. It was found very recently that during their dynamics a sizeable skyrmion Hall angle (SkHA) occurs that surprisingly depends on the skyrmion velocity. [1,2] Different theoretical models have been put forward for the creep [2] and viscous flow [1] regime. By X-ray microscopy, we investigate reproducible skyrmion trajectories at varying temperatures. We find that the angle is independent of the temperature when plotted against the skyrmion velocity and identify two different mechanisms that lead to distinctly different spin Hall angles in the creep and the flow regimes. References: [1] K. Litzius et al., Nat. Phys. 13, 170-175 (2017). [2] W. Jiang et al., Nat. Phys. 13, 162-169 (2017).

TT 107.4 Fri 10:30 H 1012

Bi-stable skyrmion states in Pt/Co/Ir multilayer nanodots as a switchable information memory — •Mateusz Zelent[1], Michał Mruczkiewicza[2], Jaroslav Tóbik[2], Konstantin Guslienko[3,4], and Maciej Krawczyk[1] — [1]Faculty of Physics, Adam Mickiewicz University in Poznan, Poznan, Poland — [2]Institute of Electrical Engineering, Slovak Academy of Sciences, Bratislava, Slovakia — [3]Depto. Fisica de Materiales, Universidad del País Vasco, UPV/EHU, San Sebastian, Spain — [4]IKERBASQUE, the Basque Foundation for Science, Bilbao, Spain

The magnetic skyrmion stability was studied numerically in circular Pt/Co/Ir multilayer stacks with perpendicular magnetic anisotropy and interface Dzyaloshinskii-Moriya interaction (DMI). We have found bi-stable system which can be found in one of the two distinct skyrmion states differing in the skyrmion radius. We demonstrated that two skyrmions can be stabilized due to the different mechanism, primary DMI or primary magnetostatic interaction, leading to small and large size skyrmions, respectively. We developed a technique to compute the total energy of magnetic configurations as a function of the skyrmion diameter, which allows us to estimate the potential barrier between stable states and to explain the influence of dipolar energy contribution on bi-stable skyrmion formation in multilayer dot systems and skyrmion formation in general. Our result can open a new route to develop an efficient skyrmion based memory, with information bit coded as a skyrmion's size. Funded from the EU Horizon 2020, G.A. No. 644348.

TT 107.5 Fri 10:45 H 1012

Skyrmion lifetimes in exchange frustrated ultrathin films — •Stephan von Malottki[1], Pavel Bessarab[2], Anna Delin[3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel — [2]School of Engineering and Natural Sciences - Science Institute, University of Iceland — [3]Department of Applied Physics, School of Engineering Sciences, KTH, Kista

The thermal stability of magnetic skyrmions is a key issue for potential applications in spintronic devices. An Arrhenius law can be used to describe the skyrmion lifetime as a function of temperature, which requires knowledge of the energy barrier and the pre-exponential factor. While the energy barrier has already been adressed by several studies [1], the pre-exponential factor for the skyrmion collapse remains unexplored [2,3].

Here, we adress the dependence of the pre-exponential factor on the external magnetic field and demonstrate that it changes qualitatively when exchange frustration is taken into account. We focus on the model system Pd/Fe/Ir(111) [4], described by an atomistic spin model based on parameters from density functional theory [1]. In our approach, the minimum energy paths and thereby the energy barriers are calculated by the geodesic nudged elastic band method, while the pre-exponential factors are determined by harmonic transition state theory [3].

[1] von Malottki *et al.*, Sci. Rep. **7**, 12299 (2017)
[2] J. Wild *et al.*, Sci. Adv. **3.9**, e1701704 (2017)
[3] P. F. Bessarab *et al.*, arXiv:1706.07173v2 (2017)
[4] N. Romming *et al.*, Phys. Rev. Lett. **114**, 177203 (2015)

30 minutes break

Invited Talk TT 107.6 Fri 11:30 H 1012

Magnonics in skyrmion-hosting chiral magnetic materials — •Markus Garst — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

Chiral magnets with a Dzyaloshinskii-Moriya interaction possess spatially modulated phases of the ferromagnetic order parameter like helices and skyrmion lattices. We give an overview of the properties of spinwave excitations in such materials [1]. In the presence of a magnetic field, the magnons are characterized by an inherent nonreciprocity, i.e., their dispersion lack reflection symmetry. We discuss the evolution of non-reciprocity as a function of magnetic field, which has been determined by inelastic neutron scattering on MnSi [2,3]. Moreover, Bragg reflection off the periodicity of the magnetic textures naturally result in magnon band structures. This band structure is topologically non-trivial for the skyrmion lattice due its emergent electrodynamics, which is reflected in non-trivial Chern numbers implying the presence of robust magnon edge states [1]. In addition, we discuss the ferromagnetic resonances of the various phases [4] and their non-reciprocity, which has been experimentally probed by spin-wave spectroscopy and Brillouin light scattering.

[1] M. Garst, J. Waizner, and D. Grundler, J. Phys. D: Appl. Phys. 50, 293002 (2017) [2] M. Kugler, et al. Phys. Rev. Lett. 115, 097203 (2015) [3] T. Weber et al. arXiv:1708.02098 [4] T. Schwarze et al. Nat. Mat. 14, 478 (2015)

TT 107.7 Fri 12:00 H 1012

Field-free deterministic ultrafast creation of magnetic skyrmions by spin–orbit torques — Felix Büttner[1], Ivan Lemesh[1], Michael Schneider[2], •Bastian Pfau[2], Christian M. Günther[2,3], Piet Hessing[2], Jan Geilhufe[2], Lucas Caretta[1], Dieter Engel[2], Benjamin Krüger[4], Jens Viefhaus[5], Stefan Eisebitt[2], and Geoffrey S. D. Beach[1] — [1]Massachusetts Institute of Technology, Cambridge, USA. — [2]Max-Born-Institut, Berlin, Germany. — [3]TU Berlin, Berlin, Germany. — [4]Institut für Lasertechnologien in der Medizin und Messtechnik an der Universität Ulm, Ulm, Germany. — [5]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany.

Magnetic skyrmions are a very promising option to realize current-driven magnetic shift registers. Generation, transport and annihilation of skyrmions are fundamental operations in this context. We study the generation and intrinsic dynamics of bubble skyrmions via static and time-resolved X-ray holography, combining sub-30 nm spatial resolution with sub-100 ps temporal resolution. It is demonstrated that single skyrmions can be generated deterministically on subnanosecond timescales in magnetic racetracks using spin–orbit torque pulses. Externally applied in-plane magnetic fields are not required in the process. Furthermore, results on the GHz dynamical behavior of bubble skyrmions are presented, where precision observation of the skyrmion trajectory is indicative of the presence of an inertial mass, connected to the skyrmion topology.

TT 107.8 Fri 12:15 H 1012

Speed limits for Skyrmions — •Jan Müller[1], Ben McKeever[2,3], and Karin Everschor-Sitte[3] — [1]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Deutschland — [2]Graduate School Materials Science in Mainz, 55128 Mainz, Germany — [3]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Deutschland

Magnetic skyrmions are particle-like textures in the magnetization, characterized by a topological winding number. Nanometer-scale skyrmions have been observed at room temperature in magnetic multilayer structures. The combination of small size, topological quantization, and their efficient electric manipulation makes them interesting candidates for information carriers in high-performance memory devices which rely on mobile bits. Skyrmion racetrack memory devices have been suggested where skyrmions move in a one-dimensional nanostrip. The information in the racetracks is encoded either in the distance between skyrmions or in additional attributes of these, e.g. shifts from the center of the track or different winding numbers. In order to drive skyrmions along the racetrack, it is often suggested to apply spin-polarized currents. Besides moving the skyrmions, the applied currents, however, also deform them, which is usually assumed a negligible effect. We study these deformations and show that they trigger an instability which ultimately sets a speed limit in the racetracks.

TT 107.9 Fri 12:30 H 1012

Skyrmion-Antiskyrmion racetrack memory in rank-1 DMI materials — M. Hoffmann[1], B. Zimmermann[1], G. P. Müller[1,2], N. S. Kiselev[1], C. Melcher[3], and •S. Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — [2]Science Institute of the University of Iceland, VR-III, Reykjavík, Iceland — [3]Department of Mathematics I & JARA FIT, RWTH Aachen University, Aachen, Germany

Recently, we extended the scope of skyrmions and antiskyrmions and introduced a classification scheme of chiral magnets [1]. Typically investigated Bloch-type skyrmions in B20 alloys and Néel-type skyrmions at (111) oriented interfaces belong to isotropic rank-three DM bulk and rank-two DM film magnets with a DM interaction described by a single spiralization constant. Within this class, antiskyrmions are stable only for bulk crystals with certain point group symmetries. New are the anisotropic rank-two DMI film magnets where skyrmions and antiskyrmions can coexist while the determinant of the spiralization tensor determines which of them has lower energy. Finally, zero determinant indicates a rank-one DMI material in which skyrmions and antiskyrmions have the same energy. Here, we discuss our new classification scheme and discuss the potential of rank-one solids for the design of a racetrack memory based on the coexistence of skyrmions and antiskyrmions where the information is encoded in the object type instead of the presence or absence of a skyrmion [2].

[1] M. Hoffmann et al., Nat. Commun. 8, 308 (2017)
[2] M. Hoffmann et al., to be submitted

TT 108: Topological Superconductors

Time: Friday 9:30–12:00 Location: H 2053

TT 108.1 Fri 9:30 H 2053

Two dimensional topological superconductivity with antiferromagnetic insulators — •Jose Lado and Manfred Sigrist — Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

Two dimensional topological superconductivity has attracted great interest due to the emergence of Majorana modes bound to vortexes and propagating Majorana modes at the edges [1]. However, due to its rare appearance in natural compounds, its experimental replication relies on delicate artificial engineering by combination of helical states, magnetic fields and conventional superconductors [2]. Here we introduce a platform alternative to those mechanisms, by showing that a class of three dimensional antiferromagnets can be used to engineer a two dimensional topological superconductor. Our proposal relies on the appearance of solitonic states at the interface between an antiferromagnet and a superconductor, that become topologically gapped by intrinsic spin-orbit coupling. We show that those interfacial states do not require fine tuning between the superconducting and the antiferromagnetic exchange fields, as its existence is protected by asymptotic boundary conditions. Our findings open the venue of using three dimensional antiferromagnetic insulators as a solid state platform to engineer topological superconductivity.

[1] S. R. Elliott, M. Franz, Rev. Mod. Phys. 87, 137
[2] C. W. J. Beenakker, Annual Review of Condensed Matter Physics 2013 4:1, 113-136

TT 108.2 Fri 9:45 H 2053

Tunabale hybridization of Majorana bound states at the quantum spin Hall edge — •Felix Keidel[1], Pablo Burset[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Department of Applied Physics, Aalto University, FIN-00076 Aalto, Finland

We study the helical edge of a quantum spin Hall insulator in proximity to an s-wave superconductor (S) and ferromagnetic insulators (F). Hybrid structures of this kind are known to give rise to topological superconductivity and allow for Majorana bound states in regions where both the ferromagnetic and the superconducting gap close. This can be used to localize and couple Majorana modes.

In our work, we consider junctions with alternating S and F barriers and a system with three S barriers. The cavities between them can be understood as quantum dots hosting overlapping Majorana (MBS) and Andreev quasi-bound states (ABS). We demonstrate how the resulting hybridization and splitting depend on distinct parameters of the systems. Remarkably, we can make a close connection between the localized bound states and the induced nonlocal pairing amplitudes. The anomalous correlations provide a way to distinguish MBS and ABS and exhibit odd-frequency dominated triplet pairing for resonances associated with hybridized MBS.

TT 108.3 Fri 10:00 H 2053

The Electronic Structure and Transport Properties of Niobium Doped Bismuth Selenide — •Henriette Elisabeth Lund[1], Marco Bianchi[1], Simone Munkholm Kevy[2], Laura Wollesen[2], Martin Bremholm[2], Mark Jonas Haastrup[1], Elze Jantien Knol[3], Alexander Ako Khajetoorians[3], Steffen Wiedmann[4], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center (iNano), Aarhus University, 8000 Aarhus C, Denmark — [2]Center for Materials Crystallography, Department of Chemistry and iNano, Aarhus University, 8000 Aarhus C, Denmark — [3]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, The Netherlands — [4]High Field Magnet Laboratory, Institute for Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands

It is believed that topological superconductivity can be realized in bismuth selenide, Bi_2Se_3, doped with Cu, Sr, and Nb. Little is known about the properties of Nb doped Bi_2Se_3. In the present study, the electronic structure and transport properties of $Nb_xBi_2Se_3$ have been investigated. Angle-resolved photoemission spectroscopy, scanning tunneling microscopy and atomic force microscopy measurements point towards an inhomogeneous surface structure. Transport measurements show that samples become partly superconducting with the critical temperature ranging between 2.3 K and 3.2 K. The results indicate that the $Nb_xBi_2Se_3$ system crystallizes in an inhomogeneous manner which makes it challenging to understand the origin of the superconductivity and motivates further work on this project.

TT 108.4 Fri 10:15 H 2053

Nematic superconductivity in $Cu_xBi_2Se_3$ — •Matthias Hecker and Jörg Schmalian — KIT, Karlsruhe, Germany

$Cu_xBi_2Se_3$ is a doped topological insulator that becomes superconducting at a temperature $T_c \approx 3.8K$. Recent NMR Knight-shift measurements in the superconducting phase have revealed the spontaneous symmetry breaking of the threefold rotational symmetry of the underlying lattice, in addition to the global U(1)-symmetry. This fact is most consistent with an odd-parity two-component superconducting order parameter, as proposed by [1]. We study the role of order parameter fluctuations, and show that the system can realize a nematic phase with $T_{nem} > T_c$, where actual superconductivity is not yet present. Besides, we find that the nematic phase transition is always a first order transition. Inside this new phase, we calculate the anisotropy in the resistivity in order to provide a tool for experimental verification.

[1] Fu and Berg, PRL 105,4 097001 (2010)

TT 108.5 Fri 10:30 H 2053

Millikelvin scanning tunneling spectroscopy: electronic features of semimetals and putative topological superconductors at very low energies — •Hermann Suderow — Universidad Autonoma de Madrid, Madrid, Spain

Scanning tunneling microscopy and spectroscopy (STM/S) down to 100 mK is an efficient tool to study superconductors and semimetals. The local electronic density of states is obtained at atomic level with a resolution in energy of a few tens of micro eV. Friedel like oscillations are observed close to defects like vacancies or interstitials. Real space maps of the electronic density of states close to defects provide thus a visual account from which we can measure the wavelength of the electronic wavefunctions at the energy corresponding to the applied bias voltage. The Fourier transform of the real space maps provides the constant energy contour of the electronic dispersion relation. By making maps at different energies, below and above the Fermi level, we can in principle trace the full bandstructure. In this talk, I will discuss recent visualization experiments of scattering effects in super-

conductors and semimetals. I will focus on the typeII Weyl semimetal WTe_2, where we directly observe the signature of edge states associated to the Weyl points and recent efforts in the putative chiral d-wave superconductor URu_2Si_2.

15 min. break.

TT 108.6 Fri 11:00 H 2053

Hybrid structures of topological insulators and superconductors - a possible realization of Cooper pair splitting? — •Jacob Fuchs[1], Michael Barth[1], Raphael Kozlovsky[1], Cosimo Gorini[1], Inanc Adagideli[2], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul

Transport in hybrid structures of topological insulator (TI) nanowires and superconductors (SCs) is investigated. The main focus is on TI-SC-TI-like structures and the question how such devices can be used to split Cooper pairs into two spatially separated electrons. On the one hand, the utilization of the spin-momentum locking in combination with the spin-singlet nature of the Cooper pairs is discussed. On the other hand, magnetic fields parallel to the TI nanowire can cause vortices in the SC leading to Majorana modes at the TI-SC boundary. These enable the splitting of Cooper pairs. Using a T-shaped junction, the splitting can be observed via a negative differential resistance.

TT 108.7 Fri 11:15 H 2053

Creation of spin-triplet Cooper pairs in the absence of magnetic ordering — •Daniel Breunig[1], Pablo Burset[2], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics and Astrophysics, *University of Würzburg, D-97074 Würzburg, Germany — [2]Department of Applied Physics, Aalto University, FIN-00076 Aalto, Finland

In superconducting spintronics, it is essential to generate spin-triplet Cooper pairs on demand. Up to now, proposals to do so concentrate on hybrid structures in which a superconductor (SC) is combined with a magnetically ordered material (or an external magnetic field). We, instead, identify a novel way to create and isolate spin-triplet Cooper pairs in the absence of any magnetic ordering. This achievement is only possible because we drive a system with strong spin-orbit interaction–the Dirac surface states of a strong topological insulator (TI)–out of equilibrium. In particular, we consider a bipolar TI-SC-TI junction, where the electrochemical potentials in the outer leads differ in their overall sign. As a result, we find that nonlocal singlet pairing across the junction is completely suppressed for any excitation energy. Hence, this junction acts as a perfect spin triplet filter across the SC generating equal-spin Cooper pairs via crossed Andreev reflection.

TT 108.8 Fri 11:30 H 2053

Nonequilibrium Andreev bound states population in short superconducting junctions coupled to a resonator — •Raffael L. Klees[1], Gianluca Rastelli[1,2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Zukunftskolleg, Universität Konstanz, D-78457 Konstanz, Germany

Inspired by recent experiments [1], we study a short superconducting junction of length $L \ll \xi$ (coherence length) inserted in a dc-SQUID containing an ancillary Josephson tunnel junction. We evaluate the nonequilibrium occupation of the Andreev bound states (ABS) for the case of a conventional junction and a topological junction [2], with the latter case of ABS corresponding to a Majorana mode. We take into account small phase fluctuations of the Josephson tunnel junction, acting as a damped LC resonator, and analyze the role of the distribution of the quasiparticles of the continuum assuming that these quasiparticles are in thermal distribution with an effective temperature different from the environmental temperature. We also discuss the effect of strong photon irradiation in the junction leading to a nonequilibrium occupation of the ABS. We systematically compare the occupations of the bound states and the supercurrents carried by these states for conventional and topological junctions.

[1] L. Bretheau *et al.*, Nature **499**, 312 (2013);
C. Janvier *et al.*, Science **349**, 1199 (2015);
D. J. van Woerkom *et al.*, Nat. Phys. **13**, 876 (2017);
A. Murani *et al.*, Nat. Commun. **8**, 15941 (2017).
[2] R. L. Klees *et al.*, Phys. Rev. B **96**, 144510 (2017).

TT 108.9 Fri 11:45 H 2053

Waiting time distributions for hybrid junctions with topological superconductors — •Pablo Burset, Shuo Mi, and Christian Flindt — Department of Applied Physics, Aalto University, Finland

Electron waiting times are an important tool for analyzing the internal dynamics of nano-scale conductors. Here we investigate the waiting time distributions (WTDs) of superconducting hybrid junctions. We consider both conventional and topologically nontrivial superconductors, with the latter hosting Majorana bound states (MBS) at their edges. We develop a scattering matrix formalism for the WTD in multi-channel, multi-terminal scatterers. The multi-channel WTDs allow us to characterize Andreev processes that entangle electrons and holes. Using our multi-terminal approach, we analyze (i) normal-superconductor (NS) junctions featuring Andreev bound states at the NS interface, and (ii) NSN junctions where Cooper pairs can be spatially split into different leads. In both cases, we include a resonant cavity at the NS interfaces that acts as a non-interacting quantum dot. The presence of Andreev bound states in the cavities leads to oscillations of the WTD and a finite probability of a simultaneous detection of electrons and holes, which always appears for topological superconductors due to the presence of the MBS.

TT 109: Frustrated Magnets - (General) Theory

Time: Friday 9:30–12:15 Location: H 3005

TT 109.1 Fri 9:30 H 3005

The frustrated bilayer honeycomb antiferromagnet — •Wolfram Brenig[1], Marcelo Arlego[2], Carlos Lamas[2], and Hao Zhang[3] — [1]Institute for Theoretical Physics, Technical University Braunschweig, Germany — [2]IFLP - CONICET, Departamento de Física, Universidad Nacional de La Plata, Argentina — [3]National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing, China

We analalyze the spin-1/2 Heisenberg antiferromagnet on the honeycomb bilayer with frustrating next-nearest neighbor exchange. Using a combination of bond-operators, Schwinger-boson mean field theory, and dimer series expansion, we show that the competition between intra- and interlayer coupling gives rise to a rich variety of semiclassical and genuinely quantum phases. Results for ground state energies, excitation gaps, and spin-spin correlation functions will be discussed. In particular we provide new evidence for the existence of a quantum disordered lattice-nematic phase within a substantial range of intermediate intralayer frustration and interlayer coupling.

TT 109.2 Fri 9:45 H 3005

Quantum Monte Carlo Study of the Thermodynamics of the Fully Frustrated Heisenberg Bilayer — •Stefan Wessel[1], Jonas Stapmanns[1], Andreas Honecker[2], Philippe Corboz[3], Bruce Normand[4], and Frederic Mila[5] — [1]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, Germany — [2]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — [3]Institute for Theoretical Physics and Delta Institute for Theoretial Physics, University of Amsterdam, The Netherlands — [4]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — [5]Institute of Physics, Ecole Polytechnique Fédérale Lausanne (EPFL), Switzerland

We examine the thermal properties of the spin-1/2 Heisenberg model on the fully frustrated square lattice bilayer. For this purpose, we use a sign problem-free quantum Monte Carlo approach that is based on a decoupling of the Hamiltonian in an inter-layer spin dimer basis. At zero temperature, a discontinuous quantum phase transition separates a inter-layer singlet phase from an antiferromagnetic ground state forming from inter-layer triplet states. We show that this discontinuous transition extends towards finite temperatures, i.e., in the absence of long-range order. The thermodynamic behavior of this system furthermore exhibits similarities to the liquid-gas transition.

TT 109.3 Fri 10:00 H 3005

Cluster-glass phase in pyrochlore XY antiferromagnets with quenched disorder — •Matthias Vojta[1], Jose A. Hoyos[2], Eric C. Andrade[2], and Stephan Rachel[1,3] — [1]Technische Universität Dresden, Germany — [2]Universidade de Sao Paulo, Brasil — [3]University of Melbourne, Australia

We study the impact of quenched disorder (random exchange couplings or site dilution) on easy-plane pyrochlore antiferromagnets. In the clean system a magnetically ordered state is selected from a classically degenerate manifold via an order-by-disorder mechanism. In the presence of randomness, however, different states can be locally selected depending on details of the disorder configuration. Using a combination of analytical considerations and classical Monte-Carlo simulations, we argue that any long-range-ordered magnetic state is destroyed beyond a critical level of randomness where the system breaks into magnetic domains due to random exchange anisotropies, becoming therefore a glass of spin clusters, in accordance with the available experimental data.

TT 109.4 Fri 10:15 H 3005

Quenched bond disorder in a non-collinear antiferromagnet — •Santanu Dey and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

In antiferromagnets, the presence of geometric frustration often leads to classical ground states with non-collinear spin ordering. Quenched disorder is an interesting ingredient which tends to counteract spontaneous symmetry breaking in low dimensional systems. Consequently, the study of the interplay between disorder and frustration has garnered some serious attention recently [1,2]. To understand the resulting phenomena, we undertake a generic point of view and also focus on a prototypical example, the disordered triangular lattice antiferromagnet (TLAF) with next and next to nearest neighbor Heisenberg interaction. The homogeneous limit of this model hosts a phase transition between non-collinear antiferromagnetic LRO and what is believed to be a Z_2 spin liquid [3]. Combining analytical arguments and finite-system numerical simulations, we study the destruction of the LRO by bond disorder and discuss physical properties of the emergent state at low temperatures. We also connect our findings to recent experimental observations on related compounds, $YbZnGaO_4$ and $YbMgGaO_4$ [1].

[1] Z. Ma et. al, arXiv:1709.00256 (2017)
[2] H. Kawamura, K. Watanabe, T. Shimokawa, J. Phys. Soc. Jpn. 83, 103704 (2014)
[3] K. Slagle and C. Xu, Phys. Rev. B. 89, 104418 (2014)

TT 109.5 Fri 10:30 H 3005

Frustrated quantum magnetism in the Kondo-lattice on the zig-zag ladder — •Matthias Peschke, Roman Rausch, and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg

The interplay between Kondo effect, indirect magnetic interaction and geometrical frustration is studied in the Kondo lattice on the one-dimensional zig-zag ladder. Using the density-matrix renormalization group (DMRG), the ground state and various short- and long-range spin- and density-correlation functions are calculated for the model at half-filling as a function of the antiferromagnetic Kondo interaction down to $J = 0.3t$ where t is the nearest-neighbor hopping.

Geometrical frustration is shown to lead to at least two critical points: Starting from the strong-J limit, where almost local Kondo screening dominates, antiferromagnetic correlations between nearest-neighbor and next-nearest-neighbor local spins become stronger and stronger, until at $J_c^{\mathrm{dim}} \approx 0.895$ frustration is alleviated by a spontaneous breaking of translational symmetry and a corresponding transition to a dimerized state. Furthermore, within the symmetry-broken dimerized state, our data suggest a magnetic transition to a 90° quantum spin spiral with quasi-long-range order at $J_c^{\mathrm{mag}} \approx 0.84$. The quantum-critical point is characterized by a diverging spin-structure factor $S(q)$ at wave vector $q = \pi/2$ and the closure of the spin gap (based on system sizes up to $L = 40$). This is opposed to the model on the one-dimensional bipartite chain, which is known to have a finite spin gap for all $J > 0$ at half-filling.

TT 109.6 Fri 10:45 H 3005

Quantum criticality of 2d transverse-field Ising models with long-range interactions — Sebastian Fey and •Kai P. Schmidt — Lehrstuhl für Theoretische Physik I, Friedrich-Alexander-Universitaet Erlangen-Nuernberg, Germany

Most investigations on strongly correlated quantum many-body systems tackle short-range interactions. Very little is known so far on quantum criticality in the presence of long-range interactions, since such models are very hard to treat microscopically. Nevertheless, important examples of long-range interactions exist in nature, e.g. dipolar interactions in spin ice or long-range forces between cold atoms in optical lattices. Here we develop linked-cluster expansions with the help of classical Monte Carlo simulations to investigate the quantum-critical properies of the transverse-field Ising model with long-range interactions on two-dimensional lattices. In the unfrustrated cases we find different kinds of universality classes corresponding to the nearest-neighbor model, mean-field theory, as well as continuously varying critical exponents. In the frustrated cases our results agree with the scenario that the quantum-critical properties are always given by the model with nearest-neighbor interactions.

TT 109.7 Fri 11:00 H 3005

$\mathbb{Z}_2$ Topological quantum paramagnet on a honeycomb bilayer — •Darshan G. Joshi and Andreas P. Schnyder — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Topological quantum paramagnets are exotic states of matter with trivial paramagnetic ground states hosting topological excitations. Here we show that a simple model of quantum spins on a honeycomb bilayer hosts a $\mathbb{Z}_2$ topological quantum paramagnet in the presence of spin-orbit coupling. The $\mathbb{Z}_2$ invariant is the same as that in the case of the fermionic quantum spin Hall state. We further show that upon making one of the Heisenberg couplings stronger the system undergoes a topological quantum phase transition, where the $\mathbb{Z}_2$ invariant vanishes, to a different topological quantum paramagnet. In this case the edge states are disconnected from the bulk excitations and the phase is characterized by a different topological invariant. This physics is amenable to experiments, where an anisotropic coupling can be induced under pressure.

15 min. break.

TT 109.8 Fri 11:30 H 3005

Thermodynamics of the Two-Dimensional Shastry-Sutherland Model for $SrCu_2(BO_3)_2$ — •Andreas Honecker[1], Jonas Stapmanns[2], Ido Niesen[3], Philippe Corboz[3], Bruce Normand[4], Frédéric Mila[5], and Stefan Wessel[2] — [1]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — [2]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, Germany — [3]Institute for Theoretical Physics and Delta Institute for Theoretical Physics, University of Amsterdam, The Netherlands — [4]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, Villigen, Switzerland — [5]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

$SrCu_2(BO_3)_2$ is famous for its rich physical properties and as a realization of the two-dimensional spin-1/2 Shastry-Sutherland model. In the latter model, an orthogonal arrangement of dimers gives rise both to an exact dimer ground state and geometric frustration that renders quantitatively reliable results for the low-temperature thermodynamic properties a challenge since, e.g., conventional Quantum-Monte-Carlo (QMC) simulations suffer from a severe sign problem. A recently developed QMC method in the dimer basis alleviates the sign problem. We assess the range of applicability of this method to the two-dimensional spin-1/2 Shastry-Sutherland model by comparing it to complementary exact diagonalization and high-temperature series. Specifically, we compute the specific heat C and the magnetic susceptibility χ in the parameter regime relevant to $SrCu_2(BO_3)_2$.

TT 109.9 Fri 11:45 H 3005

Plaquette phases in an extended Shastry-Sutherland model — •Carolin Boos[1], Philippe Corboz[2], Schelto Crone[2], Frédéric Mila[3], Ido Niesen[2], and Kai Phillip Schmidt[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]University of Amsterdam, Netherlands — [3]EPF Lausanne, Switzerland

The frustrated magnet $SrCu_2(BO_3)_2$ exhibits a quantum phase transition under high pressure. Without pressure this material is well described by the two-dimensional Shastry-Sutherland model with parameters close to a phase transition towards a ground state of singlets on empty plaquettes. This state is therefore the natural candidate for the high-pressure phase. However, it has also been suggested [1] that a different plaquette phase, where singlets reside on the full plaquettes

containing a diagonal bond, is realized in $SrCu_2(BO_3)_2$. In this work we use high-order series expansions and infinite projected entangled pair states (iPEPS) to investigate the interplay between empty and full plaquette phases in an extended Shastry-Sutherland model.
[1] M. E. Zayed *et al.*, Nat. Phys. **13** (2017) 962

TT 109.10 Fri 12:00 H 3005

Spin model of the Heisenberg antiferromagnet $Li_3Ni_2SbO_6$: the relevance of third-neighbor exchanges — •Oleg Janson — Institut für Festkörperphysik, TU Wien, Österreich

The quasi-2D $S = 1$ Heisenberg antiferromagnet $Li_3Ni_2SbO_6$ exhibits a small Weiss temperature of 8 K and a zigzag magnetic ground state below $T_N = 15$ K [1,2]. At the same time, the experiments indicate the presence of a short-range magnetic order up to 80 K [2]. The experimental behavior was rationalized in terms of a honeycomb lattice model with inequivalent nearest-neighbor (NN) exchanges [1]: antiferromagnetic J_1 forming dimers and ferromagnetic J_1' (J_2 in the notation of [1]) forming chains. Puzzled by the drastic dissimilarity of J_1 and J_1', we performed microscopic magnetic modeling and found that both NN exchanges are ferromagnetic. The antiferromagnetism and magnetic frustration are induced by two sizable third-neighbor exchanges, J_3 and J_3', that are mediated by the nonmagnetic SbO_6 octahedra in the voids of the honeycomb lattice. The resulting J_1-J_1'-J_3-J_3' model provides a simple and natural explanation for the observed zigzag state. This work has been supported by the Austrian Science Fund (FWF) through the Lise Meitner programme, project no. M2050.
[1] E. A. Zvereva *et al.*, Phys. Rev. B **92**, 144401 (2015).
[2] A. I. Kurbakov *et al.*, Phys. Rev. B **96**, 024417 (2017).

TT 110: Superconductivity: Fe-based Superconductors - 1111 and Others

Time: Friday 9:30–11:45 Location: H 3010

TT 110.1 Fri 9:30 H 3010

Nematicity and structure in single-crystalline LaFeAsO — •Sven Sauerland[1], Francesco Scaravaggi[2,3], Liran Wang[1,2], Rhea Kappenberger[2,3], Saicharan Aswartham[2], Anja U.B. Wolter[2], Bernd Büchner[2,3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden IFW, Dresden, Germany — [3]Institute for Solid State Physics, TU Dresden, Germany

We report the temperature dependence of the elastic shear modulus response and the thermal expansion of detwinned LaFeAsO single crystals. The orthorhombic distortion parameter is derived. While the evolution of orthorhombic distortion at $T_S \sim 150$ K is associated with strong uniaxial pressure dependencies in particular along the a- and b-axes as well as sizeable volume effects, our data imply much smaller lattice effects at the antiferromagnetic ordering temperature T_N. By means of the three-point bending technique in the capacitance dilatometer, we obtain the nematic susceptibility from the shear modulus response in LaFeAsO. Similar to $BaFe_2As_2$, the shear modulus softens well above T_S implying a Curie-Weiss-like behaviour of the nematic susceptibility. The relation of the nematic susceptibility in LaFeAsO to spin, structure and orbital degrees of freedom is discussed.

TT 110.2 Fri 9:45 H 3010

Determination of nematic, magnetic and superconducting phase transitions in Co doped LaOFeAs single crystals by NMR — •Piotr Lepucki, Rhea Kappenberger, Saicharan Aswartham, Adam Paul Dioguardi, Bernd Büchner, and Hans-Joachim Grafe — IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Single crystals are a prerequisite to perform angular dependent NMR measurements in solids. However, these were not available in sufficient size for doped LaOFeAs until recently [1]. Here we present such NMR measurements on single crystals of LaOFeAs doped with 3.4% , 4.1% , and 6.2% Co. The underdoped samples show clear signatures of the nematic transition in the ^{75}As NMR linewidth as well as in the spin lattice relaxation rate, T_1^{-1}, and its anisotropy. At lower temperatures, a peak in T_1^{-1} signals the onset of long-range magnetic order, whereas the superconducting transition cannot be determined unambiguously in a magnetic field of 7 T, which has been applied for the NMR measurements. In contrast, the optimally doped sample with 6.2% Co shows neither nematic nor long range magnetic order. Instead, T_1^{-1} decreases at the superconducting transition, indicating bulk superconductivity at $T_c = 12$ K even in an applied field of 7 T. Our NMR results in Co doped LaOFeAs single crystals are broadly consistent with those obtained in Co doped $BaFe_2As_2$.
[1] R. Kappenberger et al., J. Cryst. Growth 483, 9 (2018)

TT 110.3 Fri 10:00 H 3010

Interplay between electronic order and superconductivity in pnictides: The case of NdFeAs(OF) — •Mahmoud Abdel-Hafiez[1], H. K. Mao[2], Masaki Mito[3], Agnes Adamski[1] und Cornelius Krellner[1] — [1]Institute of Physics, Goethe University Frankfurt, 60438 Frankfurt/M, Germany — [2]Center for High Pressure Science and Technology Advanced Research, Shanghai, 201203, China — [3]Graduate School of Engineering, Kyushu Institute of Technology, Kitakyushu 804-8550, Japan

One of the crucial issues to elucidate the mechanism leading to high-temperature superconductivity is the nature of pairing, e.g., the symmetry and structure of the superconducting order parameter. Recently, we have reported on the superconducting gap in the newly synthesized single crystals of F-doped NdFeAsO. Our observations clearly show that the superconducting energy gap is nodeless. Additionally, pressure has long been recognized as a versatile tuning parameter which can sensitively change the electron correlations in materials. Through an extensive transport study under high-pressure up to 50 GPa, we have clarified in bulk NdFeAs(OF) the competition between ferromagnetism (FM) and superconductivity, where FM is induced by the 4f moments of Nd upon compression. We construct a comprehensive pressure-temperature phase diagram which shows a crossover from Fermi-liquid to non-Fermi-liquid to Fermi-liquid (FL-NFL-FL) alongside a monotonic suppression of the superconductivity with increasing the pressure, before the FM appears at pressures above.

TT 110.4 Fri 10:15 H 3010

The nematic phase in $LaFe_{1-x}Co_xAsO$ probed by thermal expansion — •Francesco Scaravaggi[1,2], Sven Sauerland[3], Rhea Kappenberger[1,2], Liran Wang[1,3], Saicharan Aswartham[1], Sabine Wurmehl[1,2], Rüdiger Klingeler[3], Anja U. B. Wolter[1], and Bernd Büchner[1,2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany — [2]Institute for Solid State Physics, TU Dresden, Dresden, Germany — [3]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany

Nematicity in electron doped 1111 systems $LaFe_{1-x}Co_xAsO$ (x > 0) has been studied on polycrystalline samples, revealing a rich phase diagram. Measurements suggest an abrupt suppression of the AFM/orthorhombic phase with doping upon approaching the superconducting dome, but signatures of the nematic phase could still be detected in the underdoped region. In order to better understand the unique La-1111 phase diagram among the Fe-based superconductors, we report a systematic investigation of the evolution of the nematic state of Co-doped LaFeAsO single crystals. The availability of macroscopic phase pure single crystals for different doping compositions allows us to directly probe structural changes via high resolution dilatometry. Detwinning of the crystals, achieved by the application of a small uniaxial force in the dilatometer, permits us to probe thermal expansion in different crystallographic directions (a,b,c). From this we can obtain information about the structural order parameter (δ) as a function of temperature and doping, thus allowing us to study the nematic phase at different regions in the phase diagram.

TT 110.5 Fri 10:30 H 3010

Equivalence of hydrostatic and chemical pressure? Suppression of the magnetism in CeFeAsO — •Philipp Materne[1,2], Wenli Bi[2,3], Esen Ercan Alp[2], Jiyong Zhao[2], Michael Yu Hu[2], Dongzhou Zhang[2], Til Goltz[1], Anton Jesche[4], Christoph Geibel[4], Rhea Kappenberger[5], Saicharan Aswartham[5], Sabine Wurmehl[5,1], Bernd Büchner[5,1], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, D-01069 Dresden, Germany — [2]Argonne National Laboratory, Argonne, IL

60439, USA — [3]Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA — [4]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [5]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, D-01069, Germany

We present a detailed study of the equivalence of hydrostatic and chemical (due to As by P substitution) pressure in CeFeAsO by means of energy- and time-domain Mössbauer spectroscopy. We observed a nearly linear suppression of the magnetic hyperfine field to zero between 0 and 40 % P-substitution level while the field is reduced by 25 % between 0 and 4.5 GPa followed by an abrupt decrease to zero at 5.2 GPa. We found a quantitatively equal suppression of the magnetic order below a P-substitution level of 5 % and hydrostatic pressures below 0.3 GPa. Above these values the suppression is qualitatively different. Our findings set an upper boundary for the equal treatment of chemical and hydrostatic pressure in this system.

15 min. break.

TT 110.6 Fri 11:00 H 3010

FeSi: a new building block for iron-based superconductivity — •Andres Cano — CNRS, France

We report the synthesis and characterization of the novel silicide hrydride LaFeSiH displaying superconductivity with onset at 11 K. We find that this pnictogen-free compound is isostructural to LaFeAsO, with a similar low-temperature tetragonal to orthorhombic distortion. Using density functional theory we show that this system is also a multiband metal in which the orthorhombic distortion is likely related to single-stripe antiferromagnetic order. Electrical resistivity and magnetic susceptibility measurements reveal that these features occur side-by-side with superconductivity, which is suppressed by external pressure.

[1] F. Bernardini, G. Garbarino, A. Sulpice, M. Núñez-Regueiro, E. Gaudin, B. Chevalier, A. Cano, S. Tencé; arXiv:1701.05010

TT 110.7 Fri 11:15 H 3010

Unconventional Superconductivity in Poly- and Single Crystal YFe_2Ge_2 — •Jiasheng Chen[1], Konstantin Semeniuk[1], Monika Gamza[2], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK — [2]Jeremiah Horrocks Institute for Mathematics, Physics and Astrophysics, University of Central Lancashire, Preston PR1 2HE, UK

The d-electron system YFe_2Ge_2 exhibits an unusually high Sommerfeld coefficient C/T $\sim$ 100 mJ/(molK^2) at low temperatures, indicative of strong electronic correlations. Although superconductivity in YFe_2Ge_2 has been widely observed in electrical measurements below 1.8 K, it is strongly sample-dependent and fragile against disorders [1, 2]. Until now, thermodynamic signatures of bulk superconducting transitions have only been reported in polycrystals with residual resistance ratios (RRR) above 70 [2], but not in single crystals. Detail studies on the structures and electrical properties of polycrystals with varying nominal compositions have shed light on the origins of this strong sample dependence. It also led to our success in producing a new generation of single-crystal YFe_2Ge_2 with RRR reaching $\sim$ 170 which shows bulk superconductivity as seen in high quality polycrystals. This thus allows for further investigations into the nature of its apparently unconventional superconductivity by means of heat capacity, penetration depth and quantum oscillation measurements.

[1] Y. Zou et al., Physica Status Solidi - Rapid Research Letters 8, 928 (2014),
H. Kim et al., Philos Mag 95, 804 (2015).
[2] J. Chen et al., PRL 116, 127001 (2016)

TT 110.8 Fri 11:30 H 3010

Low temperature heat capacity in the iron-based superconductor YFe_2Ge_2 — •Keiron Murphy[1], Jiasheng Chen[1], Jacintha Banda[2], Jordan Baglo[1], Manuel Brando[2], Michael Sutherland[1], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]MPI Chemical Physics of Solids, Nöthnitzer Strasse 40, Dresden

Unconventional superconductivity is rare in transition metal compounds outside the layered iron pnictide/chalcogenide and cuprate material families. These systems typically have highly anisotropic electronic properties and nearly 2D Fermi surface geometries. The iron based unconventional superconductor YFe_2Ge_2, by contrast, displays a comparatively isotropic, 3D electronic structure. Its Sommerfeld ratio C/T, is enhanced by an order of magnitude above the band structure value to $\gamma \sim 100$ mJ/(mol K^2) at low temperature, and it displays an anomalous form for the temperature dependence of the resistivity, $\rho(T) = \rho 0 + AT^{3/2}$. Theoretical proposals for the pairing mechanism in YFe_2Ge_2 include both triplet [1] and singlet, s* order parameter wave functions [2], prompting a renewed effort to examine the heat capacity well below the transition temperature in newly available bulk superconducting single crystals.

[1] D. J. Singh, Phys. Rev. B 89, 024505 (2014).
[2] A. Subedi, Phys. Rev. B 89, 024504 (2014).

TT 111: Frontiers of Electronic-Structure Theory: Correlated Electron Materials VIII (joint session O/TT/MM/DS/CPP)

Organizers: Silke Biermann, Ecole Polytechnique, Palaiseau cedex, France; Paul R. Kent, Oak Ridge National Laboratory, USA; Matthias Scheffler, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

(Synopsis provided with part I of this session)

Time: Friday 10:30–12:45 Location: HL 001

TT 111.1 Fri 10:30 HL 001

Ab initio photoluminescence in 2D materials — •Pedro Melo[1,4], Andrea Marini[2,4], Matthieu Verstraete[1,4], and Zeila Zanolli[3,4] — [1]NanoMat / CESAM, ULiege Belgium — [2]ISM CNR, Italy — [3]RWTH Aachen Germany — [4]ETSF

The theoretical study of photoluminescence (PL) has been hindered in the past due to lack of predictive ab initio numerical techniques [1,2,4]. We present a complete theoretical framework for the computation of PL where electrons, nuclei, and photons are quantised. The intrinsic non-equilibrium nature of the process is fully taken into account [3]. Starting from the Keldysh contour, we arrive at a set of equations for the Green's functions of electrons, phonons, and photons where the different kinds of interactions are treated on the same footing. These equations are then simplified by using the generalised Baym-Kadanoff ansatz and the completed collision approximation [3]. This reduces the problem to a set of decoupled equations for the density matrix that describe all kinds of static and dynamical correlations. We show how the micro-macro connection relates the observable spectrum with the time-dependent microscopic dynamics, via the Bethe-Salpeter equation. Finally, we present the results of our numerical studies on 2D materials, such as WS2, where we relate the evolution of the carrier populations in the Brillouin zone with the changes in the PL spectrum of the material, for a range of experimental setups. [1] M. F. Pereira and K. Henneberger, PRB 58, 2064 (1998). [2] K. Hannewald, et al, PRB 67, 233202 (2003). [3] P. M. M. C. de Melo and A. Marini, PRB 93, 155102 (2016). [4] S. W. Koch, et al, Nat Mat 5, 523 (2006).

TT 111.2 Fri 10:45 HL 001

Strain on molybdenum disulfide sheets with defects from first principles — •Mohammad Bahmani[1], Mahdi Faghihnasiri[2], and Thomas Frauenheim[1] — [1]BCCMS, Physics Department, Bremen University, Bremen, Germany — [2]Physics Department, Shahrood University of Technology, Shahrood, Iran

Single layer of transition metal dichalcogenides(TMDCs) are under intense investigations since the discovery of unique characteristics of 2D and Vann der Waals layered materials. They are predicted to be the most promising structure for various future nanoscale devices. They have also novel applications in spintronic and optoelectronic. As a result of thermal equilibrium and the kinetics of processing, all real materials contain structural defects which show significant effects on

their electrical, optical, vibrational, magnetic, and chemical properties. Besides, mechanical strain has very much influence on the electronic properties of 2D materials, particularly TMDCs. For example, 0.5% biaxial strain force direct band gap in molybdenum disulfide(MoS2) to become indirect since it breaks the crystalline symmetry. Therefore, I study different types of point defects such as single and double sulfur(S), single molybdenum(Mo) vacancies, and removing a Mo with its three upper S neighbors. I also substitute a Mo vacancy with one and two S atoms. Furthermore, as the second aim of this study, I showed the modification of defect states under uniaxial and biaxial compression and tensile strain. For the case of one S vacancy, this moves shallow states into the valance band and importantly breaks the degeneracy of degenerate states.

TT 111.3 Fri 11:00 HL 001

Competion of magnetic interactions and in-field behavior of cycloidal Uranium compound UPtGe. — •Leonid Sandratskii — Max Planck Institute of Microstructure Physics, Halle, Germany

Stimulated by recent high-field experiment [1] performed on unique actinide system with cycloidal magnetic structure, UPtGe, I performed a series of calculations aiming to understand the nature of the sequence of magnetic phase transitions caused by the applied magnetic field. The physics of the system is determined by the fine balance of the exchange interaction, magnetic anisotropy, and Dzyaloshinskii-Moriya interaction. This balance of interactions governs, in particular, the in-field behavior of the system. The physical consequences of the variation of the localization of the U 5f electrons is investigated.

[1] A. Miyake, A. Nakamura, Y. Shimura, Y. Honma, D. Li, F. Honda, M. Tokunaga, D. Aoki, doi.org/10.11316/jpsgaiyo.71.1.0_2062.

TT 111.4 Fri 11:15 HL 001

Electron correlation effects in the electronic structure of 4f-atoms adsorbed on metal and Graphene substrates — •Alexander B. Shick[1], Dmitry S. Shapiro[2], and Alexander I. Lichtenstein[3] — [1]Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]nstitute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow — [3]Institute of Theoretical Physics, University of Hamburg, Germany

Surface supported single magnetic atoms, the so-called "single-atom magnets", open new opportunities in a quest for the ultimate size limit of magnetic information storage. Initially, the research mainly focused on 3d-atoms on surfaces. Recently, the attention was turned to the 4f-atoms, culminating in the experimental discovery of magnetically stable Ho atom on MgO(001) substrate [1], and Dy atom on graphene/Ir(111)[2]. We address the electronic and magnetic character of 4f-atoms on metal and Graphene substrate making use of a combination of the DFT with the exact diagonalization of Anderson impurity model (DFT+ED) [3]. The spin and orbital magnetic moments of Dy@Ir(111) and Dy/Graphene/Ir(111) are evaluated and compared with experimental XMCD data. The magnetic anisotropy energy is estimated, and the magnetic stability is discussed. The role of 5d-4f interorbital exchange polarization in modification of the 4f-shell energy spectrum is emphasized. [1] F. Donati et al., Science 352, 318 (2016). [2] R. Baltic et al., Nano Lett. 16, 7610 (2016). [3] A. B. Shick, D. S. Shapiro, J. Kolorenc, A. I. Lichtenstein, Sci. Rep. 7, 2751 (2017).

TT 111.5 Fri 11:30 HL 001

Interlayer trions in the MoS_2/WS_2 van der Waals heterostructure — •Thorsten Deilmann and Kristian Sommer Thygesen — CAMD, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localisation of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type.

Here we investigate the complete set of interlayer excitations in a MoS_2/WS_2 heterostructure using a novel ab-initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers.

TT 111.6 Fri 11:45 HL 001

The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining — •Miguel Marques[1] and Antonio Sanna[2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Microstrukture Physics, Weinberg 2, 06120 Halle, Germany

Starting from the experimental data contained in the inorganic crystal structure database, we use a statistical analysis to determine the likelihood that a chemical element A can be replaced by another B in a given structure. This information can be used to construct a matrix where each entry (A,B) is a measure of this likelihood. By ordering the rows and columns of this matrix in order to reduce its bandwidth, we construct a one-dimension ordering of the chemical elements, analogous to the famous Pettifor scale. The new scale shows large similarities with the one of Pettifor, but also striking differences, especially in what comes to the ordering of the non-metals.

TT 111.7 Fri 12:00 HL 001

Novel two-dimensional topological insulators from first principles materials screening — •Thomas Olsen and Kristian Thygesen — Technical University of Denmark

We have applied first principles calculations to find new stable two-dimensional materials with non-trivial band topology. The novel materials include more than 10 quantum spin Hall insulators, quantum anomalous Hall insulators and topological crystalline insulators protected by mirror symmetry. We also discuss the dual topological nature of the band structure in the presence of both time-reversal and mirror symmetry and show that odd mirror Chern numbers always imply a quantum spin Hall effect.

TT 111.8 Fri 12:15 HL 001

Nanoparticles Classification with Self-Organisation Map (SOM) on 3D Electrostatic Potential Surface (EPS) — •Baichuan Sun and Amanda Barnard — Molecular & Materials Modelling, Data61 CSIRO, Door 34 Goods Shed, Village St, Docklands, VIC 3008, Australia

State-of-the-art deep learning (DL) algorithms are having tremendous impact across all scientific fields, and Material Science (MS) is no exception. A combination of computational chemistry simulations and DL techniques requires a hybrid computation/data research workflow, which represents a revolutionary approach to MS studies. There is a gap between the ab initio characterisation of nanomaterials with electronic structure simulations and its analytics with DL frameworks which stems from difficulties in representing quantum mechanical properties in such a way that is suitable for artificial neural networks. To overcome this issue we are evaluating the efficiency of visualising the 3-D Electrostatic Potential Surface (EPS) with Self-organising Maps (SOM), and integrating them directly into reliable DL frameworks. A Self-organisation Map classifies high-dimensional data into low-dimensional (normally 2D) space without supervision, while retaining the intrinsic topological relationship of the data set. As we will show, it is possible to represent a 3D molecular EPS with a single 2D snapshot, or "fingerprint" of the particle, provided they are orientationally invariant. In this study we demonstrate how Ag nanoparticles 3-D EPS self-organising texture maps can be used to classify nanoparticles based on the energy of the Fermi level.

TT 111.9 Fri 12:30 HL 001

Regulation of structure and high thermoelectric performance of 1D SnTe via encapsulation within single-walled carbon nanotube — Andrij Vasylenko[1], •Jamie Wynn[2], Sam Marks[1], Paulo V. C. Medeiros[3], Quentin M. Ramasse[4], Andrew J. Morris[4], Jeremy Sloan[1], and David Quigley[1] — [1]University of Warwick, Coventry, UK — [2]University of Cambridge, Cambridge, UK — [3]Daresbury Campus, Darsbury, UK — [4]University of Birmingham, Birmingham, UK

We present the extreme case of nanostructuring, exploiting capillarity of single-walled carbon nanotubes (SWCNTs) for synthesis of the smallest possible thermoelectric SnTe nanowires with cross sections as small as a single atom. By adapting high-throughput ab initio random structure searching, we discover several structures of SnTe that can be formed within SWCNT and compare results with experimentally obtained encapsulated SnTe nanowires. From first principles, we demonstrate that by choosing the appropriate diameter of a template SWCNT, we can manipulate the structure of 1D SnTe and its thermoelectric performance. The demonstrated technique opens a practical

route towards nanostructural manipulation of electrical and thermoelectric properties of the 1D materials. The best candidate 1D SnTe structures demonstrate strongly enhanced ZT over a unprecedentedly broad temperature range with a maximum value of 3.25.