Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture halls HSZ 03, HSZ 103, HSZ 201, HSZ 204, HSZ 304; Poster P2)

Plenary Talks

PLV VIII	Wed	14:00–14:45	HSZ 01	**Revealing the topological nature of transport at mesoscopic scales with quantum interferences** — •Hélène Bouchiat
PLV XIII	Thu	14:00–14:45	HSZ 02	**A Path Towards Room Temperature Superconductivity?** — •Mikhail Eremets

Invited Talks of the Joint Symposium SYSD (SKM Dissertation-Prize 2020)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited Talks of the Joint Symposium SYAS

See SYAS for the full program of the symposium.

SYAS 1.1	Mon	15:00–15:30	HSZ 02	**Ultrafast Coherent Spin-Lattice Interactions in Ferromagnets** — •Steven L. Johnson
SYAS 1.2	Mon	15:30–16:00	HSZ 02	**Ab-initio treatment of ultrafast spin-dynamics** — •Sangeeta Sharma
SYAS 1.3	Mon	16:00–16:30	HSZ 02	**Light-wave driven Spin Dynamics** — •Martin Schultze
SYAS 1.4	Mon	16:45–17:15	HSZ 02	**All-coherent subcycle switching of spins by THz near fields** — •Christoph Lange
SYAS 1.5	Mon	17:15–17:45	HSZ 02	**Ultrafast optically-induced spin transfer in ferromagnetic alloys** — •Stefan Mathias

Invited Talks of the Joint Symposium SYWH

See SYWH for the full program of the symposium.

SYWH 1.1	Wed	15:00–15:30	HSZ 02	**Engineering 2D materials with a twist** — •Cory Dean
SYWH 1.2	Wed	15:30–16:00	HSZ 02	**Flat Bands and Correlated Electronic States in Two Dimensional Atomic Crystals** — •Eva Y. Andrei

SYWH 1.3	Wed	16:00–16:30	HSZ 02	**Lightwave electronics and valleytronics in van der Waals layered materials** — •Rupert Huber
SYWH 1.4	Wed	16:30–17:00	HSZ 02	**Interaction and Topological Effects in Atomically Thin Two-dimensional Materials** — •Steven G. Louie
SYWH 1.5	Wed	17:00–17:30	HSZ 02	**Excitons in 2D Semiconductors and Heterostructures** — •Alexander Högele

Invited Talks of the Joint Symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch
SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Focus Session "Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers"

TT 11.1	Mon	15:00–15:30	HSZ 03	**Quantum simulations with linear ion crystals interacting with laser light** — •Christian Roos
TT 11.2	Mon	15:30–16:00	HSZ 03	**Entanglement spectroscopy on the IBM quantum computer** — •Titus Neupert
TT 11.3	Mon	16:00–16:30	HSZ 03	**Simulating quantum many-body systems on a quantum computer** — •Adam Smith
TT 11.4	Mon	16:45–17:15	HSZ 03	**Quantum computing and its applications in chemistry and physics** — •Ivano Tavernelli
TT 11.5	Mon	17:15–17:45	HSZ 03	**Randomized measurements: A toolbox for probing quantum simulators and quantum computers** — •Benoit Vermersch

Focus Session "The Nickel Age of Superconductivity: Cuprates Reloaded or Something New?"

TT 20.1	Tue	9:30–10:00	HSZ 03	**Superconductivity in infinite layer nickelates** — •Harold Hwang
TT 20.2	Tue	10:00–10:30	HSZ 03	**Materials design of dynamically stable d^9 layered nickelates** — •Ryotaro Arita
TT 20.3	Tue	10:30–11:00	HSZ 03	**Superconductivity in Nickelates: Similarities and Differences from Cuprates** — •Michael Norman
TT 20.4	Tue	11:15–11:45	HSZ 03	**Comparing the electronic structure and magnetism of hole doped Nickelate and Cuprate superconductorslate and Cuprate superconductors** — •George Sawatzky
TT 20.5	Tue	11:45–12:15	HSZ 03	**Doping infinite-layer nickelates: A superlattice approach** — •Eva Benckiser

Focus Session "Frontiers in Cryogenic Particle Detection"

TT 39.1	Wed	15:00–15:30	HSZ 03	**Magnetic Micro-Calorimeters: Present success stories, concepts and visions** — •Andreas Fleischmann
TT 39.2	Wed	15:30–16:00	HSZ 03	**Ultra-Sensitive Microwave Kinetic Inductance Detectors from the Optical to the Far Infrared** — •Jochem Baselmans
TT 39.3	Wed	16:00–16:30	HSZ 03	**LTS dc-SQUID sensors for TES and MMC readout** — •Jörn Beyer
TT 39.4	Wed	16:45–17:15	HSZ 03	**CRESST and NUCLEUS: The low-energy frontier of Dark Matter and neutrino physics** — •Raimund Strauss
TT 39.5	Wed	17:15–17:45	HSZ 03	**Large Array of Superconducting Transition-Edge Sensors for High Sensitive Photon and Particle Detectors** — •Luciano Gottardi

Invited Talks not included in Focus Sessions

TT 4.1	Mon	9:30–10:00	HSZ 204	**Towards an *ab-initio* theory of Anderson localization with correlated electrons** — •Liviu Chioncel
TT 14.1	Mon	15:00–15:30	HSZ 204	**Magnetotransport and 2D Superconductivity in Heterostructures of $BaBiO_3$ and $BaPbO_3$** — •German Hammerl
TT 35.1	Wed	9:30–10:00	HSZ 304	**Field-induced magnetic order in the Kitaev material α-$RuCl_3$** — •Lukas Janssen
TT 38.1	Wed	11:00–11:30	HSZ 103	**Nematic superconductivity in the superconducting doped topological insulators $Nb_xBi_2Se_3$ and $Sr_xBi_2Se_3$** — •Kristin Willa
TT 41.1	Wed	15:00–15:30	HSZ 201	**Probing unconventional superconductivity using the field dependent magnetic penetration depth** — •Joseph A. Wilcox
TT 55.1	Thu	9:30–10:00	HSZ 204	**Probing Triplet Superconductivity by Scanning Tunneling Spectroscopy** — •Elke Scheer
TT 63.1	Thu	15:00–15:30	HSZ 304	**Linear magnets: a structure-property-relation for finding unquenched orbital moments** — •Anton Jesche
TT 60.7	Thu	16:45–17:15	HSZ 103	**Heat and Work Fluctuations in a Quantum Heat Engine** — •Patrick P. Potts
TT 69.1	Fri	9:30–10:00	HSZ 03	**Microwave Optomechanics with Superconducting Quantum Interference Cavities** — •Daniel Bothner

Sessions

TT 1.1–1.12	Mon	9:30–12:45	HSZ 03	**Topological Insulators 1 (joint session TT/HL)**
TT 2.1–2.12	Mon	9:30–12:45	HSZ 103	**Superconductivity: Sample Preparation, Characterization, Properties and Electronic Structure**
TT 3.1–3.13	Mon	9:30–13:00	HSZ 201	**Complex Oxides: Bulk Properties (joint session TT/MA/HL)**
TT 4.1–4.6	Mon	9:30–11:15	HSZ 204	**Disordered Quantum Systems**
TT 5.1–5.13	Mon	9:30–13:00	HSZ 304	**Frustrated Magnets - General 1 (joint session TT/MA)**
TT 6.1–6.15	Mon	9:30–13:15	HSZ 401	**Cooperative Phenomena and Phase Transitions (joint session MA/TT)**
TT 7.1–7.7	Mon	9:30–11:15	HSZ 403	**Micro- and Nanostructured Materials (joint session MA/TT)**
TT 8.1–8.8	Mon	9:30–11:30	POT 6	**Topological Phenomena (joint session MA/TT)**
TT 9.1–9.13	Mon	10:00–13:30	HÜL 186	**Many-body Systems: Equilibration, Chaos and Localization I (joint session DY/TT)**
TT 10.1–10.6	Mon	11:30–13:00	HSZ 204	**Nanotubes and Nanoribbons**
TT 11.1–11.7	Mon	15:00–18:15	HSZ 03	**Focus Session: Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers (joint session TT/DY)**
TT 12.1–12.7	Mon	15:00–16:45	HSZ 103	**Topological Insulators 2 (joint session TT/HL)**
TT 13.1–13.13	Mon	15:00–18:30	HSZ 201	**Graphene (joint session TT/DY/HL)**
TT 14.1–14.11	Mon	15:00–18:15	HSZ 204	**Superconductivity: Theory 1**
TT 15.1–15.4	Mon	15:00–16:00	HSZ 304	**Frustrated Magnets - General 2 (joint session TT/MA)**
TT 16.1–16.48	Mon	15:00–19:00	P2/EG	**Poster Session Superconductivity, Cryogenic Particle Detectors, Cryotechnique**
TT 17.1–17.19	Mon	15:00–19:00	P2/EG	**Poster Session Correlated Electrons 1**
TT 18.1–18.8	Mon	16:15–18:15	HSZ 304	**Skyrmions (joint session TT/MA)**
TT 19.1–19.6	Mon	17:00–18:30	HSZ 103	**Low Dimensional Systems: Other Topics**
TT 20.1–20.7	Tue	9:30–12:45	HSZ 03	**Focus Session: The Nickel Age of Superconductivity: Cuprates Reloaded or Something New?**

TT 21.1–21.13	Tue	9:30–13:00	HSZ 103	**Topological Semimetals 1**
TT 22.1–22.14	Tue	9:30–13:15	HSZ 201	**Quantum Dots, Quantum Wires, Point Contacts**
TT 23.1–23.13	Tue	9:30–13:00	HSZ 204	**Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)**
TT 24.1–24.13	Tue	9:30–13:00	HSZ 304	**Frustrated Magnets - Spin Liquids 1 (joint session TT/MA)**
TT 25.1–25.12	Tue	9:30–13:00	POT 6	**Skyrmions I (joint session MA/TT)**
TT 26.1–26.7	Tue	14:00–15:45	HSZ 02	**Complex Oxides: Surfaces and Interfaces (joint session TT/MA/HL)**
TT 27.1–27.7	Tue	14:00–15:45	HSZ 103	**Topological Semimetals 2**
TT 28.1–28.7	Tue	14:00–15:45	HSZ 201	**Twisted Bilayer Graphene (joint session TT/HL)**
TT 29.1–29.8	Tue	14:00–16:00	HSZ 204	**Nonequilibrium Quantum Many-Body Systems 2 (joint session TT/DY)**
TT 30.1–30.5	Tue	14:00–15:15	HSZ 304	**Frustrated Magnets - Spin Liquids 2 (joint session TT/MA)**
TT 31.1–31.13	Wed	9:30–13:00	HSZ 03	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 1**
TT 32.1–32.5	Wed	9:30–10:45	HSZ 103	**Superconductivity: Theory 2**
TT 33.1–33.12	Wed	9:30–12:45	HSZ 201	**Correlated Electrons: Method Development 1**
TT 34.1–34.13	Wed	9:30–13:00	HSZ 204	**Correlated Electrons: f-Electron Systems and Heavy Fermions 1**
TT 35.1–35.12	Wed	9:30–13:00	HSZ 304	**Frustrated Magnets - Strong Spin-Orbit Coupling 1 (joint session TT/MA)**
TT 36.1–36.13	Wed	9:30–13:00	HÜL 186	**Many-body Systems: Equilibration, Chaos and Localization II (joint session DY/TT)**
TT 37.1–37.12	Wed	9:30–13:00	POT 6	**Skyrmions II (joint session MA/TT)**
TT 38.1–38.6	Wed	11:00–12:45	HSZ 103	**Topological Superconductors**
TT 39.1–39.8	Wed	15:00–18:30	HSZ 03	**Focus Session: Frontiers in Cryogenic Particle Detection**
TT 40.1–40.8	Wed	15:00–17:00	HSZ 103	**Topological Josephson Junctions**
TT 41.1–41.14	Wed	15:00–19:00	HSZ 201	**Unconventional Superconductors**
TT 42.1–42.10	Wed	15:00–17:45	HSZ 204	**Correlated Electrons: f-Electron Systems and Heavy Fermions 2**
TT 43.1–43.10	Wed	15:00–17:45	HSZ 304	**Frustrated Magnets - Strong Spin-Orbit Coupling 2 (joint session TT/MA)**
TT 44.1–44.14	Wed	15:00–19:00	HÜL 186	**Quantum Chaos (joint session DY/TT)**
TT 45.1–45.13	Wed	15:00–18:30	POT 6	**Skyrmions III (joint session MA/TT)**
TT 46.1–46.22	Wed	15:00–19:00	P2/2OG	**Poster Session: Frustrated Magnets, Quantum Magnets, Charge Order and Complex Oxids**
TT 47.1–47.30	Wed	15:00–19:00	P2/3OG	**Poster Session Correlated Electrons 2**
TT 48.1–48.12	Wed	15:00–19:00	P2/4OG	**Poster Session: Many Body Systems, Quantum Critical Phenomena**
TT 49.1–49.7	Wed	17:15–19:00	HSZ 103	**Topolectric Circuits and Quantum Hall Systems**
TT 50.1–50.4	Wed	18:00–19:00	HSZ 204	**Many-Body Localization**
TT 51.1–51.4	Wed	18:00–19:00	HSZ 304	**Molecular Electronics and Photonics (joint session TT/CPP)**
TT 52.1–52.11	Thu	9:30–12:30	HSZ 03	**Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 2 (joint session TT/HL)**
TT 53.1–53.14	Thu	9:30–13:15	HSZ 103	**Topology: Majorana Physics**
TT 54.1–54.14	Thu	9:30–13:15	HSZ 201	**Fe-based Superconductors**
TT 55.1–55.11	Thu	9:30–12:45	HSZ 204	**Superconductivity: Tunnelling and Josephson Junctions**
TT 56.1–56.13	Thu	9:30–13:00	HSZ 304	**Correlated Electrons: Quantum-Critical Phenomena**
TT 57.1–57.7	Thu	9:30–11:15	POT 6	**Skyrmions IV (joint session MA/TT)**
TT 58.1–58.6	Thu	10:30–12:00	GER 37	**Graphene I: Growth, Structure and Substrate Interaction (joint session O/TT)**
TT 59.1–59.13	Thu	15:00–18:30	HSZ 03	**Correlated Electrons: Quantum Impurities and Kondo Physics; Other Materials**
TT 60.1–60.9	Thu	15:00–17:45	HSZ 103	**Cryotechnique: Refrigeration and Thermometry**
TT 61.1–61.10	Thu	15:00–17:45	HSZ 201	**Ultrafast Dynamics of Light-Driven Systems (joint session TT/MA)**
TT 62.1–62.5	Thu	15:00–16:15	HSZ 204	**Correlated Electrons: Method Development 2**
TT 63.1–63.10	Thu	15:00–18:00	HSZ 304	**Quantum Magnets and Molecular Magnets (joint session TT/MA)**

TT 64.1–64.9	Thu	15:00–18:00	P1A	**Poster: Active Matter and Microswimmers (joint session DY/TT)**
TT 65.1–65.32	Thu	15:00–19:00	P2/EG	**Poster Session Topological Topics**
TT 66.1–66.18	Thu	15:00–19:00	P2/EG	**Poster Session Transport**
TT 67.1–67.8	Thu	16:30–18:30	HSZ 204	**Cold Atomic Gases and Superfluids**
TT 68	Thu	18:30–20:00	HSZ 03	**Annual General Meeting**
TT 69.1–69.3	Fri	9:30–10:30	HSZ 03	**Nano- and Optomechanics (joint session TT/HL/CPP)**
TT 70.1–70.5	Fri	9:30–10:45	HSZ 103	**Correlated Electrons: Charge Order**
TT 71.1–71.9	Fri	9:30–12:00	HSZ 304	**Correlated Electrons: Other Theoretical Topics**
TT 72.1–72.8	Fri	10:30–12:30	GER 37	**Graphene II: Adsorption, Intercalation and Doping (joint session O/TT)**
TT 73.1–73.5	Fri	11:00–12:15	HSZ 103	**Topology: Other Topics**

Annual General Meeting of the Low Temperature Physics Division

Thursday 18:30–20:00 Room HSZ 304

- Bericht
- Wahl
- Verschiedenes

TT 1: Topological Insulators 1 (joint session TT/HL)

Time: Monday 9:30–12:45 Location: HSZ 03

TT 1.1 Mon 9:30 HSZ 03

2D to 3D crossover in topological insulators — Corentin Morice, •Thilo Kopp, and Arno P. Kampf — University of Augsburg, Augsburg, Germany

At the heart of the study of topological insulators lies a fundamental dichotomy: topological invariants are defined in infinite systems, but their main footprint, surface states, only exists in finite systems. In systems in the slab geometry, namely infinite in two dimensions and finite in one, the 2D topological invariant was shown to display three different types of behaviours. In the limit of zero Dirac velocity along z, these behaviours extrapolate to the three 3D topological phases: trivial, weak and strong topological insulators. We show analytically that the boundaries of these regions are topological phase transitions of particular significance, and allow one to fully predict the 3D topological invariants from finite-thickness information. Away from this limit, we show that a new phase arises, which displays surface states but no band inversion at any finite thickness, disentangling these two concepts closely linked in 3D.

TT 1.2 Mon 9:45 HSZ 03

Correlated Ground States in Maximally Symmetric Flat Bands of 2D Topological Insulators — •Nikolaos Stefanidis and Inti Sodemann — Max-Planck-Institut für Physik komplexer Systeme,Nöthnitzer Str. 38, 01187 Dresden

We study the many body-problem in partially filled topological flat bands that are maximally symmetric realisations of two dimensional time-reversal invariant insulators. These bands can be viewed as two flat bands with opposite Chern numbers that are forced to be degenerate by time-reversal-symmetry. For half-filled bands we develop a mean field description of states that spontaneously break time reversal symmetry and their competition with translationally broken symmetry states and superconductors. At general fillings we prove a rigorous theorem dictating the absence of exact topological degeneracy for any translational and time reversal invariant two-body Hamiltonian. We also solve exactly the two body problem, which turns out to display a remarkable correlation between the center-of-mass and relative-coordinate degrees of freedom of the two particles.

TT 1.3 Mon 10:00 HSZ 03

Dynamic impurities in two-dimensional topological insulator edge states — •Simon Wozny[1], Martin Leijnse[1], Karel Vyborny[4], Wolfgang Belzig[3], and Sigurdur I. Erlingsson[2] — [1]Division of Solid State Physics and NanoLund, Lund University, Box 118, S-22100 Lund, Sweden — [2]School of Science and Engineering, Reykjavik University, Menntavegi 1, IS-101 Reykjavik, Iceland — [3]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [4]Institute of Physics, Academy of Science of the Czech Republic, Cukrovarnická 10, Praha 6, Czech Republic

Two-dimensional topological insulators give host one-dimensional helical states at the edges. These are characterized by spin-momentum locking and time-reversal symmetry protects the states from backscattering by potential impurities. Magnetic impurities break time-reversal symmetry and allow for backscattering. In an earlier work we investigated the effects of random, static, aligned magnetic impurities [1] on the spectrum and found that for fixed magnetic impurity strength the gap in the density of states closes with rising potential strength. We are now moving on to investigate the effect of random, aligned but harmonically rotating magnetic impurities. This is done by calculating the density of states via the time dependent Green's function for the system.

[1] S. Wozny, K. Vyborny, W. Belzig, and S. I. Erlingsson, Phys. Rev. B 98, 165423 (2018)

TT 1.4 Mon 10:15 HSZ 03

Topology and boundary physics in one dimensionional insulators — •Herbert Schoeller, Niclas Müller, Dante Kennes, and Mikhail Pletyukhov — RWTH Aachen University, Germany

Alternative to the characterization of topological insulators in terms of mathematical invariants we present a practical version via the explicit solution of the Schrödinger equation for a generic half-infinite system in one dimension. We show how the boundary condition can be fulfilled by taking appropriate linear combinations of Bloch eigenstates for the infinite system with complex quasimomentum [1]. Via this scheme all edge and bulk states can be explicitly constructed. In the presence of chiral or particle-hole symmetry the existence and stability of zero-energy edge states together with the bulk-boundary correspondence is established, proving the consistency with the standard classification scheme. Without symmetry constraints, we find generically edge states at finite energy in the gap and show that many bulk states are superpositions of Boch waves and exponentially decaying parts, implying interesting boundary physics at finite energy [2].

[1] D.M. Kennes et al., Phys. Rev. B 100, 041103 (2019).
[2] N. Müller et al., arXiv:1911.02295.

TT 1.5 Mon 10:30 HSZ 03

Topological invariants to characterize universality of boundary charge in one-dimensional insulators beyond symmetry constraints — •Mikhail Pletyukhov[1], Dante Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and Herbert Schoeller[1] — [1]RWTH Aachen University, Germany — [2]University of Basel, Switzerland

We address universal properties of the boundary charge Q_B for a wide class of tight-binding models with non-degenerate bands in one dimension [1]. We provide a precise formulation of the bulk-boundary correspondence by splitting Q_B via a gauge invariant decomposition in a Friedel, polarisation, and edge part. We reveal the topological nature of Q_B by proving the quantization of a topological index $I = \Delta Q_B - \bar{\rho}$, where ΔQ_B is the change of Q_B when shifting the lattice by one site towards a boundary and $\bar{\rho}$ is the average charge per site. For a single band we find this index to be given by the winding number of the fundamental phase difference of the Bloch wave function between two adjacent sites. For a given chemical potential we establish a central topological constraint $I \in \{-1, 0\}$ related to charge conservation and particle-hole duality.

[1] M. Pletyukhov et al, arXiv: 1911.06886, 1911.06890

TT 1.6 Mon 10:45 HSZ 03

Interaction effects in band insulators with topological properties — •Yen-Ting Lin, Volker Meden, Herbert Schoeller, and Dante M. Kennes — Institute for Theory of Statistical Physics, RWTH Aachen, and JARA- Fundamentals of Future Information Technology

One-dimensional models for band insulators such as the Su-Schrieffer-Heeger model or the Rice-Mele model currently regain attention as they show topological properties. We investigate the spinless versions of these models complemented by a two-particle interaction. To study the bulk as well as boundary and topological properties we use the functional renormalization group. The bulk gap shows the interaction dependent scaling predicted by an effective field theory. The density oscillations of an open boundary are modified by the interaction. The decay length of the exponential part is reduced and the inverse square root behavior of the pre-exponential function is altered. In addition, we present results for the boundary charge and the local single-particle spectral function.

TT 1.7 Mon 11:00 HSZ 03

Magnetoconductance, Quantum Hall Effect, and Coulomb Blockade in Topological Insulator Nanowires — •Raphael Kozlovsky, Ansgar Graf, Denis Kochan, Klaus Richter, and Cosimo Gorini — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Three-dimensional topological insulator (3DTI) nanowires host topologically non-trivial surface states wrapped around an insulating bulk. We investigate the transport properties of such wires subject to external electric and magnetic fields using effective surface Dirac Hamiltonians. By considering shaped (tapered, curved) 3DTI nanowires, we go beyond the well-studied cylindrical geometry [1] and thereby access intriguing mesoscopic transport phenomena: While the conductance of a wire in perpendicular magnetic field is in general quantized due to higher-order topological hinge states, the conductance in longitudinal magnetic field depends on the precise wire geometry. For rotationally symmetric nanowires with varying radius, a coaxial magnetic field leads to a spatial variation of the enclosed magnetic flux giving rise to a non-trivial mass potential along the wire direction. Depending on the radial profile of the wire, this mass potential leads, for instance,

to a conductance governed by the transmission through Dirac Landau levels, or to Coulomb blockade.
[1] arxiv:1909.13124 (2019)

15 min. break.

TT 1.8 Mon 11:30 HSZ 03

Electronic structure and properties of the surface of $TlBiSe_2$ in dependence on the coverage by Fe — •Svitlana Polesya[1], Sergiy Mankovsky[1], Alexander Liebig[2], Franz Giessibl[2], and Hubert Ebert[1] — [1]Dept. Chemistry, LMU Munich, Butenandtstrasse 11, D-81377 Munich, Germany — [2]Inst. Expt. and Appl. Physics, University Regensburg, Regensburg, Germany

We will present the results of investigations on the electronic structure of the surface of of the topological insulator $TlBiSe_2$ with different terminations by means of the tight binding KKR band structure method (TB KKR). The appearance of the topologically protected surface states at the Γ point is found in agreement with ARPES experiment. The modification of these states due to Fe adatoms deposited on top of the surface having different terminations, was investigated as a function of the degree of surface coverage by Fe. This study was performed via the CPA (Coherent Potential Approximation) alloy theory, assuming random occupation of the surface positions by Fe. The exchange coupling parameters have been calculated for different amount of Fe atoms covering the surface in order to determine the magnetic structure of the Fe overlayer, that can be probed by STM experiments.

TT 1.9 Mon 11:45 HSZ 03

MBE-grown Sb_2Te_3/Bi_2Te_3 heterostructures - Tuning of the topological surface states — Vanda M. Pereira, Chi-Nan Wu, Liu Hao Tjeng, and •Simone G. Altendorf — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Topological insulators (TIs) are bulk insulators with the bulk band gap only intersected by conducting, Dirac-cone like surface states that are topologically protected. For many materials, the Dirac point of these surface states lays buried in the bulk bands which hinders an experimental observation of the various theoretically predicted topological quantum effects, like the quantum anomalous Hall effect.

In our study, we combine two TIs, namely Sb_2Te_3 and Bi_2Te_3, in a heterostructure which allows for a tuning of the position of the Dirac point to the Fermi level by varying the layer thicknesses. Using the optimized layer structure, we investigate the changes of the TI properties when interfaced with a magnetic substrate. We will present a characterization of the MBE-grown Sb_2Te_3/Bi_2Te_3 heterostructures on non-magnetic and magnetic substrates by RHEED, XPS, ARPES, XMCD, and transport measurements.

TT 1.10 Mon 12:00 HSZ 03

Topological insulator interfaced with ferromagnetic insulators: Bi_2Te_3 thin films on magnetite and iron garnets — V. M. Pereira[1], S. G. Altendorf[1], C. E. Liu[1], S. C. Liao[1], A. C. Komarek[1], M. Guo[2], H. -J. Lin[3], C. T. Chen[3], M. Hong[4], J. Kwo[2], L. H. Tjeng[1], and •C. N. Wu[1,2] — [1]MPI CPfS, Dresden, Germany — [2]Dept. of Phys., NTHU, Hsinchu, Taiwan — [3]NSRRC, Hsinchu, Taiwan — [4]Dept. of Phys., NTU, Taipei, Taiwan

We report on our study about the growth and characterization of Bi_2Te_3 thin films on top of $Y_3Fe_5O_{12}(111)$, $Tm_3Fe_5O_{12}(111)$, $Fe_3O_4(111)$, and $Fe_3O_4(100)$ single crystal substrates. Using molecular beam epitaxy, we were able to prepare the topological insulator / ferromagnetic insulator heterostructures with no or minimal chemical reaction at the interface. We observed the anomalous Hall effect on these heterostructures and also a suppression of the weak antilocalization in the magnetoresistance, indicating a topological surface state gap opening induced by the magnetic proximity effect. However, we did not observe any obvious x-ray magnetic circular dichroism (XMCD) on the Te M_{45} edges. The results suggest that the ferromagnetism induced by the magnetic proximity effect via Van der Waals bonding in Bi_2Te_3 is too weak to be detected by XMCD, but still can be observed by electrical transport measurements. This is in fact not inconsistent with reported density-functional calculations on the size of the gap opening.

TT 1.11 Mon 12:15 HSZ 03

Time dependent Rashba coupling at the helical edge — •Lorenzo Privitera[1], Niccolò Traverso ZIani[2], Simone Barbarino[3], Jan Carl Budich[3], and Björn Trauzettel[1] — [1]Institute for Theoretical Physics, University of Würzburg, 97074 Würzburg, Germany — [2]Dipartimento di Fisica, Università di Genova, and SPIN-CNR, Via Dodecaneso 33, 16146 Genova, Italy — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Time-dependent effects in the edges of quantum spin Hall insulators (QSHI) have been the subject of intense research in the last years. In particular, it was recently pointed out that the interplay of electromagnetic temporal noise with Rashba impurities might play a prominent role in the observed breaking of perfect conductance quantization. In this work we study the conductance of a QSHI edge subjected to the time-periodic oscillations of the strength of a single Rashba impurity. We investigate the perturbative regime of the impurity and examine the effects of repulsive interactions through bosonization. The resulting backscattering current is the sum of three different power laws in driving frequency and voltage, marking a clear distinction from nonhelical Luttinger liquids. Furthermore, we find that backscattering can become stronger for weak interactions upon tuning the frequency of the driving. Our results provide a further step in the understanding of time-dependent perturbations in 1d electronic liquids and are of particular interest in view of the technological applications arising from the time-dependent manipulation of topological edge states.

TT 1.12 Mon 12:30 HSZ 03

Thermoelectric effects in a helical edge coupled to a quantum magnet — •Peter Silvestrov[1], Piet Brouwer[2], and Patrik Recher[1,3] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Physics Department and Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [3]Laboratory for Emerging Nanometrology Braunschweig, 38106 Braunschweig, Germany

We explore the analogy between a helical edge current interacting with a microscopic magnet and the adiabatic quantum motor[1-3], with special emphasis on thermal effects. These include a thermal engine, in which the thermal gradient is converted directly into mechanical work, a device producing an AC current from the temperature gradient, and an electron refrigerator.
[1] Q. Meng, S. Vishveshwara, and T. L. Hughes, Phys. Rev. B **90**, 205403 (2014).
[2] L. Arrachea and F. von Oppen, Physica E **74**, 596 (2015).
[3] P. G. Silvestrov, P. Recher, and P. W. Brouwer, Phys. Rev. B **93**, 205130 (2016).

TT 2: Superconductivity: Sample Preparation, Characterization, Properties and Electronic Structure

Time: Monday 9:30–12:45 Location: HSZ 103

TT 2.1 Mon 9:30 HSZ 103

Magnetic proximity effect in Nb/Gd superlattices seen by neutron reflectometry — •Yury Khaydukov[1,2,3], Evgeny Kravstov[4,5], Vladimir Zhaketov[6], Vyacheslav Progliado[4], Gideok Kim[1], Yury Nikitenko[6], Thomas Keller[1,2], Vladimir Ustinov[4,5], Viktor Aksenov[6], and Bernhard Keimer[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Max Planck Society Outstation at the Heinz Maier-Leibnitz Zentrum (MLZ), D-85748 Garching, Germany — [3]Skobeltsyn Institute of Nuclear Physics, Moscow State University, Moscow 119991, Russia — [4]Institute of Metal Physics, Ekaterinburg 620180, Russia — [5]Ural Federal University, Ekaterinburg 620002, Russia — [6]Joint Institute for Nuclear Research, Dubna 141980, Russia

We used polarized neutron reflectometry to investigate the magnetization profile of superlattices composed of ferromagnetic Gd and superconducting Nb layers [1]. Below the superconducting (S) transition of the Nb layers we observed a partial suppression of ferromagnetic

(F) order of Gd layers in [Gd(d_F)/Nb(25nm)]$_{12}$ superlattices. The amplitude of the suppression decreases with increasing d_F. By analyzing the neutron data we conclude that the observed effect has an electromagnetic origin - the proximity-coupled S layers screen out the external magnetic field and thus suppress the F response of the Gd layers. Our investigation demonstrates significance of electromagnetic effects, and potential of elemental S/F multilayers as simple model systems for ferromagnetic superconductors.

[1] Khaydukov et al., Phys. Rev. B 99, 140503 (R) (2019)

TT 2.2 Mon 9:45 HSZ 103

Interface effects in magnetic and superconducting heterostructures — •Sebastian Kölsch and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany

Niobium-based thin films in combination with non-collinear ferromagnetic layers offer the potential for applications in superconducting spintronics, especially in superconducting spin valves (SSV) [1]. Regarding the interface between these two different layers, a gapless and odd-in-frequency superconducting ground state may be stabilized, where the Cooper-pairs remain in a spin-triplett configuration.

Considering potential applications, a reduction of complexity in terms of a single magnetic layer in SVVs is mandatory. In this case the binary compounds of manganese-silicon appear as an ideal partner due to their rich magnetic phase diagram [2]. Here we present recent results on the successful growth of manganese-silicon thin films on a superconducting niobium layer.

[1] N.G. Pugachet al. Appl. Phys. Lett. 111, 162601 (2017)
[2] I. I. Lobanova et al. Scientific Reports 6, 22101 (2016)

TT 2.3 Mon 10:00 HSZ 103

Investigating the proximity effects in chiral molecules on conventional superconductors — Hen Alpern[1], •Roman Hartmann[2], Nir Sukenik[1], Shira Yochelis[1], Itai Keren[1], Hadar Steinberg[1], Zaher Salman[3], Elke Scheer[2], Yossi Paltiel[1], Oded Milo[1], and Angelo Di Bernardo[2] — [1]Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, 91904 Israel — [2]Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany — [3]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Superconducting spintronics is emerging as an alternative technology that can overcome the main limitations of conventional spintronic devices related to their high current dissipations. It has developed after the recent discovery that Cooper pairs with parallel-aligned spins (spin-triplets) can be generated at the interface between a conventional superconductor (S) and a magnetically inhomogeneous ferromagnet (F). More recently, by performing low-temperature STM measurements of the density of states of chiral molecules (ChMs) adsorbed on the surface of a Nb (S) thin film, we have observed subgap features due to spin-triplet states in such system, without an F layer. Based on these results, we have carried out low-energy muon spectroscopy on ChMs/Nb demonstrating evidence for an inverse (paramagnetic) Meissner state meaning an increase in the local field above the applied field in the superconducting state, with an amplitude variation depending on the Nb thickness. This provides spectroscopic evidence for spin-triplet pairing in ChMs/Nb and paves the way for novel superconducting devices.

TT 2.4 Mon 10:15 HSZ 103

STM and STS studies of superconducting 1T-TaSeS — •Marion A. van Midden[1], Yaroslav Gerasimenko[1,2], Petra Šutar[1], Erik Zupanič[1], and Dragan Mihailovic[1,2] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]Center of Excellence in Nanoscience and Nanotechnology, Ljubljana, Slovenia

In 1T-TaS_2, similarly to many high-temperature superconductors, superconductivity, charge density waves (CDW) and Mott insulating (MI) states coexist. The MI state is suppressed upon doping [1], substitution [2] or pressure [3]. Until recently, it has been believed that this, together with the formation of CDW domain walls, is crucial for the onset of superconductivity. However, recent studies at T > T_{SC} have challenged this hypothesis in 1T-TaS_2 and 1T-$TaSe_xS_{2-x}$ [4]. We study superconducting 1T-TaSeS close to optimal T_{SC} = 3.5 K using high-resolution scanning tunneling spectroscopy (STS) both below and above T_{SC}. In contrast to pure 1T-TaS_2 we observe a finite density of states inside the Mott gap both inside the domains and at the domain walls. STS at T = 1.2 K shows a small 1-2 meV gap at the Fermi level that vanishes at T > 5K, strongly suggesting it is related to SC. It is clearly uncorrelated with the CDW domain walls of any kind in clear contrast with the simple domain wall picture. This suggest a different, correlated picture of SC onset.

[1] L. J. Li et al., European Physics Letters 97, 67005 (2012).
[2] Y. Liu et al., Applie Physics Letters. 102, 192602 (2013).
[3] B. Sipos et al., Nature Materials 7, 960 (2008).
[4] J. Skolimowski, Y. Gerasimenko and R. Žitko, PRL, 122 (2019).

TT 2.5 Mon 10:30 HSZ 103

Detection and control of phase slip lines in plain superconducting $NbSe_2$ devices — •Nicola Paradiso[1], Michaela Eichinger[1], Christian Bäuml[1], Kenji Watanabe[2], Takashi Taniguchi[2], and Christoph Strunk[1] — [1]University of Regensburg — [2]National Institute for Materials Science, Tsukuba, Japan

In ordinary superconductors the dissipationless state is destroyed when the current density reaches a critical value, known as depairing current. On the other hand, it was recently found [1,2] that in superconducting 2D materials as $NbSe_2$, dissipation emerges as a sequential nucleation of so-called phase slip lines (PSL). Such nucleation occurs for current densities well below the depairing value. Here we study PSLs on plain few-layer $NbSe_2$ crystals. By transport measurements we can observe the repulsive interaction between PSLs. Moreover, by using a carbon nanotube as a local heater, we can locally tune the critical current for the nucleation of one individual PSL. Our observations show that PSLs are localized and interacting objects, whose nucleation can be locally controlled.

[1] N. Paradiso *et al.*, 2D Materials, **6**, 025039 (2019);
[2] S. Tran *et al.*, arXiv:1903.00453v3 (2019).

TT 2.6 Mon 10:45 HSZ 103

Transport measurements on microstructured samples of neodymium doped $CeCoIn_5$ — •J. Stirnat[1,2], S. Hamann[1,3], M. Winter[1,2], M. König[3], L. Bischoff[4], C. Petrovic[5], T. Helm[1,3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Technische Universität Dresden (TUD), Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe (MPI CPfS), Dresden, Germany — [4]Ionenstrahlzentrum (IBC), HZDR, Dresden, Germany — [5]Brookhaven National Laboratory, Upton, USA

$CeCoIn_5$ is known to host d-wave heavy-fermion superconductivity and also a high-field superconducting phase, the Q phase. In neodymium the $4f$-electrons do not hybridize with the conduction electrons. Therefore, substituting a certain amount of the cerium atoms in $CeCoIn_5$ with neodymium, spin density waves and antiferromagnetic order can be induced. Previous de Haas-van Alphen measurements show that with increasing Nd doping the Fermi surfaces of $CeCoIn_5$ are reconstructed from a quasi-two-dimensional to a three-dimensional topology. Such a dramatic change may also be reflected by the electrical transport anisotropy. In order to gain access to different conduction-channel directions, we fabricated micrustructures of Nd-doped $CeCoIn_5$ using focused ion beam (FIB) microfabrication. Our goal is to study the effect of Nd doping on the resistivity anisotropy in high magnetic fields. In this talk I will present first preliminary results in fields of up to 16 T and at ^{3}He temperatures.

TT 2.7 Mon 11:00 HSZ 103

Crystal structure and superconducting properties of $Sc_5Ir_6Sn_{18}$ — •Manuel Feig[1,2], Volodymyr Levytskyi[1,3], Lev Akselrud[2,3], Walter Schnelle[2], Andreas Leithe-Jasper[2], Vadim Dyadkin[4], Dmitry Chernyshov[4], and Roman Gumeniuk[1,2] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]Ivan Franko National University of Lviv. Kyrala and Mefodiya Str. 6, UA-79005, Lviv, Ukraine — [4]Swiss-Norwegian Beamline at ESRF, CS 40220, 38043 Grenoble Cedex 9, France

High quality single crystals of $Sc_5Ir_6Sn_{18}$ were grown from Sn melt. A split variant of the $Tb_5Rh_6Sn_{18}$ structure type (SG: $I4_1/acd$, $a \approx 13.6$ Å, $c \approx 27.2$ Å) was obtained from both single crystal and powder X-ray diffraction. The instability of the crystal structure without splits could be confirmed by DFT calculations. Measurements of the magnetic susceptibility, specific heat capacity and electrical resistivity revealed $Sc_5Ir_6Sn_{18}$ to be a metallic diamagnet with a superconducting transition temperature $T_c = 2.64$ K. The obtained values for the second critical field $B_{c2} = 3.2$ T, the specific heat jump $\Delta c_p/\gamma_N T_c = 1.73$ and the energy-gap ratio $\Delta(0)/k_B T_c = 1.85$ indicate this compound to be a weakly coupled s-wave BCS superconductor.

15 min. break.

TT 2.8 Mon 11:30 HSZ 103

The electronic structure of infinite-layer nickelates — •Matthias Hepting[1,8], Danfeng Li[1], Chunjing Jia[1], Haiyu Lu[1], Eugenio Paris[2], Yi Tseng[2], Xiao Feng[1], Motoki Osada[1], Emily Been[1], Yasuyuki Hikita[1], Yi-De Chuang[3], Zahid Hussain[3], Ke-Jin Zhou[4], Abhishek Nag[4], Mirian Garcia-Fernandez[4], Matteo Rossi[1], Hsiao-Yu Huang[5], Di-Jing Huang[5], Zhi-Xun Shen[1,6], Thorsten Schmitt[2], Harold Hwang[1], Brian Moritz[1], Jan Zaanen[7], Thomas Devereaux[1], and Wei-Sheng Lee[1] — [1]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, USA — [2]PSI, Switzerland — [3]ALS, LBNL, USA — [4]Diamond Light Source, United Kingdom — [5]NSRRC, Hsinchu Science Park, Taiwan — [6]Geballe Lab, Stanford University, USA — [7]Instituut-Lorentz for Theoretical Physics, Leiden University, Netherlands — [8]Max Planck Institute for Solid State Research, Germany

The recent discovery of superconductivity in the Sr-doped infinite-layer nickelate $NdNiO_2$ has revived the search for materials with physical properties similar to cuprate high-temperature superconductors. We have used x-ray spectroscopy and density functional theory to show that the electronic structure of the undoped parent compound RNiO2 (R = La, Nd), while similar to the cuprates, includes significant distinctions [1]. The material can be regarded as a Kondo- or Anderson-lattice-like oxide-intermetallic, replacing the Mott insulator as the reference state from which superconductivity emerges upon doping.

[1] M. Hepting *et al.*, arXiv:1909.02678 (2019).

TT 2.9 Mon 11:45 HSZ 103

Properties of sputtered films of the electron-doped $Nd_{2-x}Ce_xCuO_{4-d}$ superconductor — •Angela Nigro[1], Anita Guarino[2], Pasquale Marra[3,4], Antonio Leo[1], and Gaia Grimaldi[2] — [1]Dipartimento di Fisica E. R. Caianiello, Università degli Studi di Salerno, 84084 Fisciano (Salerno), Italy — [2]CNR-SPIN, c/o Dipartimento di Fisica E. R. Caianiello, Università degli Studi di Salerno, 84084 Fisciano (Salerno), Italy — [3]Graduate School of Mathematical Sciences, The University of Tokyo, Tokyo,Japan — [4]Department of Physics, Keio University, 4-1-1 Hiyoshi, Yokohama, Kanagawa 223-8521, Japan,Japan

In $RE_{2-x}Ce_xCuO_{4-d}$ (RE =rare earth) electron-doped cuprates, the superconductivity is harder to achieve since as-grown samples are antiferromagnetic up to high doping levels, and become superconducting only after a special annealing process. The role of the annealing treatment still constitutes an open question for n-type superconductors. We investigate the electrical and structural properties of $Nd_{2-x}Ce_xCuO_4$ films grown by a sputtering technique in an oxygen deficient environment, in order to obtain information on the complete oxygen-phase diagram. The as-grown samples are non-superconducting and the structural properties are consistent with a deficiency of the oxygen content. Unexpectedly, a reducing thermal treatment at high temperature is able to induce superconductivity in these films. Our data seem to support the picture that the high-temperature annealing procedure induces a peculiar oxygen atoms distribution triggering the superconducting transition in these compounds.

TT 2.10 Mon 12:00 HSZ 103

Evidence for an orbital dependent Mott transition in the ladders of $(La, Ca)_xSr_{14-x}Cu_{24}O_{41}$ derived by electron energy-loss spectroscopy — •Friedrich Roth[1], Udo Ammerahl[2], Alexandre Revcolevschi[2], Bernd Büchner[3], Martin Knupfer[3], and Jörg Fink[3,4,5] — [1]Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Straße 23, D-09599 Freiberg, Germany — [2]Laboratoire de Physico-Chimie de l'État Solide, Université Paris-Sud, 91405 Orsay, France — [3]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [4]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [5]Institute for Solid-State and Material Physics, Technical University Dresden, D-01062 Dresden, Germany

The knowledge of the charge carrier distribution among the different orbitals of Cu and O is a precondition for the understanding of the physical properties of various Cu-O frameworks. We employ electron energy-loss spectroscopy to elucidate the charge carrier plasmon dispersion in $(La, Ca)_xSr_{14-x}Cu_{24}O_{41}$ in dependency of x as well as temperature. We observe that the energy of the plasmon increases upon increasing Ca content, which signals an internal charge redistribution between the two Cu-O subsystems. Moreover, a comparison of the experimental plasmon excitations with RPA-like calculations indicates that the holes which are transferred to the Cu_2O_3 ladders are mainly located on O orbitals in the rungs and to a much lesser extent in those in the legs. This is related to a different filling of the bonding and antibonding band leading to an orbital dependent Mott transition.

TT 2.11 Mon 12:15 HSZ 103

Combinatorial Laser Molecular Beam Epitaxy System Integrated with Specialized Low-temperature Scanning Tunneling Microscopy — •Ge He[1,2], Zhongxu Wei[1,2], Zhongpei Feng[1,2], Xiaodong Yu[1,2], Beiyi Zhu[1], Li Liu[1], Kui Jin[1,2,3,4], Jie Yuan[1,3,4], and Qing Huan[1,3,4,5] — [1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China — [4]Key Laboratory for Vacuum Physics, University of Chinese Academy of Sciences, Beijing 100190, China — [5]CAS Center for Excellence in Topological Quantum Computation, University of Chinese Academy of Sciences, Beijing 100190, China

We describe the setting-up and the performance of a newly developed combined system of combinatorial laser molecular beam epitaxy and low-temperature ultra-high vacuum scanning tunneling microscopy. This facility aims at accelerating the materials research in a highly efficient way, by advanced high-throughput film synthesis techniques and subsequent fast characterization of surface morphology and electronic states. During five years efforts, the system has exhibited good stability on both combi-film deposition and STM measurements, and decidedly appreciated advantages in both exploring new materials and investigating novel physical phenomenon.

TT 2.12 Mon 12:30 HSZ 103

Raman signatures of the Higgs mode in d-wave superconductors — •Matteo Puviani and Dirk Manske — Max Planck Institute for Solid State Research, Stuttgart, Germany

The amplitude mode (so called "Higgs" mode) in superconductors originates from the Anderson-Higgs mechanism in the symmetry-broken phase and consists of the oscillation of the order parameter with twice the gap energy[1]. Electronic Raman scattering in superconductors probes charge excitations across the superconducting gap, and thus is a valid candidate to provide information about the modes of the order parameter[2,3].

We investigated the role of the Higgs oscillations in d-wave superconductivity with the theoretical simulation of the Raman response for different light polarizations. In particular, we calculated the full Raman vertices' corrections in the amplitude channel: our results show the presence of a relevant Higgs contribution for the A1g spectrum which could solve the A1g problem[4].

Moreover, with the same theoretical approach, we are able to explain the very last experimental results of the current-assisted activation of the Higgs mode in superconductors[5].

[1] P.B. Littlewood and C.M. Varma, Phys. Rev. B 26, 4883 (1982)
[2] M.V. Klein and S.B. Dierker, Phys. Rev. B 29, 4976 (1984)
[3] T. Cea and L. Benfatto, Phys. Rev. B 90, 224515 (2014)
[4] T.P. Devereaux et al., Phys. Rev. Lett. 72, 396 (1994)
[5] S. Nakamura et al., Phys. Rev. Lett. 122, 257001 (2019)

TT 3: Complex Oxides: Bulk Properties (joint session TT/MA/HL)

Time: Monday 9:30–13:00 Location: HSZ 201

TT 3.1 Mon 9:30 HSZ 201

Single-crystal growth and magnetic phase diagram of $TbFeO_3$ — •Alexander Engelhardt[1], Georg Benka[1], Christian Oberleitner[1], Andreas Bauer[1], Andreas Erb[2], and Christian Pfleiderer[1] — [1]Physik Department E51, Technische Universität München, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Walther-Meißner-Str. 8, 85748 Garching, Germany

Single crystals of the multiferroic rare earth orthoferrite $TbFeO_3$ were synthesized by means of optical float-zoning. The magnetization, the longitudinal and the transverse ac susceptibility, as well as the specific heat were measured at low temperatures under large applied magnetic fields to determine the complex, anisotropic magnetic phase diagram of $TbFeO_3$ along the three major crystallographic axes. Taken together, our data are consistent with previous studies reported in the literature. As a new result we identify clear evidence in the bulk properties of the formation of a soliton lattice in a small temperature range, so far observed by means of neutron scattering only.

TT 3.2 Mon 9:45 HSZ 201

Melting of excitonic dispersion in $LaCoO_3$: theory and experiment — Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1,3], Keisuke Tomiyasu[4], Davide Betto[5], Nicholas B. Brookes[5], Yohei Uemura[2], Mahnaz Ghiasi[2], Frank M. F. de Groot[2], and •Jan Kuneš[1,6] — [1]Institute of Solid State Physics, TU Wien — [2]Debye Institute for Nanomaterials Science, Utrecht University — [3]Akhiezer Institute for Theoretical Physic, Kharkiv — [4]Department of Physics, Tohoku University — [5]European Synchrotron Radiation Facility, Grenoble — [6]Institute of Physics, Czech Academy of Sciences

We present Co L_3-edge resonant inelastic x-ray scattering (RIXS) on bulk $LaCoO_3$ across the thermally-induced spin-state crossover around 100 K. Owing to a high energy resolution of 20 meV, we observe unambiguously the dispersion of the intermediate-spin (IS) excitations in the low temperature regime. Approaching the intermediate temperature regime, the IS excitations are damped and the bandwidth reduced. The observed behavior can be well described by a model of mobile IS excitons with strong attractive interaction, which we solve using dynamical mean-field theory for hard-core bosons. Our results provide a detailed mechanism of how HS and IS excitations interact to establish the physical properties of cobaltite perovskites.

TT 3.3 Mon 10:00 HSZ 201

Spin Selective Quasi-Particle Interference in $PdCoO_2$ — •Dibyashree Chakraborti[1,2], Chi Ming Yim[1], Luke Rhodes[1], Seunghyun Khim[2], Andrew Mackenzie[1,2], and Peter Wahl[1] — [1]School of Physics and Astronomy, St. Andrews, Scotland, United Kingdom, KY169SS — [2]Max Planck Institute of Chemical Physics of Solids, Noethnitzer Strasse, Dresden -01187

The metallic delafossite $PdCoO_2$, which is among the most conductive oxides currently known (at 295 K) [1], has risen to prominence due to interesting physical effects, such as unusually long mean free paths, leading to hydrodynamic effects being observed in electron flow [2]. Further, recent Angle Resolved Photoemission Spectroscopy (ARPES) studies have reported exciting surface-physics on the CoO_2-terminated surface. The CoO_2 surface shows evidence of large Rashba spin-splitting, arising from the interplay of energy scales due to strong spin orbit coupling and inversion symmetry breaking at the surface. [3]. In this study, we have identified and investigated the CoO_2 termination of $PdCoO_2$ with low temperature Scanning Tunneling Microscopy (STM). We present and discuss the quasi-particle interference imaging of the Rashba spin-split surface state, and the implications for possible spintronics applications.

[1] C.W. Hicks et al., Phys. Rev. Lett. 109, 116401 (2012)
[2] P.J.W. Moll et al., Science 351, 1061 (2016)
[3] V. Sunko et al., Nature 549, 492 (2017)

TT 3.4 Mon 10:15 HSZ 201

Interplay of Electronic and Spin Degrees in Ferromagnetic $SrRuO_3$: Anomalous Softening of the Magnon Gap and Stiffness — •Kevin Jenni[1], Stefan Kunkemöller[1], Daniel Brüning[1], Thomas Lorenz[1], Yvan Sidis[2], Astrid Schneidewind[3], Augustinus Agung Nugroho[4], Achim Rosch[5], Daniil Iljitsch Khomskii[1], and Markus Braden[1] — [1]II. Physikalisches Institut, Universität zu Köln, Deutschland — [2]Laboratoire Leon Brillouin, Grenoble, Frankreich — [3]JCNS, Forschungszentrum Jülich, Garching, Deutschland — [4]Institut Teknologi Bandung, Indonesien — [5]Institut für Theoretische Physik, Universität zu Köln, Deutschland

We succeeded to grow large single crystals of $SrRuO_3$ using the floating-zone technique [1,2]. The first inelastic neutron scattering study of the spin dynamics on single crystals yields the expected quadratic spin wave dispersion of a ferromagnet. However the magnon gap and stiffness considerably deviate from an earlier inelastic neutron scattering study on powders [3]. In addition we find a non-monotonous temperature dependence of the anisotropy gap and a softening of the magnon stiffness upon cooling. We discuss how Weyl points caused by SOC in $SrRuO_3$ couple electronic and spin degrees of freedom and how this interplay leads to the characteristic behavior in the spin dynamics [4].

[1] S. Kunkemöller et al., Chrys. Res Tec. 51, 299 (2016)
[2] S. Kunkemöller et al., PRB 96, 220406(R) (2017)
[3] S. Itoh et al., Nat. Commun. 7, 11788 (2016)
[4] K. Jenni et al., Phys. Rev. Lett. 123, 017202 (2019)

TT 3.5 Mon 10:30 HSZ 201

Ca_2RuO_4: DFT + DMFT study of the magnetic order and dynamical susceptibility — •Dominique Geffroy[1,2], Kyo-Hoon Ahn[1], Hoshin Gong[4], and Jan Kuneš[1,3] — [1]TU Wien, Vienna, Austria — [2]Masaryk University, Brno, Czech Republic — [3]Czech Academy of Science, Prague, Czech Republic — [4]Max Planck POSTECH/Korea Research Initiative, Pohang, Korea

Relativistic Mott insulators are complex compounds in which spin and orbital degrees of freedom become entangled due to a large spin-orbit coupling. Previous studies, both experimental and theoretical[1, 2], have shown that they are good candidates for novel forms of order, including excitonic magnetism[3]. We report results on the theoretical study of the prototypical relativistic Mott insulator Ca_2RuO_4. We use a realistic ab initio DFT + DMFT approach including SU(2) Coulomb interaction and spin-orbit coupling. The emergence of antiferromagnetic order at low temperature is correctly described. We present and discuss the spectra of the the collective modes in the ordered phase within the DMFT approximation.

[1] Jain et al., Nat. Physics 13, 633 (2017)
[2] G. Zhang and E. Pavarini, Phys. Rev. B 95, 075145 (2017)
[3] A. Akbari and G. Khaliullin, Phys. Rev. B 90, 035137 (2014)

TT 3.6 Mon 10:45 HSZ 201

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Rare-Earth Nickelates — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We present a computational study of L-edge resonant inelastic x-ray scattering (RIXS) across the metal-insulator transition (MIT) of $LuNiO_3$. We apply exact diagonalization to a material specific Anderson impurity model with a by DMFT obtained hybridization function. In contrast to other available methods, this approach enables us to describe simultaneously localized (d-d) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. We reproduce the experimentally observed behaviour of fluorescence-like and Raman-like features across the MIT and provide its material specific interpretation.

TT 3.7 Mon 11:00 HSZ 201

Interplay of electronic correlations, charge disproportionation and lattice in $RNiO_3$ nickelates with R = Lu, Y, and Bi — •Ivan Leonov — M. N. Mikheev Inst. of Metal Physics, Yekaterinburg, Russia — NUST 'MISiS', Moscow, Russia

In recent years, increasing attention has been drawn to the understanding of the rare-earth-element nickelate perovskites $RNiO_3$, which exhibit a sharp metal-insulator transition (MIT). The MIT is accompanied by a structural phase transformation, complicated by the appearance of unusual charge order and non-collinear magnetic phases in the Mott insulating regime. Here, I will focus on this particular problem and will discuss an application of the DFT+DMFT method to explore the electronic structure, magnetic and lattice properties of a series of $RNiO_3$ nickelates with R = Lu, Y, and Bi. I will discuss our results for the pressure-induced Mott MIT in $RNiO_3$, which is found to be accompanied by a structural transformation. While the rare-earth and Bi $RNiO_3$ are closely related in their electronic state and crystal structure, these materials exhibit sufficiently different electronic properties. Our results for $BiNiO_3$ suggest the important role of the Bi 4s charge ordering (charge difference of $\sim$0.52 electrons), with a charge transfer between the Bi 4s and O 2p states and a stable Ni^{2+} configuration, for understanding of the MIT in $BiNiO_3$ [1]. We find that electronic correlations are important to explain the electronic structure, magnetic state, and lattice stability of $RNiO_3$ (R = Lu, Y, and Bi).

[1] I. Leonov et al., Phys. Rev. B **100**, 161112(R) (2019).

15 min. break.

TT 3.8 Mon 11:30 HSZ 201

Origin of orbital ordering in $LaTiO_3$ and $YTiO_3$ — •Xuejing Zhang and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

The origin of orbital ordering (OO) in correlated oxides is strongly debated. Two main mechanisms have been proposed as possible explanation for OO phenomena. The first is the classical Jahn-Teller effect and the second is the electronic super-exchange, introduced by Kugel-Khomskii. In the case of the paradigmatic e_g systems $KCuF_3$ and $LaMnO_3$ it has been shown that the electronic Kugel-Khomskii mechanism is not sufficient to drive the OO transition alone, at the temperatures at which orbitally order is typically observed by the co-operative Jahn-Teller distortion.[1,2] In the case of t_{2g} compounds, however, the problem remains open. In these systems both the electron-lattice coupling and the hopping integrals are typically smaller than those for e_g compounds; on the other hand, orbital degeneracy is larger, which enhances the effects of super-exchange. Here we investigate representative t^1_{2g} systems in which OO is observed, the Mott insulators $LaTiO_3$ and $YTiO_3$. We show that the Kugel-Khomskii transition temperature is about 390 K, comparable to the one of $KCuF_3$. This shows that static distortions are needed to explain the presence of OO at high temperature.

[1] E. Pavarini, E. Koch and A. I. Lichtenstein, Phys. Rev. Lett. 101, 266405 (2008).
[2] E. Pavarini and E. Koch, Phys. Rev. Lett. 104, 086402 (2010).

TT 3.9 Mon 11:45 HSZ 201

Charge transport in oxygen-deficient $EuTiO_3$: The emerging picture of dilute metallicity in quantum-paraelectric perovskite oxides — •Johannes Engelmayer[1], Xiao Lin[1], Christoph Grams[1], Raphael German[1], Tobias Fröhlich[1], Joachim Hemberger[1], Kamran Behnia[2], 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

Quantum paraelectric $SrTiO_3$ is a large-gap band insulator that becomes metallic upon electron doping already at extremely small charge-carrier concentrations $\simeq 5\times10^{17}\mathrm{cm}^{-3}$. The observed T^2 resistivity in this material challenges conventional theories for electron–electron scattering. We report on a study of charge transport in the related compound $EuTiO_3$ where the carrier density is tuned via reduction. Because of a lower electric permittivity, the metal–insulator transition (MIT) in $EuTiO_{3-\delta}$ occurs at higher carrier densities compared to doped $SrTiO_3$. The critical carrier concentration n_c for the MIT is discussed in the context of the so-called Mott criterion and compared with other doped perovskite compounds with a quantum-paraelectric parent. Similar to doped $SrTiO_3$, $EuTiO_{3-\delta}$ shows a distinct AT^2 resistivity, where the prefactor A scales with n. Using a simple three-band model, the $A(n)$ behavior in doped perovskite titanates can be described over a large range of n.

Funded by DFG via CRC1238 and via ANR-DFG LO 818/6-1 and HE 3219/6-1.

TT 3.10 Mon 12:00 HSZ 201

Magnetic Phase diagram and thermal expansion studies of $NiTiO_3$ — •Kaustav Dey[1], Sven Sauerland[1], Johannes Werner[1], Rabindranath Bag[2], Surjeet Singh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics , Heidelberg University, Germany — [2]IISER Pune, Maharashtra, India

We report the magnetic phase diagram of $S = 1$ magnetodielectric $NiTiO_3$ single crystals grown by the optical floating zone technique. The high-quality single crystals have been studied by specific heat, by magnetometry up to 60 T, and by thermal expansion and magnetostriction measurements up to 15 T, respectively. The compound evolves long-range antiferromagnetic order at $T_N = 22.5$ K with spins lying in the $ab-$plane. Pronounced anomalies in the thermal expansion coefficients $(\alpha_i, (i = a, b))$ at T_N indicate strong magnetoelastic coupling in $NiTiO_3$. Magnetic length and entropy changes as detected by α and c_p obey Grüneisen scaling which evidences one dominant (spin) degree of freedom driving the transitions. In addition, the magnetic phase diagram features a spin-reoriented phase below $B_c = 1.2$ T which suggests the presence of a small in-plane anisotropy. Notably, spin-reorientation is associated with a first-order-like anomaly in the magnetostriction. The high-field behavior of magnetization is linear and isotropic with saturation at 36 T thereby facilitating constructing the entire magnetic phase diagram.

TT 3.11 Mon 12:15 HSZ 201

Low-Energy Excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ Probed by Antiferromagnetic Resonance — •Martin Jonak, Kaustav Dey, Johannes Werner, Changhyun Koo, and Rüdiger Klingeler — Kirchhoff Institute of Physics, Heidelberg University, Heidelberg, Germany

We study magnetic excitations in $NiTiO_3$ and $Ni_{0.25}Mn_{0.75}TiO_3$ by means of X-band and high-frequency electron spin resonance spectroscopy. Our data for $NiTiO_3$ show that in the antiferromagnetically ordered and spin-reoriented phase, i.e. below T_N and in external magnetic fields above the spin-reorientation field $B_C = 1.13(8)$ T, antiferromagnetic resonance (AFMR) modes are well described by a two-sublattice model with an easy ab-plane. Correspondingly, two zero-field excitation gaps are deduced at $\Delta_1 \approx 15$ GHz and $\Delta_2 = 185(2)$ GHz, respectively. At $B < B_C$, an additional magnon mode is observed, which rules out a simple two-sublattice model, thereby contradicting the presently established picture of the low-field ground state. The strongly Mn-doped $Ni_{0.25}Mn_{0.75}TiO_3$ exhibits at least two antiferromagnetically ordered phases. The low-temperature phase shows AFMR modes of a two-sublattice antiferromagnet with anisotropy gaps $\Delta_1 = 29(1)$ GHz and $\Delta_2 = 139(3)$ GHz.

TT 3.12 Mon 12:30 HSZ 201

Electronic transformations in the semi-metallic transitional oxide Mo_8O_{23} — •Venera Nasretdinova[1], Yaroslav Gerasimenko[1,2], Jernej Mravlje[2], Gianmarco Gatti[3], Petra Sutar[2], Damjan Svetin[1,2], Anton Meden[4], Viktor Kabanov[2], Alexander Kuntsevich[5,6], Marco Grioni[3], and Dragan Mihailovic[1,2] — [1]CENN Nanocenter, Ljubljana, Slovenia — [2]JSI, Ljubljana, Slovenia — [3]Institute of Physics, EPFL, Lausanne, Switzerland — [4]University of Ljubljana, Slovenia — [5]LPI of RAS, Moscow, Russia — [6]HSE, Moscow, Russia

Mo_8O_{23} is a low-dimensional stoichiometric transitional metal oxide from MoO_{3-x} family. Its room-temperature phase associated with charge density wave (CDW) is accompanied by non-monotonic resistivity at low temperatures well below structural transitions. Using tunneling and angle-resolved spectroscopy, transport measurements and density functional calculations we reveal electronic transformations leading to a multi-band correlated ground state [1, 2]. We observe the metal-to-insulator transition at 343 K in resistivity, consistent with CDW onset. At low temperatures, the picture with the only CDW order parameter is broken by the onset of the correlated ground state visible both in transport and spectroscopic probes. Spatially-resolved tunneling spectroscopy studies reveal the emergent electronic texture. We discuss the possible origins of the electronic order that emerge in the absence of any structural or magnetic transitions.

[1] V. Nasretdinova et al., Phys.Rev. B 99, 085101 (2019)
[2] V. Nasretdinova et al., Sci. Rep. 9, 15959 (2019)

TT 3.13 Mon 12:45 HSZ 201

Cr and Ce magnetic ordering in $CeCrO_3$:revisited — •Neetika Sharma[1], Reinhard K. Kremer[1], Clemens Ritter[2], and Fereidoon S. Razavi[3] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institute Laue Langevin, Grenoble 38000, France — [3]Department of Physics, Brock University, St. Catharines, ON, L2S 3A1, Canada

We have investigated the magnetic structure of $CeCrO_3$ using neutron powder diffraction (NPD). $CeCrO_3$ crystallizes with the $GdFeO_3$ structure-type (Pbnm). Earlier neutron diffraction measurements on $CeCrO_3$ have proposed a G-type afm structure for the Cr and a C-type for the Ce sublattice. The analysis of the magnetic structure for the Ce sublattice had been based on one magnetic peak (102) at d ∼ 3.152 Å. However, the proposed C-type coupling for Ce will generate primarily two magnetic Bragg peaks (100) at d ∼ 5.47 Å and (102) at d ∼ 3.152 Å. We have collected NPD patterns on a sample of $CeCrO_3$ using ILL's D20 high-intensity medium resolution diffractometer and did observe the previously reported magnetic Bragg peak at d ∼ 3.152 Å, however significantly less intense than reported before. Simulations indicate that only the presence of magnetic coupling of C-type on the Cr- and the Ce- sublattices can lead to a situation where the magnetic peak (102) at d ∼ 3.152 Å is a lot stronger than the (100) Bragg peak at d ∼ 5.47Å. Following this proposal we have analyzed our neutron diffraction data very carefully at low temperature (1.5K), and conclude a CyGz type magnetic ordering for the Cr sub-lattice with a very small Cy-component and Cy type coupling for Ce - sublattice.

TT 4: Disordered Quantum Systems

Time: Monday 9:30–11:15 Location: HSZ 204

Invited Talk TT 4.1 Mon 9:30 HSZ 204

Towards an *ab-initio* theory of Anderson localization with correlated electrons — •Liviu Chioncel — Uni. Augsburg

Great progress has been made in recent years towards understanding the properties of disordered electronic systems. This is made possible by recent advances in quantum effective medium methods which include Dynamical Mean-Field Theory and the Coherent Potential Approximation, and their cluster extension, the Dynamical Cluster Approximation. The recently developed typical medium dynamical cluster approximation captures disorder-induced localization and provides an order parameter for the Anderson localized states. We present an overview of various recent applications of the typical medium single-site and dynamical cluster approximation to the Hubbard model, and its combination to realistic systems in the framework of Density Functional Theory.

TT 4.2 Mon 10:00 HSZ 204

Electrically Biased Resonators for Investigations of Dielectric Low Temperature Properties of Amorphous Solids — •Benedikt Frey, Marcel Haas, Marius Lutz, Diana Körner, 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, which can be described as two-level systems (TLS) with a distribution of their energy splitting E, as assumed by the phenomenological standard tunneling model. Recent interest in these systems due to their deteriorative effects on the performance of superconducting quantum devices have been leading to novel experimental investigations of atomic tunneling systems also driven by novel measurement techniques.

We use microfabricated superconducting resonators in a bridge-type setup to study the dielectric rf-response of the amorphous sample in the presence of an electric bias field. The bias field modifies the energy splitting E of a TLS and allows to probe different regions of the TLS distribution. This technique enables various opportunities for studying TLS more in-depth. We see a correlation between the dielectric loss and the bias field sweep rate, which can be well described within a theory based on Landau-Zener transitions. Moreover, a desaturation of the TLS occupation number also occurs, when noise is used as the bias signal. These results are compared to detailed numerical simulations, showing in general a good agreement.

TT 4.3 Mon 10:15 HSZ 204

Dielectric Polarization Echoes of Glasses Containing Large Nuclear Quadrupole Moments — •Andreas Schaller, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

Many properties of amorphous solids at low temperatures can be explained by the standard tunneling model, which is based on atomic tunneling systems, described as two-level systems. Tunneling systems with an electric dipole moment couple resonantly to electric fields and can thus be studied using dielectric two-pulse polarization echoes to learn about their dynamics and coherence. 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 moments. Furthermore, measurements of the dielectric constant of glasses with large nuclear quadrupole moments point towards a so far unconsidered relaxation process.

We present results of dielectric two-pulse polarization echo measurements carried out on different multi-component glasses and polymers containing large nuclear quadrupole moments. For all these samples the two-pulse-echo amplitude is small and the decay occurs on a shorter timescale compared to samples containing no or just small nuclear quadrupole moments. We compare the results to simulations obtained by a Monte Carlo method approach.

TT 4.4 Mon 10:30 HSZ 204

Ab initio typical medium theory of substitutional disorder — •Andreas Östlin[1], Yi Zhang[2,3], Hanna Terletska[4], Florian Beiuseanu[5], Voicu Popescu[6], Krzysztof Byczuk[7], Levente Vitos[8,9,10], Mark Jarrell[2], Dieter Vollhardt[1], and Liviu Chioncel[1,11] — [1]University of Augsburg, Augsburg, Germany — [2]Louisiana State University, Baton Rouge, USA — [3]Kavli Institute for Theoretical Sciences, Beijing, China — [4]Middle Tennessee State University, Murfreesboro, USA — [5]University of Oradea, Oradea, Romania — [6]Sophie-Scholl-Gymnasium Oberhausen, Oberhausen, Germany — [7]University of Warsaw, Warszawa, Poland — [8]KTH Royal Institute of Technology, Stockholm, Sweden — [9]Uppsala University, Uppsala, Sweden — [10]Research Institute for Solid State Physics and Optics, Budapest, Hungary — [11]Augsburg Center for Innovative Technologies, Augsburg, Germany

By merging single-site typical medium theory with density functional theory we introduce a self-consistent framework for electronic structure calculations of materials with substitutional disorder which takes into account Anderson localization. The scheme and details of the implementation are presented and applied to the hypothetical alloy Li(c)Be(1-c), and the results are compared with those obtained with the coherent potential approximation. Furthermore we demonstrate that Anderson localization suppresses ferromagnetic order for a very low concentration of (i) carbon impurities substituting oxygen in MgO(1-c)C(c), and (ii) manganese impurities substituting magnesium in Mg(1-c)Mn(c)O for the low-spin magnetic configuration.

TT 4.5 Mon 10:45 HSZ 204

Slow Dynamics in the Charge-Glass Forming Organic Conductors θ-(BEDT-TTF)$_2$MM′(SCN)$_4$ — •Tatjana Thomas[1], Yassine Agarmani[1], Tim Thyzel[1], Hungwei Sun[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2], Hiroshi Yamamoto[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute for Materials Research, Tohoku University, Japan — [3]Institute for Molecular Science, Okazaki, Japan

The organic charge-transfer salts θ-(ET)$_2$MM′(SCN)$_4$ are considered as model systems to study strongly correlated electron systems under the influence of geometric frustration. Due to strong Coulomb interactions the system exhibits a charge ordering transition, which can be kinetically avoided by fast cooling resulting in a charge-glass state without long-range order [1]. The required cooling rate depends on the degree of charge frustration, where a higher frustration on the triangular lattice within the conducting layers promotes the charge-glass forming ability [2]. Fluctuation spectroscopy has proven to be a powerful tool to study the charge carrier dynamics at low frequencies [3], which have shown to become very slow and heterogeneous when approaching the glass transition, similar to conventional glass-forming liquids [4]. Here, we present systematic noise studies on three compounds MM′=CsCo, RbZn, TlZn with high, medium and low frustration, respectively. From the power spectral density we extract characteristic energies and time scales dominating the resistance noise and compare the results with the quenched states.

[1] Adv. Mater. **29**, 1601979;
[2] JPSJ **83**, 083602
[3] Crystals **8**, 166

[4] Science **357**, 1381

TT 4.6 Mon 11:00 HSZ 204

Universal quantum glass transition on the Bethe lattice — •Izabella Lovas[1], Catalin Pascu Moca[2,3], and Gergely Zarand[2] — [1]Technical University of Munich, Garching, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]University of Oradea, Oradea, Romania

We study the Coulomb glass behavior emerging from the interplay of interactions and disorder, by examining a model of spinless fermions at half filling on the Bethe lattice. We consider the limit of infinite coordination number, where we combine dynamical mean field theory with a Hartree-Fock approximation to investigate the glass transition and the properties of the glassy phase in the presence of full replica symmetry breaking. This approach allows us to study the opening of the Efros-Shklovskii pseudogap in the glassy phase, and also grants us access to the spectral function. In particular, we demonstrate the universal scaling collapse of the pseudogap and the spectral function at close to zero temperatures, where the melting of the glass is governed by the quantum fluctuations induced by the hopping of fermions between lattice sites. We show that this quantum scaling function differs from the classical scaling function of the thermal phase transition of the spin glass limit. Our results should be relevant for the glassy dynamics observed in Si inversion layers, persisting in the metallic phase.

TT 5: Frustrated Magnets - General 1 (joint session TT/MA)

Time: Monday 9:30–13:00 Location: HSZ 304

TT 5.1 Mon 9:30 HSZ 304

Pressure tuning of the ground state of a frustrated Kondo lattice investigated by Muon Spin Relaxation / Rotation spectroscopy — •Mayukh Majumder[1], Ritu Gupta[2], Philipp Gegenwart[1], Oliver Stockert[3], and Veronika Fritsch[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [3]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Formation of novel quantum states driven by magnetic frustration are of strong current interest. For metallic Kondo lattices tuned to a quantum critical point (QCP), strong frustration is predicted to cause a severe breakdown of Fermi liquid behavior and a possible metallic spin liquid state. CePdAl is a prototype frustrated Kondo lattice with incommensurate long-range magnetic order (LRO) at about 2.7 K involving only 2/3-rd of the 4f moments. The LRO can be suppressed by hydrostatic pressure exceeding 1 GPa [1] and an extended non-Fermi liquid ground state has been observed up to a pressure of about 1.7 GPa [2]. We have employed Muon Spin Relaxation / Rotation (μSR) at milli-Kelvin temperatures and pressures up to 1.62 GPa as a local technique to determine the nature of the magnetic moments across the quantum critical point in CePdAl.

[1] H. Kitazawa et al. Phys. B, 28, 199 (1994)
[2] Zhao et al. Nature Phys. 10.1038/s41567-019-0666-6 (2019)

TT 5.2 Mon 9:45 HSZ 304

Microscopic meaning of the Goodenough-Kanamori-Anderson (GKA) rule in frustrated cuprates — •Stefan-Ludwig Drechsler[1], Liviu Hozoi[1], Ravi Yadav[1], Satoshi Nishimoto[1,2], Rolf Schumann[2], Jan M. Tomczak[3], Dijana Miloslavlevic[4], and Helge Rosner[4] — [1]IFW-Dresden, D-01171 Dresden Germany — [2]TU Dresden, Germany — [3]Vienna University of Technology, Vienna, Austria — [4]MPI-cPfS, Dresden, Germany

Within the multiband (pd) Hubbard model we consider the influence of the ferromagnetic (fm) intersite exchange K_{pd} and that of the intra-site Hund's rule exchange J_H on bridging O in between two Cu-sites on the NN exchange J_1 within a spin-model for cuprates with edge-sharing elements. Based on quantum chemistry (QC), DFT, GW, and exact calculations for small clusters and extended systems we determine the main interactions and transfer integrals for several representative cuprates with edge-sharing elements. In most such compounds with Cu-O-Cu bond angles near 90^o the relatively large $-J_1 > 230$ K is dominated by a *nonuniversal* $K_{pd} > 100$ meV, i.e. significantly larger than 50 meV adopted previously /1/. In contrast to common belief, $J_H < 0.8$ eV is moderate and somewhat screened. It plays only a *minor* role in the GKA. Moderate J_H-values are in accord with results for superoxides /2/. Enlarged K_{pd} ~200 meV agree with QC for corner-sharing cuprates /3/ and empirically with $CuGeO_3$ ($\sim$ 100 meV) /2/.

[1] Y. Mizuno *et al.*, Phys. Rev. B **57**, 5326 (1998).
[12] M. Matsuda *et al.*, ibid. **100** 104415 (2019) and references therein.
[3] M.S. Hybertsen *et al.*, ibid. **45**, 10032 (1992).

TT 5.3 Mon 10:00 HSZ 304

Magnetic interactions in the new double perovskite Nd_2ZnIrO_6, probed by Resonant Elastic X-ray Scattering (REXS) — •Florian Heinsch[1,2], Morgan Allison[2], Sonia Francoual[3], Jochen Geck[2], Florian Rasch[4], Tobias Ritschel[2], Quirin Stahl[2], Raman Thiyagarajan[1,2], Michael Vogl[4], Eugen Weschke[5], and Sabine Wurmehl[4] — [1]HZDR, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]DESY, Hamburg, Germany — [4]IFW, Dresden, Germany — [5]HZB, Berlin, Germany

The unique interplay of spin-orbit coupling, crystal field splitting and Coulomb repulsion have made double perovskites of the general formula $A_2BB'O_6$ with a 5d transition metal sitting on the B'-site a subject of intense research. Recently a new series Ln_2ZnIrO_6 with Ln = Nd, Sm, Eu and Gd and Ir as 5d-elment could be synthesized [1]. In this series, Nd_2ZnIrO_6 stands out because of its particularly intriguing magnetic properties.

Here we present results of REXS experiments on a Nd_2ZnIrO_6 single crystal, conducted at P09 at PETRA III and UE46 PGM-1 at BESSY. The combined capabilities of both facilities provided us with temperature (down to ~5K) and magnetic field (up to ~13T) dependent data that elucidate the particularly strong correlation between the two magnetic sublattices of the Nd^{3+} and Ir^{4+} ions. An outlook will be given on how to put the found field dependent anisotropy in a comprehensive picture of the magnetic ground state of Nd_2ZnIrO_6 and how that relates to compounds with different Ln.

[1] M. Vogl et al., arXiv:1910.13552

TT 5.4 Mon 10:15 HSZ 304

Crystal growth and characterization of $ZrFe_4Si_2$ — •Katharina M. Zoch, Isabel Reiser, Alexander Bodach, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universitaet Frankfurt, 60438 Frankfurt, Germany

The crystal structure of $ZrFe_4Si_2$ consists of edge-linked Fe-tetrahedra along the crystallographic *c*-direction. This type of arrangement is prone to show frustration and low dimensional fluctuations. First results indicate that $ZrFe_4Si_2$ displays some sort of weak magnetic order at unusual low temperatures for a Fe-based compound, as well as deviant behavior in specific heat and resistivity measurements [1]. To further investigate these features, we are in need of good quality single crystals. The crystal growth is a challenging subject since the compound is strongly peritectic melting and its melted elements are reactive with common crucible materials under crystal growth conditions. We show first results of the crystal growth from a levitating melt using the Czochralski method. Furthermore, we present the characterization of the obtained samples especially near the suspected magnetic order.

[1] K. Weber: Intermetallic 3d systems close to a magnetic instability: new unusual cases, Dissertation TU Dresden (2017)

TT 5.5 Mon 10:30 HSZ 304

Orientation dependence of the magnetic phase diagram of $Gd_2Ga_5O_{12}$ — •Markus Kleinhans, Christopher Duvinage, and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

The magnetic properties of $Gd_2Ga_5O_{12}$ (GGG) originate in large, classical spins ($J = S = 7/2$) that interact antiferromagnetically on two interpenetrating hyperkagome lattices. It has long been recognized that this implies, on a classical level, a high degree of frustration with some kind of classical spin liquid at low temperatures. Yet, dipolar interactions are large and may normally be expected to relieve the effects of geometric frustration. Therefore, it has been considered surprising that GGG at zero magnetic field exhibits spin-freezing without evidence for long-range order, where the recent observation of antiferromagnetic correlations on ten-spin rings, suggests a nematic order parameter, or director. We report vibrating coil magnetometry of the orientation dependence of the magnetic phase diagram of GGG down to mK temperatures, where the applied magnetic field stabilizes a complex sequences of cross-overs and phase transitions that reflect the underlying antiferromagnetic interactions.

TT 5.6 Mon 10:45 HSZ 304

Effective chainlike physics in frustrated $S = \frac{1}{2}$ spin-trimer Heisenberg magnets $Na_2Cu_3Ge_4O_{12}$ and $K_2Cu_3Ge_4O_{12}$ — •Oleg Janson[1] and Satoshi Nishimoto[1,2] — [1]Leibniz Institute für Festkörper- und Werkstoffforschung (IFW Dresden) — [2]Technische Universität Dresden (TU Dresden)

The trimerized $S = \frac{1}{2}$ Heisenberg magnet $Na_2Cu_3Ge_4O_{12}$ exhibits an incommensurate magnetic order below $T_N = 2\,K$ [1], which is nearly two orders of magnitude smaller than the Weiss temperature $\theta_W \simeq 200\,K$. Its potassium sibling $K_2Cu_3Ge_4O_{12}$ features similar structural Cu_3O_8 trimers, but their connectivity is different. Here, despite the sizable antiferromagnetic $\theta_W = 49\,K$, the magnetic susceptibility $\chi(T)$ reveals no sign of long-range magnetic ordering down to 2.5 K [2]. For both materials, $\chi(T)$ data can not be described within the Heisenberg trimer model. To provide a microscopic insight into the spin models of both materials, we perform microscopic modeling by means of DFT band structure calculations. We find, besides the dominant intertrimer exchange J_1, three (two) further antiferromagnetic exchanges that give rise to a quasi-1D frustrated model in $Na_2Cu_3Ge_4O_{12}$ ($K_2Cu_3Ge_4O_{12}$). The ground states of the spin Hamiltonians are studied using exact diagonalization and DMRG. We also compute the central charge c and the static structure factor $S(q)$, and discuss the possibility to describe the physics of these highly frustrated materials within an effective Heisenberg chain model.

[1] Y. Yasui *et al.*, J. Appl. Phys. **115**, 17E125 (2014).
[2] C. Stoll *et al.*, Inorg. Chem. **57**, 14421 (2018).

TT 5.7 Mon 11:00 HSZ 304

Low-temperature thermal conductivity in the frustrated spin chain mineral Linarite — •Matthias Gillig[1], Xiaochen Hong[1], Gaël Bastien[1], Anja U.B. Wolter[1], Bernd Büchner[1,2], and Christian Hess[1,2] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Center for Transport and Devices, TU Dresden, Germany

Motivated by recent theoretical results which predict a finite thermal Drude weight in frustrated spin chains, we have studied the thermal conductivity of the mineral Linarite $PbCuSO_4(OH)_2$ at low temperature. This well-studied material forms a monoclinic structure where a sequence of $Cu(OH)_2$ units forms a S=1/2 spin chain. Competing FM nearest-neighbor and AFM next-nearest-neighbor interactions in this low dimensional spin structure create a magnetically frustrated system which orders below $T_N = 2.8$ K in an elliptical spiral ground state. Upon applying magnetic field along the spin chain direction, other magnetically ordered phases can be induced. For fields of 10 T and higher the spin system is fully polarized. Our results reveal that the thermal conductivity κ in zero field is dominated by a phononic contribution. As a function of magnetic field κ shows a peculiar nonmonotonic behavior. Whenever the magnetic field value approaches a critical field, κ is highly suppressed. This trend can be explained by strong magnetic fluctuations which are expected near a phase boundary and which reduce thermal conductivity by phonon scattering.

15 min. break.

TT 5.8 Mon 11:30 HSZ 304

Magnetic properties and phase diagram of the triangular-lattice antiferromagnet $KCeS_2$ — •Bastian Rubrecht[1,2], Gael Bastien[1], Anja U.B. Wolter[1], Sven Luther[3], Hannes Kühne[3], Philipp Schlender[4], Ellen Häussler[4], Thomas Doert[4], and Bernd Büchner[1,2] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

Triangular-lattice(TL) antiferromagnets are well-known canditates for frustrated magnetism. By introducing different magnetic rare-earth ions, one can change the magnetic interactions to reinforce frustration in these systems. This may lead to the realization of a quantum spin liquid state or to various competing ordered phases, e.g. an oblique version of the 120° state or a collinear up-up-down phase. The delafossite $KCeS_2$ is a new contender realizing anisotropic magnetic interactions. From magnetization measurements of $KCeS_2$-crystals, we observe a strong anisotropy between the basal plane and the c axis. This cannot be explained by g-factor values obtained from single site CASSCF calculations and suggests anisotropic magnetic interactions. Furthermore, our He3 specific heat studies at zero field reveal a phase transition at $T_N = 0.38$ K, which follows a non-monotonous shift as function of an applied in-plane field, resulting in three different magnetic phases in fields up to 9 T. We construct the magnetic phase diagram of $KCeS_2$ and discuss the possible nature of the occurring phases.

TT 5.9 Mon 11:45 HSZ 304

Typical Pure Quantum states and the thermodynamics of highly frustrated quantum magnets — •Andreas Honecker[1] and Alexander Wietek[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

Reliable computation of the low-temperature thermodynamic properties of highly frustrated quantum magnets remains a considerable challenge. Here we explore the power of Thermal Pure Quantum (TPQ) states implemented in the framework of a Lanczos method using examples of frustrated two-dimensional $S = 1/2$ spin models. In particular, we present accurate results for the specific heat and magnetic susceptibility 2D $S = 1/2$ Shastry-Sutherland model with up to 40 sites in the parameter regime relevant to $SrCu_2(BO_3)_2$ [1] that had remained inaccessible over the previous two decades.

[1] A. Wietek, P. Corboz, S. Wessel, B. Normand, F. Mila, and A. Honecker, Phys. Rev. Research **1**, 033038 (2019).

TT 5.10 Mon 12:00 HSZ 304

Strain-induced order in highly frustrated magnets — •Mary Madelynn Nayga and Matthias Vojta — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

One defining feature of highly frustrated magnets is a massively degenerate manifold of classical ground states. Here we study how inhomogeneous strain can lift this degeneracy and induce magnetic order in frustrated magnets. We provide explicit examples of strain-induced ordered states and characterize their observable properties, both static and dynamic.

TT 5.11 Mon 12:15 HSZ 304

Quantum criticality of an extended XY-chain with long-range interactions in a transverse field — •Patrick Adelhardt and Kai Phillip Schmidt — Friedrich-Alexander Universität, Erlangen, Germany

The critical breakdown of a one-dimensional quantum magnet with long-range interactions is studied by investigating an extended XY-model in a transverse field for the ferro- and antiferromagnetic case. While for the the limiting case of the pure long-range XY-model we can extract the elementary one-particle excitation analytically, for the long-range Ising limit as well as in the intermediate regime we use perturbative continuous unitary transformations on white graphs in combination with classical Monte Carlo simulations [1] for the graph embedding on the chain to extract high-order series expansions. This allows us to determine the quantum-critical regime including critical exponents.

[1] S. Fey, S.C. Kapfer, K.P. Schmidt, Phys. Rev. Lett. 122, 017203 (2019)

TT 5.12 Mon 12:30 HSZ 304

Quantum criticality of the transverse-field Ising model with long-range interactions on triangular-lattice cylinders — •Jan Koziol, Sebastian Fey, Sebastian C. Kapfer, and Kai P. Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universitaet Erlangen-Nuernberg, D-91058 Erlangen, Germany

To gain a better understanding of the interplay between frustrated long-range interactions and zero-temperature quantum fluctuations, we investigate the ground-state phase diagram of the transverse-field Ising model with algebraically decaying long-range Ising interactions on quasi-one-dimensional infinite-cylinder triangular lattices. Technically, we apply various perturbative approaches including low- and high-field series expansions, as well as quantum Monte-Carlo stochastic series expansion simulations. For the classical long-range Ising model, we investigate cylinders with an arbitrary even circumference. We show the occurrence of gapped stripe-ordered phases emerging out of the infinitely degenerate nearest-neighbor Ising ground-state space on the two-dimensional triangular lattice. For the full long-range transverse-field Ising model, we concentrate on cylinders with circumference four and six. The ground-state phase diagram consists of several quantum phases in both cases including an x-polarized phase, stripe-ordered phases, and clock-ordered phases which emerge from an order-by-disorder scenario already present in the nearest-neighbor model. In addition, the generic presence of a potential intermediate gapless phase with algebraic correlations and associated Kosterlitz-Thouless transitions is discussed for both cylinders.

TT 5.13 Mon 12:45 HSZ 304

Dynamic Structure Factor of Disordered Coupled-Dimer Heisenberg models — •Max Hörmann and Kai Phillip Schmidt — Institut für Theoretische Physik, Universität Erlangen-Nürnberg, Staudtstraße 7, D-91058 Erlangen

We investigate the impact of quenched disorder on the zero-temperature dynamic structure factor of coupled-dimer Heisenberg models on two-dimensional bilayers on the square, triangular and Kagome lattice. Using perturbative continuous unitary transformations, the effects on quasiparticles are investigated [1]. The disorder leads to intriguing quantum structures in dynamical correlation functions well observable in spectroscopic experiments.

[1] M. Hörmann, P. Wunderlich, K. P. Schmidt, Phys. Rev. Lett. 121, 167201 (2018)

TT 6: Cooperative Phenomena and Phase Transitions (joint session MA/TT)

Time: Monday 9:30–13:15 Location: HSZ 401

TT 6.1 Mon 9:30 HSZ 401

Driving the magnetic transition by chemical substitution in $\mathbf{Cs_{1-x}Rb_xFeCl_3}$ — •Lena Stoppel[1], Shohei Hayashida[1], Zewu Yan[1], Severian Gvasaliya[1], Andrey Podlesnyak[2], and Andrey Zheludev[1] — [1]Laboratory for Solid State Physics, ETH Zurich, Switzerland — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennesse

We report the observation of a chemical-substitution driven phase transition from a gapped quantum paramagnetic phase to one with long range order in $Cs_{1-x}Rb_xFeCl_3$. The $x = 0$ compound in this series of triangular-lattice antiferromagnets has a spin-singlet ground state due to strong easy-plane magnetic anisotropy. In contrast, the $x = 1$ material orders magnetically in a 120° structure [1]. Calorimetric and magnetic experiments performed on a series of samples with $0 \leq x \leq 1$ reveal that in the low-temperature limit magnetic order appears at $x \sim 0.35$. Inelastic neutron scattering experiments show that this coincides with the closure of the gap in the spin excitation spectrum. It appears that disorder effects in this material are more pronounced than those in the only other known phase transition of this type, namely in DTNX [2].

[1] S. Hayashida L. Stoppel et al., Phys. Rev. B 99, 224420 (2019).
[2] K. Yu. Povarov et al., Phys. Rev. B 92, 024429 (2015).

TT 6.2 Mon 9:45 HSZ 401

Lattice effects in pyrochlore compounds $\boldsymbol{A_2B_2O_7}$ — •M. Doerr[1], T. Stoeter[1,2], S. Granovsky[1], S. Zherlitsyn[2], and J. Wosnitza[1,2] — [1]Institut für Festkörper- und Materialphysik, TU Dresden — [2]Hochfeld-Magnetlabor Dresden, Helmholtz-Zentrum Dresden-Rossendorf

The magnetic character of pyrochlores $A_2B_2O_7$ (A = rare earths, B = transition metals or p-elements, *e.g.* Ti, Zr, Hf, Sn) strongly depends on the lattice. The ionic radii determine their existence and stability. The question of whether the ground state is degenerated or magnetically ordered is decisively determined by the ratio of dipole and exchange interaction. We present investigations of thermal expansion, magnetostriction and relaxation processes at temperatures down to 0.05 K. $Dy_2Ti_2O_7$ and $Ho_2Ti_2O_7$ show a number of anomalies that can be explained with both exchange and crystal-field effects. These anomalies reflect as well the magnetic properties via magnetoelastic coupling. Thus, statements on the monopole dynamics can be derived from relaxation processes. Relaxation times in the order of 10^3 s evidence the formation and annihilation of monopoles in the kagome-ice and saturated phase, in accordance with the known magnetic phase diagram. In contrast, the lattice effects in $Dy_2Sn_2O_7$ and $Ho_2Sn_2O_7$ are rather negligible. At last, measurements on $Pr_2Zr_2O_7$, $Gd_2Zr_2O_7$ and $Nd_2Hf_2O_7$ allow the direct comparison of classical spin-ice compounds to pyrochlores with light rare earths. A representation-theoretic investigation of the symmetry group of the pyrochlore lattice could lead to a better understanding of the magnetoelastic coupling mechanisms.

TT 6.3 Mon 10:00 HSZ 401

Control of structure and physical properties of La0.7Sr0.3MnO3 thin films via oxygen stoichometry — Lei Cao[1], •Oleg Petracic[1], Paul Zakalek[1], Alexander Weber[2], Ulrich Rücker[1], Jürgen Schubert[3], Alexandros Koutsioubas[2], Stefan Mattauch[2], and Thomas Brückel[1] — [1]Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI-4), JARA-FIT Forschungszentrum Jülich GmbH, Jülich — [2]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ) Forschungszentrum Jülich GmbH, Garching — [3]Peter Grünberg Institute (PGI9-IT) JARA-Fundamentals of Future Information Technology Forschungszentrum Jülich GmbH, Jülich

Epitaxial thin films of La0.7Sr0.3MnO3 were prepared by high oxygen pressure sputter deposition on SrTiO3 substrates at various oxygen partial pressures. In addition, we performed after preparation systematic oxygen desorption and absorption studies by thermal annealing or oxygen plasma processing, respectively. We derive a phase diagram with respect to the crystal structure (Perovskite vs. Brownmillerite), the magnetic behavior (ferromagnetic vs. antiferromagnetic) and the transport properties (metallic vs. insulating) for various annealing conditions.

TT 6.4 Mon 10:15 HSZ 401

Spin-lattice coupling in a Yafet-Kittel ferrimagnetic spinel — •Atsuhiko Miyata[1,2], Hidemaro Suwa[3], Toshihiro Nomura[2], Lilian Prodan[4], Viorel Felea[2,4,5], Yurii Skourski[2], Joachim Deisenhofer[6], Hans-Albrecht Krug von Nidda[6], Oliver Portugall[1], Sergei Zherlitsyn[2], Vladimir Tsurkan[4,6], Joachim Wosnitza[2,5], and Alois Loidl[6] — [1]LNCMI, Toulouse, France — [2]HLD-HZDR, Dresden Germany — [3]University of Tokyo, Tokyo, Japan — [4]Institute of Applied Physics, Chisinau, Moldova — [5]TU Dresden, Dresden, Germany — [6]University of Augsburg, Augsburg, Germany

Since the discovery of ferrimagnetism in 1948, noncollinear ferrimagnets have been well studied in spinels, AB_2X_4. The key essence is the competition of magnetic exchanges within or between the two A and B lattices. Yafet and Kittel (YK) proposed a model for triangular-structure ground states. To realize unconventional ferrimagnetic structures beyond the YK model, one can consider that spontaneous lattice deformation will modulate these main antiferromagnetic exchanges, i.e., through a spin-lattice coupling mechanism. This kind of spin-lattice coupling mechanism, however, has not been taken into account in previous theoretical works on ferrimagnetic spinels.

In this talk, using ultrasound and magnetostriction results up to 60 T, magnetization measurements up to 110 T, and Monte Carlo calculations, we demonstrate that the spin-lattice coupling induces unconventional magnetic structures under magnetic fields in the YK spinel $MnCr_2S_4$.

TT 6.5 Mon 10:30 HSZ 401

Pressure and field tuning in low-dimensional metal-organic magnets — •Matthew Coak[1], Samuel Curley[1], David Graf[2], Jamie Manson[3], and Paul Goddard[1] — [1]University of Warwick, Coventry, United Kingdom — [2]National High Magnetic Field Laboratory, Tallahassee, FL, USA — [3]Eastern Washington University, Cheney, WA, USA

The 1D molecular magnet $Cu(pyz)(gly)ClO_4$ (gly = glycine, pyz = pyrazine) is an $S = 1/2$ dimer material with small enough exchange constants to address with accessible fields. The dimers are coupled antiferromagnetically, possessing a singlet-triplet energy-gap that can be closed upon application of an external magnetic field. When the Zeeman splitting of the degenerate triplet state initially closes the gap, the system passes through a quantum phase transition from a quantum-disordered ground state to a long-range XY-ordered phase. This excited triplet state can be described as a system of bosonic quasi-particles called 'triplons'. Under certain conditions, this triplon excited state maps onto a Bose-Einstein condensate of magnons; Cu(pyz)(gly)ClO_4, at ambient pressures, appears to conform to this picture.

We present our latest results in using hydrostatic pressure as a tuning parameter to control the inter- and intra-dimer exchange interactions and observing the effects on the temperature-field phase diagram.

TT 6.6 Mon 10:45 HSZ 401

Spin crossover in mechanically responsive Ni(II)-MOF-74 — •Dijana Žilić[1], Krunoslav Užarević[1], Senada Muratović[1], Bahar Karadeniz[1], Tomislav Stolar[1], Stipe Lukin[1], Ivan Halasz[1], Mirta Herak[2], Gregor Mali[3], Yulia Krupskaya[4], and Vladislav Kataev[4] — [1]R. Bošković Institute, Zagreb, Croatia — [2]Institute of Physics, Zagreb, Croatia — [3]National Institute of Chemistry, Ljubljana, Slovenia — [4]Leibniz IFW, Dresden, Germany

The metal-organic frameworks (MOFs) are the subject of intensive research not only due to potential applications but also due to unresolved magnetic properties. We present here very detailed study of structural and magnetic properties of Ni(II)-MOF-74 compound, investigated by powder X-ray diffraction, infrared and Raman spectroscopy, magnetization measurements, X-band and multifrequency high-field electron spin resonance and solid state nuclear magnetic resonance spectroscopy. Our results show that Ni-MOF-74 can be described as a zig-zag spin chain system with ferromagnetic intrachain and weaker antiferromagnetic (AFM) interchain interaction, with long-range AFM phase transition around 17 K. We also studied how desolvation and amorphization process can influence the chemical and physical properties of Ni-MOF-74. The observed strong differences in magnetic properties of amorphous Ni-MOF-74 were explained by spin crossover from high-spin to low-spin state of Ni(II) ions.

Supported by HRZZ (UIP-2014-09-4744 and IP-2018-01-3168) and DAAD-MZO projects "Magneto-structural correlations in molecular magnetic complexes studied by electron spin resonance spectroscopy".

TT 6.7 Mon 11:00 HSZ 401

Atomistic simulations of spin-state switching in multinuclear spin-crossover molecules — •Robert Meyer, Christian Mücksch, Juliusz A. Wolny, Volker Schünemann, and Herbert M. Urbassek — Physics Department & Research Center OPTIMAS, University Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Spin-crossover materials exhibit the unique ability to switch between a low-spin and a high-spin state, indicating their potential as possible organic storage devices. A switch between the low and the high spin state is reflected by a frequency shift in the phonon density of states. This makes the phonon density of states an interesting tool to analyze spin-crossover materials.

We use a molecular dynamics approach to calculate the phonon density of states for both spin states. In particular, we are interested in the spin-switch behaviour of multinuclear SCO-compounds. We report on spin-switch dynamics depending on chain-length and number of switched atoms.

TT 6.8 Mon 11:15 HSZ 401

Noncoplanar magnetic order induced absence of large anomalous Hall effects in Mn_3Sn — •Xiao Wang[1], Fengfeng Zhu[1], Junda Song[1], Yixi Su[1], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

Recent experimental realizations of large anomalous Hall effect (AHE) at room temperature[1] in the non-collinear antiferromagnet (AFM) Mn_3Sn have attracted strong interests on this compound due to its potential applications in antiferromagnetic spintronics devices. We have prepared high quality Mn_3Sn single crystals [2] and studied its physical properties and magnetic structure by various methods. Surprisingly, below a magnetic phase transition at 280 K, the AHE vanished completely along with the emergence of two incommensurate phases. Our further polarized neutron scattering studies show the low temperature magnetic structures are noncoplanar order. Based on the polarized analysis results, we propose several possible magnetic structure models below 280 K. Moreover, we will discuss the reason for disappearance of AHE in the low temperature noncoplanar structures with magnetic symmetry analysis[3] and scalar spin chirality theory.

[1] S. Nakatsuji, et al., Nature 527, 212 (2015). [2] N.H. Sung, et al., Appl. Phys. Lett. 112, 132406 (2018). [3] M.-T. Suzuki, et al. Phys. Rev. B 95, 094406 (2017).

TT 6.9 Mon 11:30 HSZ 401

Magnetic structures and interplay between Eu and Mn in Dirac material EuMnBi2 — •Fengfeng Zhu[1], Xiao Wang[1], Junda Song[1], Thomas Müller[1], Yixi Su[1], and Thomas Brückel[2] — [1]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science JCNS and Peter Grünberg Institut PGI, JARA-FIT, Jülich, Germany

We report here a comprehensive determination of the antiferromagnetic (AFM) structures of Eu and Mn magnetic sub-lattices by using both polarized and non-polarized single-crystal neutron diffraction methods. All the magnetic moments are orientated along c axis, the magnetic propagation vector is (0,0,1) for Eu sub-lattice and (0,0,0) for Mn sub-lattice. With proper neutron absorption correction, the ordered moments are refined as about 7.7 μ_B and 4.1 μ_B for the Eu and Mn ions, respectively, at 3K. In addition, a spin-flop phase transition of Eu moments was confirmed at field B_c ∼5.3T along c axis which is constant with previous reported work [1] and the evolution of magnetic moment orientations were also determined. In the spin-flop process, we found a clear kink in the field dependence of magnetic diffraction (1,0,1) of Mn, which unambiguously indicates the existence of strong coupling between Eu and Mn moments [2].

[1] H. Masuda et al., Sci. Adv. 2, e1501117 (2016) [2] A. F. May et al., Phys. Rev. B 90, 075109 (2014)

TT 6.10 Mon 11:45 HSZ 401

Ferrimagnetism in $CeSb_2$: Measuring bulk magnetic properties with an STM — •Christopher Trainer[1], Paul Canfield[2], and Peter Wahl[1] — [1]University of St Andrews, School of Physics and Astronomy, St Andrews, Fife, UK — [2]Iowa state University, Department of Physics and Astronomy, Ames, Iowa, US

$CeSb_2$ is one of a family of rare earth magnetic materials that exhibit metamagnetism where the magnetic state can be changed by an applied magnetic field. At low temperature it exhibits a complex phase diagram with multiple magnetically ordered phases for many of which the order parameter is only poorly understood. In this talk I will report Scanning Tunneling Microscopy and magnetization measurements of $CeSb_2$. I introduce a new mode of STM measurements which allows for the characterization of the sample magnetostriction and thus the construction of a bulk phase diagram using an STM. From the magnetostriction measurement, we determine the bulk phase diagram and validate it by comparison with magnetization measurements. Our magnetostriction and magnetisation measurements indicate the low temperature ground state at zero field is ferrimagnetic. Quasiparticle interference mapping showing how the electronic behaviour develops through the phase diagram will also be discussed.

TT 6.11 Mon 12:00 HSZ 401

Spin-reorientation in CuCr2S4 from μSR — •Elaheh Sadrollahi[1,2], Jochen Litterst[2,3], Vladimir Tsurkan[4], and Alois Loidl[4] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Physik der kondensierten Materie, Technische Universität Braunschweig, 38110 Braunschweig, Germany — [3]Centro Brasileiro de Pesquisas Físicas, 22290-180, Rio de Janeiro, RJ, Brazil — [4]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Muon Spin Relaxation and Rotation (μSR) experiments have been performed on the thio-spinel CuCr2S4 for further clarifying the long-standing controversy regarding its electronic and magnetic states [1,2]. Long regarded as ferromagnet (Tc=378 K) with magnetic moments residing only on Cr, CuCr2S4 is nowadays considered a ferrimagnetic with small magnetic moments on the Cu sites [3]. In addition to the transition at Tc, our μSR data reveal transitions around 50 K and 100 K with changes in spontaneous rotation signals and in relaxation behaviour. There is a close resemblance between these μSR results with those found for Fe1-xCuxCr2S4 with high Cu concentrations [4]. We interpret the transitions with spin re-orientations and will discuss

Jahn-Teller effect as a possible reason. [1] F. K. Lotgering et al., J. Phys. Chem. Solids 30, 799 (1969) and Solid State Commun. 2, 55 (1964). [2] J. B. Goodenough, Solid State Commun. 5, 577 (1967) and J. Phys. Chem. Solids 30, 261 (1969). [3] A. Kimura et al., Phys. Rev. B 63,224420 (2001). [4] E. Sadrollahi, Doctoral Thesis (2018): https://publikationsserver.tubraunschweig.de/receive/dbbs_mods_00066058.

TT 6.12 Mon 12:15 HSZ 401

Epsilon iron as a spin-smectic state — Tommaso Gorni[1] and •Michele Casula[2] — [1]Laboratoire de Physique et d'Étude des Matériaux, École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris, Université Paris Sciences et Lettres, 75005 Paris, France — [2]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

By first-principles and spin-model calculations, we study the high-pressure epsilon phase of iron. We reveal the existence of a modulated spin pattern, lower in energy than the previous results, where spin fluctuations lead to the formation of antiferromagnetic bilayers separated by null spin bilayers. This pattern is analogous to the smectic phase found in liquid crystals. The magnetic bilayers are likely orientationally disordered, owing to the soft interlayer excitations and the near-degeneracy with other smectic phases. This possible lack of long-range correlation agrees with neutron powder diffraction and could be integral to explaining its puzzling superconductivity.

TT 6.13 Mon 12:30 HSZ 401

Frustration induced highly anisotropic magnetic patterns in classical XY model on kagome lattice — •Alexei Andreanov[1] and Mikhail Fistul[1,2] — [1]IBS PCS, Daejeon, Korea — [2]Russian Quantum Center, Moscow, Russia

We predict and observed novel highly anisotropic magnetic patterns obtained in the classical XY model on kagome lattice. The frustration is provided by the presence of both ferromagnetic (FM) and antiferromagnetic interactions between adjacent magnetic moments. At a critical value of frustration $f_{cr} = 3/4$ the system exhibits a transition from the ferromagnetic state to highly-degenerated ground state. In this regime, $f_{cr} < f \leq 1$, the average magnetization $\langle \vec{M} \rangle \simeq N^{-1/4}$ (N is the number of spins). This scaling originates from highly anisotropic character of the groundstates with the FM ordering along the y-direction, and short-range correlations along the x-direction. These features are explained by the presence of the double-degenerate ground state in a single triangle of the kagome lattice supplied witg a large number of constraints. We anticipate the implementation of this model in various systems, e.g. natural magnetic molecular clusters, artificially prepared Josephson junctions networks, trapped-ions and/or photonic crystals.

TT 6.14 Mon 12:45 HSZ 401

Concept of geometrically controlling artificial magnetoelectric materials — •Oleksii M. Volkov[1], Ulrich K. Rössler[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Dresden, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e. V. (IFW Dresden), Dresden, Germany

Magnetoelectric materials combine coupled magnetic and electrical order parameters, that allowed to control magnetic states via electrical influence and vice versa [1]. This offers exciting prospectives for energy efficient memory, logic and sensor devices. Here, we propose a new approach to electric field controlled nanomagnets [2], where the manipulation of magnetic states is done geometrically via modification of mesoscale Dzyaloshinskii-Moriya interaction and curvature-induced anisotropy [3]. The concept refers to geometrically curved helimagnetic springs embedded in a piezoelectric matrix or sandwitched between two piezoelectric layers. The electric field induces tiny changes of geometrical parameters, that leads to the transition between homogeneous and periodic helimagnetic states. This results in the appearance of strong converse magnetoelectric effect (CME) 15×10^{-3} (A m^{-1})/(V m^{-1}), which is five times higher than CME for best laminated magnetoelectric composites 2.9×10^{-3} (A m^{-1})/(V m^{-1}).

[1] W. Eerenstein et al., Nature **442**, 759 (2006).
[2] O. Volkov et al., J. Phys. D: Appl. Phys. **52**, 345001 (2019).
[3] O. Volkov et al., Scientific Reports **8**, 866 (2018).

TT 6.15 Mon 13:00 HSZ 401

Orthomagnons and Quantum Weak Ferromagnetism in Kagome Antiferromagnets — •Robin R. Neumann[1], Alexander Mook[2], Jürgen Henk[1], and Ingrid Mertig[1,3] — [1]Institut für Physik, Martin-Luther-Universität, D-06120 Halle — [2]Department of Physics, University of Basel, CH-4056 Basel — [3]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle

Magnons are charge-neutral spin carriers that appear as excitations in magnetically ordered systems. The magnetic moment they carry is often thought to be antiparallel to the localized magnetic moments in the ground state, causing magnons in collinear (or coplanar) magnets to carry only those magnetic moment components offered by the texture.

In this talk, we lift the aforementioned limitation by introducing "orthomagnons," whose magnetic moment has a component orthogonal to the magnetic texture. We demonstrate that the notion of orthomagnons appears naturally in coplanar antiferromagnets on the kagome lattice. As a consequence, both quantum and thermal fluctuations introduce a weak out-of-plane magnetic moment. In the limit of zero temperature, this gives rise to quantum weak ferromagnetism.

TT 7: Micro- and Nanostructured Materials (joint session MA/TT)

Time: Monday 9:30–11:15 Location: HSZ 403

TT 7.1 Mon 9:30 HSZ 403

Magnetization properties of individual 3D Fe-Co Nanostructures — •Mohanad Al Mamoori[1,2], Fabrizio Porrati[1], Michael Huth[1], Christian Schröder[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Institute of Materials Science, Technical University of Darmstadt, Germany — [3]Institute for Applied Materials Research, Bielefeld University of Applied Sciences, Germany

The transition from 2D to 3D nanomagnetism may bring with it the emergence of novel physical effects and enable future magnetic memory and sensing applications. In [1,2], we have employed focused electron beam induced deposition (FEBID) to grow 3D nanomagnets as nanocubes and nano-trees directly onto a micro-Hall sensor acting both as substrate and high-resolution detection device of small magnetic stray fields. We find that the magnetisation reversal propagates by multi-vortex switching scenarios. In this presentation, firstly, we report systematic measurements of magnetic stray fields of newly grown Fe-Co tetrahedral structures as building blocks of diamond lattices as a function of temperature and magnetic field applied at different angles. Secondly, in order to gain further insights in the hysteresis loops, (irreversible) magnetic interaction effects and coercivity distributions, first-order-reversal curves (FORC) of these 3D nanomagnets supported will be shown. Finally, an outlook to the future design of such structures towards the realization of 3D artificial spin ice architectures will be given. [1] L.Keller et al., *Sci. Rep.* **8** , 6160 (2018). [2] M. Al Mamoori et al., *Materials* **11**, 289 (2018).

TT 7.2 Mon 9:45 HSZ 403

Magnetization reversal in round and square nanodots — •Andrea Ehrmann[1] and Tomasz Blachowicz[2] — [1]Bielefeld University of Applied Sciences, Faculty of Engineering and Mathematics, Bielefeld, Germany — [2]Silesian University of Technology, Institute of Physics - Center for Science and Education, Gliwice, Poland

Ferromagnetic nanodots in different shapes can be applied in data storage, spintronics, neuromorphic computing, etc. Especially the possibility to create vortex states is of high technological interest since these states have significantly reduced stray fields and correspondingly less interaction with neighboring nanodots. Whether a vortex state occurs in the absence of an external magnetic field, depends on the dimensions of the nanodots and, in case of not round nanoparticles, on the shape, since the shape anisotropy significantly influences magnetization reversal processes.

Here we give an overview of magnetization reversal processes in square [1] and round nanodots [2], often including a single-vortex state, while in some cases two, three or even more vortex-antivortex pairs can be found. We also show the stability of single vortex ground states, i.e. the states usually suggested for data storage, which depends strongly on the dot geometry.

[1] A. Ehrmann, T. Blachowicz, Hyperfine Interactions 239, 8 (2018)
[2] A. Ehrmann, T. Blachowicz, J. Magn. Magn Mater. 475, 727-733 (2019)

TT 7.3 Mon 10:00 HSZ 403

Experimentally observable curvature-induced effects in parabolic nanostripes — •Oleksii M. Volkov[1], Attila Kákay[1], Florian Kronast[2], Ingolf Mönch[1], Mohamad-Assaad Mawass[2], Jürgen Fassbender[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum-Dresden-Rossendorf, Dresden, Germany — [2]Helmholtz-Zentrum Berlin für Materialen und Energie, Berlin, Germany

Dzyaloshinskii-Moriya interaction (DMI) is a key aspect in magnetism that can lead to the appearance of chiral effects, such as the topological Hall effect [1], or to the formation of chiral noncollinear magnetic textures, as skyrmions or chiral domain walls [1]. Curvature effects in magnetism offer means to create chiral interactions like DMI based on the geometry of thin films [2]. This extrinsic tailoring of the DMI (strength and spatial orientation) is in stark contrast to conventional approaches, where chiral interactions are tuned relying on extensive material screening. Very recently, we provide the very first experimental confirmation of the existence of curvature-induced DMI in parabola-shaped Permalloy nanostripes [3,4]. The magnitude of the effect can be tuned by the parabola's curvature and width, while its value is comparable with those experimentally reported for asymmetric Co sandwiches.

[1] N. Nagaosa and Y. Tokura, Nat. Nanotechnol. **8**, 899 (2013).
[2] Y. Gaididei et al., PRL **112**, 257203 (2014).
[3] O. Volkov et al., PRL **123**, 077201 (2019).
[4] O. Volkov et al., PSS-RRL **13**, 1800309 (2019).

TT 7.4 Mon 10:15 HSZ 403

Giant Photovoltaic Effect in Magnetic Materials — •Oles Matsyshyn and Inti Sodemann — MPI PKS, Dresden, Germany

We investigate a rectification process present in materials that break both inversion and time reversal symmetries. At second order in electric fields, this effect is inverseley proportional to the relaxation rate, and, therefore, the rectified current would be infinity in a "naive" ideal clean and zero temperature limit. Employing Floquet theory, we show, however, that there is a non-perturbative correction in the electric field strength that regularises this divergence, but, which ultimately leads to a giant photo-current generation. Therefore, this effect offers a promising alternative paradigm for solar cell technologies.

TT 7.5 Mon 10:30 HSZ 403

Microscopic origin of improved magnetic fluid hyperthermia performance of CFO-Pd heterodimers: Element-specific investigations of structural, electronic, and magnetic characteristics — •S. Fatemeh Shams[1], Detlef Schmitz[2], Alevtina Smekhova[2], Eugen Weschke[2], Kai Chen[2], Chen Luo[2], Amir. H. Tavabi[3], Sussane Pettinger[4], Konrad Siemensmeyer[2], Gil Westmeyer[4], Rafal E. Dunin-Borkowski[3], Florin Radu[2], and Carolin Schmitz-Antoniak[1] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Institute of Biological and Medical Imaging (IBMI), Helmholtz Zentrum München, 85764 Neuherberg, Germany

Cobalt ferrite nanoparticles were synthesized and randomly decorated with approximately 2 wt.% of Pd particles. After careful structural and compositional characterization, X-ray absorption spectroscopy was used to investigate their element-specific magnetic properties. A significant increase in the effective spin and orbital magnetic moments of both the Fe and the Co ions was found upon decoration with Pd, leading to an increase in total magnetic moment per formula unit by 60% for the larger nanoparticles and by 200% for the smaller ones at 300 K. XMCD measurements show that the magnetic field dependence of the Co moment is much steeper at lower magnetic fields, leading to an enhanced maximum heating power in hyperthermia experiments.

TT 7.6 Mon 10:45 HSZ 403

Strain induced orientation of hematite nanospindles studied via Mössbauer spectroscopy — •Damian Günzing[1], Julian Seifert[2], Samira Webers[1], Joachim Landers[1], Annette M. Schmidt[2], and Heiko Wende[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen — [2]Department of Chemistry, Institute of Physical Chemistry, University of Cologne

Magnetic nanoparticles embedded in different matrices are a promising hybrid material class with the opportunity of tayloring the magneto-elastic properties. For an efficiently working hybrid material, it is mandatory to understand the particle matrix interaction on the nanoscale. In this work spatial particle ordering of anisotropic hematite nanospindels [1] is induced via applied strain to an elastomer matrix with incorporated particles. To study the ordering process the focus lies on the element specific Mössbauer spectroscopy with and without an applied magnetic field. With this technique we obtain information about the spin orientation and Brownian diffusion simultaneously from the measured spectra. The distributions in spin orientation are further compared to Monte-Carlo simulations calculating the degree of ordering. As a complementary method, small angle x-ray scattering measurements are performed on the sample systems to determine the ordering parameter from the spatial particle distribution. This work is financially supported by the DFG priority program SPP1681 (WE2623/7-3).

[1] J. Landers et al., J. Phys. Chem. C 119, 20642-20648 (2015)

TT 7.7 Mon 11:00 HSZ 403

Cellulose nanocomposite with $SrFe_{12}O_{19}$ nanoparticles as a novel magnetic nanopaper source — •Andrei Chumakov[1], Calvin Brett[1,2], Artem Eliseev[3], Evgeny Anokhin[3], Lev Trusov[3], Lewis Akinsinde[4], Marc Gensch[1,5], Dirk Menzel[6], Matthias Schwartzkopf[1], Micheal Rübhausen[4], and Stephan Roth[1,2] — [1]DESY, Hamburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]MSU, Moscow, Russia — [4]CFEL, Universität Hamburg, Hamburg, Germany — [5]TUM, Garching, Germany — [6]TU Braunschweig, Braunschweig, Germany

The combination of biocompatible cellulose nanofibrils (CNF) with magnetic nanoparticles provides a promising magnetic composite material for flexible and electromechanical devices. Superparamagnetic ferrite nanoparticles are used as a magnetic material for such composites. We combined CNF with a novel type of stable magnetic colloids based on disc-like (diameter 40 nm, thickness 5 nm) hard magnetic hexaferrite ($SrFe_{12}O_{19}$) particles, electrostatically stabilized in aqueous solution. Each particle carries a large permanent magnetic moment oriented perpendicularly to the plate surface (Ms = 50 emu/g, Hc = 4500 Oe). As a result of the interaction of positively charged magnetic particles with a negatively charged surface of the CNF (1360 μmol/g), a thin film of the magnetic composite material was fabricated by spray deposition. The structure was studied by imaging, X-ray scattering and the magnetic techniques of such a composite showed a uniform distribution of single hexaferrite nanoparticles in a cellulose matrix.

TT 8: Topological Phenomena (joint session MA/TT)

Time: Monday 9:30–11:30 Location: POT 6

TT 8.1 Mon 9:30 POT 6

Complex magnetism and colossal magnetoresistance in wallpaper fermion candidate Eu5In2Sb6 — •Marein Rahn[1,2], Sonia Francoual[4], Alessandro Bombardi[5], Pascal Manuel[6], Larissa Veiga[7], Morgan Allison[1], Marc Janoschek[3], Jochen Geck[1], Filip Ronning[2], and Priscila Rosa[2] — [1]IFMP, Technische Universität Dresden, 01069 Dresden, Germany — [2]LANL, Los Alamos, NM 87545, USA — [3]PSI, 5232 Villigen, Switzerland — [4]DESY, 22607 Hamburg, Germany — [5]Diamond Light Source, Didcot OX11 0DE, UK — [6]ISIS Neutron an Muon Source, Didcot OX11 0QX, UK —

[7]LCN, University College London, London WC1H 0AH, UK

A new type of hourglass topological surface state has been predicted to be protected by non-symmorphic structural symmetries in Ba5In2Sb6. Following this prediction, we synthesized the isostructural Eu5In2Sb6, which promises to combine the potential for novel electronic topology with the 8 muB magnetic moment of Eu2+. Indeed, we find unusual unusual electronic properties, such as 99% negative magnetoresistance and a two-step magnetic ordering process. We present our complementary use of neutron powder diffraction, Eu L3-edge resonant elastic x-ray scattering and muon spin-rotation to reveal the mechanism of this unusual magnetic ground state, which may form a basis for understanding of the relevance of topological surface states in this material.

TT 8.2 Mon 9:45 POT 6

Large magnetic gap at the Dirac point and spin polarization control in $Bi_2Te_3/MnBi_2Te_4$ heterostructures — •Friedrich Freyse[1], Emile Rienks[1], Stefan Wimmer[2], Andreas Ney[2], Hubert Steiner[2], Valentine Volobuev[2], Heiko Groiss[2], Günther Bauer[2], Andrei Varykhalov[1], Oliver Rader[1], Gunther Springholz[2], and Jaime Sánchez-Barriga[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, Linz, Austria

Using spin- and angle-resolved photoemission, we investigate the electronic and spin structure of the topological surface state (TSS) of $Bi_2Te_3/MnBi_2Te_4$ heterostructures as a function of temperature. By cooling below the Curie temperature T_C, we observe how a magnetic surface gap opens at the Dirac point of the initially gapless TSS, a requirement which is crucial to enable the quantum anomalous Hall effect. The spectrum of the gapped Dirac point measured in remanence after field cooling (M+) is clearly spin polarized, with spin orientation perpendicular to the surface plane and spin split by a large value of $\Delta = 56 \pm 4$ meV at 6 K. Subsequent measurement at room temperature shows that the spin polarization completely disappears, whereas subsequent cooling in an oppositely oriented field (M-) leads to a reversal of the spin polarization.
[1] J.Sánchez-Barriga *et al.* Nature (2019), in press

TT 8.3 Mon 10:00 POT 6

Magnetic properties of antiferromagnetic topological insulators — •Martin Hoffmann[1], Mikhail M. Otrokov[2,3,4,5], Arthur Ernst[1], and Evgueni V. Chulkov[2,4,5,6] — [1]Institute for Theoretical Physics, Johannes Kepler Universität, Linz, Austria. — [2]Centro de Física de Materiales (CFM-MPC), Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain. — [3]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain. — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain. — [5]Saint Petersburg State University, Saint Petersburg, Russia. — [6]Departamento de Física de Materiales UPV/EHU, San Sebastián, Spain.

The doping of nonmagnetic topological insulators with magnetic transition metal elements exhibits less desired strongly inhomogeneous magnetic and electronic properties, which restricts the observation of important effects to very low temperatures. Well ordered intrinsic magnetic topological insulators can be the solution to those problems as they show higher magnetic phase transition temperatures as theoretically predicted and experimentally confirmed for the antiferromagnetic (AFM) topological insulator $MnBi_2Te_4$. Here, we report about the *ab initio* results and calculated magnetic properties of this prediction. $MnBi_2Te_4$ forms septuple-layer blocks including a Mn layer. A three-dimensional AFM order establishes below the Néel temperature of $T_N = 25.4$ K obtained by Monte Carlo simulations. This AFM order causes the different Mn layer to align their moments antiparallel due to weak out-of-plane magnetic exchange coupling constants, while the intralayer magnetic order is ferromagnetic.

TT 8.4 Mon 10:15 POT 6

A Family of Intrinsic Magnetic Topological Insulators $(MnBi_2Te_4)(Bi_2Te_3)_n$, $n = 0, 1, 2$ — •Anna Isaeva[1,2], Alexander Zeugner[3], Anja U. B. Wolter[1], Bernd Büchner[1], and Hendrik Bentmann[4] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, Dresden, Germany — [2]Faculty of Physics, Technische Universität Dresden, Dresden, Germany — [3]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Dresden, Germany — [4]Experimental Physics VII, Universität Würzburg, Würzburg, Germany

In a quest to harness quantum effects for technological advances, new realizations of materials for quantum anomalous Hall effect are pursued. A family of van-de-Waals $(MnBi_2Te_4)(Bi_2Te_3)_n$ compounds derive from the 3D topological insulator Bi_2Te_3 and feature an ordered Mn sublattice. They are the first intrinsic magnetic topological insulators [1]. We obtain high-quality crystals for all n. $(MnBi_2Te_4)(Bi_2Te_3)_n$ are thermodynamically stable in narrow temperature ranges near 873 K. We establish ubiquitous off-stoichiometry of the materials, e.g. $Mn_{1-x}Bi_{2+2x/3}Te_4$ ($x = 0.15$). Temperature- and field-dependent magnetization measurements show a 3D antiferromagnetic order ($T_N = 24$ K) in $MnBi_2Te_4$. It originates from an AFM interlayer coupling of Mn(II) layers with ferromagnetic intralayer coupling. This magnetic ground state and a centrosymmetric space group $R\bar{3}m$ entail the $Z_2 = 1$ topological classification and render $MnBi_2Te_4$ the first AFM TI [1]. [1] M. Otrokov et al. Nature (2019), in press, arxiv.org: 1809.07389.

TT 8.5 Mon 10:30 POT 6

Intriguing magnetic ground state of $MnBi_4Te_7$: a Bi_2Te_3 derivative with a periodic Mn sublattice — •Laura T. Corredor-Bohórquez[1], Vilmos Kocsis[1], Anja U. B. Wolter[1], M. Hossein Haghighi[1], Nicolás Pérez[2], Jorge Facio[3], Bernd Büchner[1,4], and Anna Isaeva[1,4] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, 01069 Dresden, Germany — [2]Institute for Metallic Materials, Leibniz IFW Dresden, 01069, Dresden, Germany — [3]Institute for Theoretical Solid State Physics, Leibniz IFW Dresden, 01069, Dresden, Germany — [4]Faculty of Physics, Technische Universität Dresden, Dresden, Germany

Materials with a combination of non–trivial band topology and long-range magnetic order have been long desired, since it is expected the appearance of novel spintronic phenomena. Following theoretical advances material candidates are emerging. $MnBi_2Te_4$ is the first antiferromagnetic topological insulator [1] and the progenitor of a modular (Bi_2Te_3)n$(MnBi_2Te_4)$ series. For n = 1, it is established an antiferromagnetic state below 13 K followed by a state with net magnetization and ferromagnetic–like hysteresis below 5 K. Through static and dynamic magnetic characterization of single crystals, we build up a picture of the intriguing magnetic ground state of this new compound. Our results render $MnBi_4Te_7$ as a band inverted material with an intrinsic net magnetization and a complex magnetic phase diagram providing a versatile platform for the realization of different topological phases. [1] M. Otrokov et al. Nature (2019), in press. Arxiv.org:1809.07389.

TT 8.6 Mon 10:45 POT 6

Dynamic magnetic properties of a magnetic topological insulator material $MnBi_4Te_7$ — •Kavita Mehlawat[1,3], Alexey Alfonsov[1,3], Anna Isaeva[1,2,3], Bernd Buechner[1,2,3], and Vladislav Kataev[1,3] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, Dresden, Germany — [2]Faculty of Physics, Technische Universität Dresden, Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat

A van der Waals compound $MnBi_4Te_7$ belongs to the family of (Bi_2Te_3)n$(MnBi_2Te_4)$, (n = 0, 1, 2) heterostructures and is a candidate magnetic topological insulator [1]. It is the first magnetic material that features both, the intrinsic net magnetization and a band inversion. Static magnetic susceptibility (χ) and magnetization (M) measurements as a function of the applied field (H) on $MnBi_4Te_7$ single-crystals show an antiferromagnetic state at $T_N = 13$ K and a ferromagnetic-like hysteresis occurring upon cooling below 5 K [1]. We performed electron spin resonance (ESR) spectroscopy measurements in wide frequency and temperature ranges to explore the dynamic magnetic properties of $MnBi_4Te_7$. From high-frequency ESR measurements, we obtain evidence that $MnBi_4Te_7$ is an easy-axis type ferromagnet and ferromagnetic spin correlations persist up to T = 30 K on the time scale of an ESR experiment (10^{-10} - 10^{-11} s). [1] Raphael C. Vidal et. al, Topological electronic structure and intrinsic magnetization in $MnBi_4Te_7$: a Bi_2Te_3-derivative with a periodic Mn sublattice, arXiv:1906.08394.

TT 8.7 Mon 11:00 POT 6

Spin orbit torque with topological insulator and ferro/antiferromagnetic heterostructures — •sumit ghosh[1,2] and aurelien manchon[2] — [1]PGI-1 and IAS-1, Forschungszentrum, Jülich 52425, Germany — [2]PSE, King Abdullah University of Science and Technology, Thuwal 23955, Saudi Arabia

Due to the robust spin-orbit coupling emerging at the surfaces, topological insulators like Bi2Se3 have become a strong source of spin-orbit torque [1,2]. However in the vicinity of a magnetic element the topological protection and hence the interfacial spin-orbit coupling change drastically. In this presentation, we are going to see some of the interesting phenomena arising at the interface of a topological insulator and ferro/antiferromagnet heterostructure [3,4]. Using a simplified tight binding model we are going to show how the interfacial spin texture is modified in the presence of a magnetic element and its impact on the non-equilibrium spin density within the linear response framework. We show how the non-equilibrium spin density changes while moving from surface dominated regime to bulk dominated regime. We also explain the origin of the large spin-Hall angle for the topological insulator ferromagnet heterostructure. Finally, we show their robustness against the scalar impurity to demonstrate their superiority against their heavy metal counterpart.

[1] A. R. Mellnik et. al., Nature, 511, 449 (2014).
[2] D. C. Mahendra et. al. Nature Materials, 17, 800 (2018).
[3] S. Ghosh and A. Manchon, Phys. Rev. B 97, 134402 (2018).
[4] S. Ghosh and A. Manchon, Phys. Rev. B 100, 014412, (2019).

TT 8.8 Mon 11:15 POT 6

Magneto-electrically controllable spin-orbit torque in topological insulator thin films — •Ali G. Moghaddam[1,2], Alireza Qaiumzadeh[3], Anna Dyrdal[4,2], and Jamal Berakdar[2] — [1]Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran — [2]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [4]Faculty of Physics, Adam Mickiewicz University, ul. Umultowska 85, 61-614 Poznan, Poland

We investigate the inverse spin-galvanic effect (ISGE) in topological insulator thin films and the resulting spin-orbit torque (SOT) in the hybrid structures with magnetic layers. Considering in-plane magnetizations inside the magnetic layers which can shift the Dirac dispersion of surface states in the two sides, we find anisotropic ISGE and SOT with a strong dependence on the chemical potential and the magnetization. Then the magnetization-dependence of current-induced spin densities gives rise to a nonlinear field-like SOT which can be controlled by varying the magnetization and applying external gate voltages to change the chemical potential. Also, the mathematical relations between current-induced spin densities and the conductivity of this system results in similar anisotropic features in the magneto-conductance of TI thin film.

TT 9: Many-body Systems: Equilibration, Chaos and Localization I (joint session DY/TT)

Time: Monday 10:00–13:30 Location: HÜL 186

Invited Talk TT 9.1 Mon 10:00 HÜL 186

Dynamically probing winding numbers of Floquet toplogical insulators in optical lattices — •André Eckardt — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden

The classification of topological Floquet systems with time-periodic Hamiltonians transcends that of static systems. For example, spinless fermions in periodically driven two-dimensional lattices are not completely characterized by the Chern numbers of the quasienergy bands, but rather by a set of winding numbers associated with the quasienergy gaps [Phys. Rev. X 3, 031005 (2013)]. I will present two schemes for probing these winding numbers in experiments with ultracold atoms in driven optical lattices. The first one relies on the quench-based tomography [PRL 113, 045303 (2014), Science 352, 1091 (2016)] of band-touching singularities occurring, when adiabatically connecting the driven system to a trivial high-frequency regime [PRL 122, 253601 (2019)]. The second one is based on observing the far-from equilibrium micromotion of the driven system within two driving periods after a sudden quench into the target Hamiltonian and relies on the identification of the winding numbers with an Hopf invariant characterizing the micromotion operator [Phys. Rev. Research 1, 022003(R) (2019)]. Together with the measurement of Chern numbers from the far-from equilibrium dynamics monitored in stroboscopic steps of the driving period [Nat. Comms. 10, 1728 (2019)], it provides a full characterization of the system.

TT 9.2 Mon 10:30 HÜL 186

Evaporative cooling and self-thermalization in an open system of interacting fermions — •Andrey Kolovsky[1,2] and Dima Shepelyansky[3] — [1]Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia — [2]Siberian Federal University, 660041 Krasnoyarsk, Russia — [3]Université de Toulouse, CNRS, 31062 Toulouse, France

We study depletion dynamics of an open system of weakly interacting fermions with two-body random interactions. In this model fermions are escaping from the high-energy one-particle orbitals, that mimics the evaporation process used in laboratory experiments with neutral atoms to cool them to ultra-low temperatures. It is shown that due to self-thermalization the system instantaneously adjusts to the new chemical potential and temperature which decreases in course of time.

TT 9.3 Mon 10:45 HÜL 186

Entanglement entropy of fractal states — •Giuseppe De Tomasi[1] and Ivan Khaymovich[2] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany

In this talk we will discuss the relations between entanglement (and Renyi) entropies and fractal dimensions D_q of many-body wave-functions.

As a simple example we introduce a new class of *sparse* random pure states being fractal in the corresponding computational basis and show that their entropies grow linearly with for fractal dimension smaller than the subsystem size ($D_q < 0.5$ for equipartitioning) and reach the upper bound of Page value otherwise, far below the ergodic limit $D_q = 1$. The latter shows that Page value entanglement entropy does not guarantee ETH.

Moreover this D_q-dependence poses an upper bound for entanglement and Renyi entropies of any multifractal states and uncovers the relation between multifractality and entanglement properties of many-body wave-functions.

TT 9.4 Mon 11:00 HÜL 186

Tripartite information, scrambling, and the role of Hilbert space partitioning in quantum lattice models — Oskar Schnaack[1], •Niklas Bölter[1], Sebastian Paeckel[1], Salvatore R. Manmana[1], Stefan Kehrein[1], and Markus Schmitt[2,3,1] — [1]Institut für Theoretische Physik, Universität Göttingen — [2]Department of Physics, University of California, Berkeley — [3]Max-Planck-Institute for the Physics of Complex Systems, Dresden

For the characterization of the dynamics in quantum many-body systems the question how information spreads and becomes distributed over the constituent degrees of freedom is of fundamental interest. We investigate the time-evolution of tripartite information as a natural operator-independent measure of scrambling, which quantifies to which extent the initially localized information can only be recovered by global measurements. Studying the dynamics of quantum lattice models we demonstrate that in contrast to quadratic models generic interacting systems scramble information irrespective of the chosen partitioning of the Hilbert space, which justifies the characterization as scrambler.

TT 9.5 Mon 11:15 HÜL 186

Moire Localization in Two Dimensional Quasi-Periodic Systems — •Biao Huang[1,2] and W Vincent Liu[1] — [1]University of Pittsburgh — [2]Max Planck Institute for the Physics of Complex Systems

Moire reconstructions of Bloch waves have led to exciting development recently, where bilayer systems with small twist angles produce new periodic structures including the flat-band induced superconductivity. Here, we point out that an incommensurate, large twist angle, realized in a recent bilayer graphene experiment, may imply a qualitatively new localized system. This includes a rapidly changing mobility edge with respect to energy distinguishing from quasi-periodic systems in 1D and 3D, and scaling exponents saturating the Harris bound formulated for a purely random system in the localization transition. Methods for engineering and signatures for detections in cold atom simulations are also discussed.

Ref: B. Huang and W. V. Liu, Phys. Rev. B 100, 144202 (2019).

TT 9.6 Mon 11:30 HÜL 186

Hierarchy of relaxation timescales in local random Liouvillians — Kevin Wang[1], •Francesco Piazza[2], and David Luitz[2] — [1]Department of Physics, Stanford University, Stanford, California 94305, USA — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden, Germany

To characterize the generic behavior of open quantum systems, we consider random, purely dissipative Liouvillians with a notion of locality. We find that the positivity of the map implies a sharp separation of the relaxation timescales according to the locality of observables. Specifically, we analyze a spin-1/2 system of size ℓ with up to n-body Lindblad operators, which are n-local in the complexity-theory sense. Without locality ($n = \ell$), the complex Liouvillian spectrum densely covers a "lemon"-shaped support, in agreement with recent findings [*Phys. Rev. Lett.* **123**, 140403;arXiv:1905.02155]. However, for *local Liouvillians* ($n < \ell$), we find that the spectrum is composed of several dense clusters with random matrix spacing statistics, each featuring a lemon-shaped support wherein all eigenvectors correspond to n-body decay modes. This implies a hierarchy of relaxation timescales of n-body observables, which we verify to be robust in the thermodynamic limit.

TT 9.7 Mon 11:45 HÜL 186

Decay of spin-spin correlations in disordered quantum and classical spin chains — •Dennis Schubert, Jonas Richter, and Robin Steinigeweg — University of Osnabrück, Germany

The real-time dynamics of equal-site correlation functions is studied for one-dimensional spin models with quenched disorder. Focusing on infinite temperature, we present a comparison between the dynamics of models with different quantum numbers $s = 1/2, 1, 3/2$, as well as of chains consisting of classical spins. Based on this comparison as well as by analysing the statistics of energy-level spacings, we show that the putative many-body localization transition is shifted to considerably stronger values of disorder for increasing s . In this context, we intro- duce an effective disorder strength, which provides a mapping between the dynamics for different spin quantum numbers. For small values of the effective disorder, we show that the real-time correlations become essentially independent of s , and are moreover very well captured by the dynamics of classical spins. Particularly for $s = 3/2$, the agreement between quantum and classical dynamics is remarkably observed even for very strong values of disorder. This behaviour also reflects itself in the appropriate spectral functions, which are obtained via a Fourier transform from the time to the frequency domain. As an aside, we also comment on the self-averaging properties of the correlation function at weak and strong disorder.
[1] arXiv:1911.09917

TT 9.8 Mon 12:00 HÜL 186

Statistics of correlations functions in the random Heisenberg chain — •Luis Colmenarez[1], David Luitz[1], Paul McClarty[1], and Masudul Haque[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden, Germany — [2]Department of Theoretical Physics, Maynooth University, Co. Kildare, Ireland

Ergodic quantum many-body systems satisfy the eigenstate thermalization hypothesis (ETH). However, strong disorder can destroy ergodicity through many-body localization (MBL) – at least in one dimensional systems – leading to a clear signal of the MBL transition in the probability distributions of energy eigenstate expectation values of local operators. We consider the full probability distribution of eigenstate correlation functions across the entire phase diagram. At intermediate disorder – in the thermal phase – we find further evidence for anomalous thermalization in the form of heavy tails of the distributions. In the MBL phase, we observe peculiar features of the correlator distributions: a strong asymmetry in $S^z_i S^z_{i+r}$ correlators skewed towards negative values; and a multimodal distribution for spin-flip correlators. A quantitative quasi-degenerate perturbation theory calculation of these correlators yields a surprising agreement of the full distribution with the exact results, revealing, in particular, the origin of the multiple peaks in the spin-flip correlator distribution as arising from the resonant and off-resonant admixture of spin configurations. The distribution of the $S^z_i S^z_{i+r}$ correlator exhibits striking differences between the MBL and Anderson insulator cases.

TT 9.9 Mon 12:15 HÜL 186

Quantum coherent dynamical extension to RKKY interaction — •Stephanie Matern and Bernd Braunecker — School of Physics and Astronomy, University of St Andrews, UK

We study the full time evolution of a pair of impurity spins coupled to a bath of itinerant electrons. Even if the spins do not interact directly they can be coupled through the bath. In its simplest form this corresponds to the RKKY interaction. However, the RKKY interaction is considered as instantaneous and disregards that the spins are not just affected by the response of the bath but have an influence on the bath itself. To capture this effect on the dynamics we take into account all temporal correlations, particularly the quantum coherent correlations building up between the spins and the bath. This immediately leads to non-Markovian dynamics and to a coupling between the spins induced by the coherent quantum excitations of the electron bath. This effective coupling can be considered as a dynamical quantum coherent extension to the RKKY interaction.

Our approach is based on a self-consistent projection operator calculation for generalised quantum master equations. This method allows us to keep track of the time evolution of both the spins and the electron bath, and therefore for the bath to go beyond the usual assumption that it is represented by a Gibbs equilibrium state.

TT 9.10 Mon 12:30 HÜL 186

Entanglement Negativity at Localization Transition — •Gergö Roosz[1], Robert Juhasz[2], and Zoltan Zimboras[2] — [1]TU Dresden — [2]Wigner RCP

We study the entanglement negativity and entanglement entropy asymptotic at the localization transition of the quasi-periodic Harper model. In the delocalized phase the scaling is identical with the scaling of the homogeneous system $S \sim \frac{1}{3}\ln l$ and $\mathcal{E} \sim \frac{1}{4}\ln l$. In the critical point the scaling is different, $S \sim \frac{\tilde{c}}{3}\ln L$ and $\mathcal{E} \sim \frac{\tilde{c}}{4}\ln L$, with $\tilde{c} \approx 0.78$ In the localized phase the length scale is set by the localization length l_{loc} and we find $S \sim \frac{\tilde{c}}{3}\ln l_{loc}$ and $\mathcal{E} \sim \frac{\tilde{c}}{4}\ln l_{loc}$. Unlike the random and aperiodic singlet phases, where the ratio of the entanglement entropy and negativity prefactor is 2, in the Harper model this ratio is identical with the homogeneous case, 3/4.

TT 9.11 Mon 12:45 HÜL 186

Signatures of excited-state quantum phase transitions in quench dynamics — •Michal Kloc — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland

Excited-state quantum phase transitions manifest themselves as singularities in the level density of the excited states. In the case of integrable or weakly chaotic systems, we show that equilibration after a rapid quantum quench is affected by these singularities. The specific features of the equilibration process are analyzed using both purely quantum and quasiclassical approaches.

TT 9.12 Mon 13:00 HÜL 186

Density dynamics in the mass-imbalanced Hubbard model — •Tjark Heitmann, Jonas Richter, and Robin Steinigeweg — Physics Department, University of Osnabrück, Germany

We consider two mutually interacting particle species on a onedimensional lattice and study how the mass ratio between the two species affects the (equilibration) dynamics of the particles. While initial nonequilibrium density distributions are known to decay for equal masses (by diffusion [1]), the lighter particles localize in an effective disorder potential when the heavy particles become infinitely heavy and thus immobile. Knowing that, what behavior can we expect in the case of intermediate mass-imbalance ratios [2,3]? To investigate this question, we prepare pure initial states featuring a sharp nonequilibrium density profile and study their real-time dynamics which, by means of dynamical quantum typicality, can be related to equilibrium correlation functions. We observe that anomalous diffusion impedes localization as soon as the heavy particles become mobile.

[1] R. Steinigeweg et al., Phys. Rev. E 96, 020105(R) (2017).
[2] N. Y. Yao et al., Phys. Rev. Lett. 117, 240601 (2016).
[3] J. Sirker, Phys. Rev. B 99, 075162 (2019).

TT 9.13 Mon 13:15 HÜL 186

Thermalization properties of closed quantum systems in linear response — •Christian Bartsch — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, D-33615 Bielefeld

Linear response theory provides a useful tool to describe nonequilibrium dynamics not too far away from equilibrium. We are able to identify different long time behavior for certain types of non-equilibrium initial conditions also with respect to the eigenstate thermalization hypothesis (ETH). Additionally, we investigate the stability of long time dynamics in driven quantum systems and its dependence on, e.g., the driving frequency. Along these lines we analyze the average energy input per driving period.

TT 10: Nanotubes and Nanoribbons

Time: Monday 11:30–13:00 Location: HSZ 204

TT 10.1 Mon 11:30 HSZ 204

Correlated or coherent - Kondo-like features in carbon nanotubes with transparent contacts — •Magdalena Margańska[1], Wei Yang[2], Carles Urgell[2], Sergio Lucio de Bonis[2], Milena Grifoni[1], and Adrian Bachtold[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93053 Regensburg, Germany — [2]ICFO - Institut De Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain

We report on electron transport measurements in high-quality carbon nanotube devices with a total transmission of about 1.5 e^2/h. At high temperatures the linear conductance exhibits moderate oscillations as a function of the gate voltage around an average value of the order the quantum of conductance. Upon decreasing temperature, we observe an intriguing fourfold increase in the period of the oscillations accompanied by an enhancement in their amplitude. This temperature dependence is rather unusual. On the one hand, the high temperature oscillations are suggestive of charging effects in an open carbon nanotube quantum dot. On the other hand the low temperature transport characteristics is reminiscent of single-particle Fabry-Pérot interference in a carbon nanotube waveguide. We reconcile these observations by attributing the four-fold increase to the interplay of resonant tunneling, interaction and quantum fluctuations, leading to an SU(4) Kondo-like enhancement in open quantum dots systems. Our work provides a comprehensive phenomenology of transport in nanotubes when both interference and interaction are involved.

TT 10.2 Mon 11:45 HSZ 204

Transport properties and Thermoelectric figure of Merit of CNT peapods — •Alvaro Rodriguez[1,2], Arezoo Dianat[1], Rafael Gutierrez[1], Leonardo Medrano[3], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Tu Dresden, 01062 Dresden, Germany. — [2]Max Planck Institute for Complex Systems, 01187 Dresden, Germany. — [3]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg.

The ability to control the electrical and thermal response in nanoscale systems represents a fundamental challenge towards the optimization of the thermoelectric figure of merit. Recent experimental studies have addressed the electrical and thermal conductivity of so called carbon nanotube (CNT) peapods, where C_{60} or larger fullerenes are encapsulated in carbon nanotubes. The reported results showed some discrepancies regarding the transport properties, suggesting either a positive or a negative effect of the fullerenes. In our computational study, we address this issue by combining electronic and vibrational structure calculations with quantum transport methods based on Green's functions to investigate the electrical, thermal and thermoelectric response of C_{60}@(8,8) CNT peapod system. We were able to calibrate the contribution of local structural deformations of the CNT surface due to the fullerene insertion; especially, we found a considerable suppression of thermal transport at low frequencies, similar to the effect found using silicon nanopillars in other nanostructures. We discuss the changes in the thermoelectric figure of merit when comparing to a pure CNT.

TT 10.3 Mon 12:00 HSZ 204

Transport spectroscopy of MoS_2 nanotubes — •Wolfgang Möckel[1], Simon Reinhardt[1], Luka Pirker[2], Christian Bäuml[1], Maja Remškar[2], and Andreas K. Hüttel[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Solid State Physics Department, Institut Jožef Stefan, Ljubljana, Slovenia

While synthesis procedures for nanotubes based on layered materials other than graphene are well-known, their transport properties are so far largely unexplored. Here, we introduce transition metal dichalcogenide (TMDC) nanotubes as a new material platform for quantum dots. We present results on optimized nanotube synthesis and device fabrication, and demonstrate low-temperature transport spectroscopy measurements on quantum dots lithographically defined in multiwall MoS_2 nanotubes. First results show clear Coulomb blockade, with charging energies of $\sim 1\,\mathrm{meV}$ and discrete conductance resonances in single electron tunneling.[1] Ongoing work targets improvement of the contact properties, the reduction of charge noise, as well as spectroscopy in magnetic fields. — [1]S. Reinhardt *et al.*, Phys. Stat. Sol. RRL **13**, 1900251 (2019).

TT 10.4 Mon 12:15 HSZ 204

Spin-Orbit Coupling modulations near edges: emergence of massive edge states — •Tineke L. van den Berg[1], M. Reyes Calvo[2], Alessandro De Martino[3], and Dario Bercioux[1,4] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [2]Departamento de Fisica Aplicada, Universidad de Alicante, 03690 Alicante, Spain — [3]Department of Mathematics, City, University of London, London EC1V 0HB, United Kingdom — [4]IKERBASQUE, Basque Foundation of Science, E-48011 Bilbao, Spain

In topological two-dimensional systems, gap modification near system edges, can lead to the appearance of massive edge states, as we have shown in earlier work [1]. In graphene, it is the Kane-Mele Spin-Orbit Coupling (SOC) that leads to the opening of a topological gap [2]. Here we will deal with systems subject to inhomogeneous SOC. In zigzag nanoribbons, smooth spatial modification of SOC near the edges results in in-gap massive edge states at the K and K' points. In armchair nanoribbons, such massive states appear at the Γ point. We analyse the properties of these states, and propose how to measure and tune them [3].

[1] C. L. Kane and E. J. Mele, PRL. 95, 226801 (2005).
[2] T. L. van den Berg, M. R. Calvo and D. Bercioux, arXiv:1911.09363.
[3] T. L. van den Berg *et al. in preparation*

TT 10.5 Mon 12:30 HSZ 204

Correlated Topological States in Graphene Nanoribbon Heterostructures — •Jan-Philip Joost[1], Antti-Pekka Jauho[2], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]CNG, DTU Physics, Kongens Lyngby, Denmark

Finite graphene nanoribbon (GNR) heterostructures host intriguing topological in-gap states [1]. These states may be localized either at the bulk edges or at the ends of the structure. Here we show that correlation effects (not included in previous density functional simulations) play a key role in these systems: they result in increased magnetic moments at the ribbon edges accompanied by a significant energy renormalization of the topological end states, even in the presence of a metallic substrate [2]. We present simulations of 7-9-AGNRs based on a Green functions method with GW self-energy applied to an effective Hubbard model. Our computed results for the differential conductance are in excellent agreement with experimental observations [3]. Furthermore, we discover a striking, novel mechanism that causes an energy splitting of the nonzero-energy topological end states for a weakly screened system. We predict that similar effects should be observable in other GNR heterostructures as well.

[1] T. Cao et al., Phys. Rev. Lett. 119, 076401 (2017)
[2] J.-P. Joost, A.-P. Jauho, M. Bonitz, Nano Letters (2019), DOI:10.1021/acs.nanolett.9b04075
[3] D. J. Rizzo et al., Nature 560, 204-208 (2018)

TT 10.6 Mon 12:45 HSZ 204

Four-terminal graphene-based nanostructures for electron quantum optical stups — Sofia Sanz[1], Pedro Brandimarte[1], Daniel Sánchez-Portal[2], •Géza Giedke[1,3], and Thomas Frederiksen[1,3] — [1]Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain — [2]Centro de Física de Materiales (CFM), CSIC-UPV/EHU, 20018 San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

Graphene nanoribbons (GNRs) an attractive basis for coherent electron transport. We study configurations that provide functionalities for simple "electron quantum optics" setups.

A central building block of such setups is the four-terminal device formed by two GNRs crossing each other at 60 degrees.

Using a tight-binding approximation and the Green's function formalism we analyze the transmission amplitudes between the four arms for low-energy electrons. Studying different widths, stackings and GNR edge topologies, we identify promising settings with suppressed back-scattering and those realizing functionalities such a 50:50 beam splitting or full transfer between the stacked ribbons. Applications for GNR-based interferometers are discussed.

TT 11: Focus Session: Simulating Quantum Many-Body Systems on Noisy Intermediate-Scale Quantum Computers (joint session TT/DY)

Time: Monday 15:00–18:15 Location: HSZ 03

Invited Talk TT 11.1 Mon 15:00 HSZ 03

Quantum simulations with linear ion crystals interacting with laser light — •Christian Roos — IQOQI Innsbruck, Innsbruck, Austria

I will describe recent quantum simulation experiments with linear ion crystals. In these experiments, ion crystals are laser-cooled to low temperatures and subjected to laser pulses that induce interactions between qubits encoded in the ions, which can be modeled as a long-range Ising interaction. I will discuss our efforts to characterize the complex entangled states that results from the non-equilibrium dynamics induced by the laser field and to apply such states for computational tasks.

Invited Talk TT 11.2 Mon 15:30 HSZ 03

Entanglement spectroscopy on the IBM quantum computer — •Titus Neupert — University of Zurich, Zurich, Switzerland

Entanglement properties are routinely used to characterize phases of quantum matter in theoretical computations. For example, the spectrum of the reduced density matrix, or so-called "entanglement spectrum", has become a widely used diagnostic for universal topological properties of quantum phases. However, while being convenient to calculate theoretically, it is notoriously hard to measure in experiments. I will discuss how IBM quantum computers allow the measurement of the entanglement spectrum using various states of one-dimensional spin systems as examples. This way, it is possible to distinguish topological states via their entanglement spectrum from paramagnetic and long-range ordered states. I will also remark on the challenges connected to the simulation of a simple interacting many-body Hamiltonian, such as the Hubbard model, on a NISQC device.

Invited Talk TT 11.3 Mon 16:00 HSZ 03

Simulating quantum many-body systems on a quantum computer — •Adam Smith[1,2], Bernhard Jobst[1], Andrew G. Green[3], and Frank Pollmann[1,4] — [1]Technical University Munich, Garching, Germany — [2]Imperial College London, London, UK — [3]University College London, London, UK — [4]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Universal quantum computers are potentially an ideal setting for simulating many-body quantum systems out of reach for classical computers. Here we discuss the practical applications to two main problems: the simulation of far out-of-equilibrium dynamics and the study of topological ground states of static Hamiltonians. In the former we demonstrate that on small scales current devices are already capable of capturing the correct qualitative physics of quantum quenches with the presence of disorder and interactions. In the latter we represent the ground states of Hamiltonians using shallow quantum circuits and observe a topological phase transition on a quantum device. Looking to the near-future, we discuss the utility of these devices for dynamics and the efficient representation of physical quantum states as we enter the noisy intermediate-scale quantum (NISQ) era.

15 min. break.

Invited Talk TT 11.4 Mon 16:45 HSZ 03

Quantum computing and its applications in chemistry and physics — •Ivano Tavernelli — IBM Research - Zurich

Quantum computing is emerging as a new paradigm for the solution of a wide class of problems that are not accessible by conventional high performance computers based on classical algorithms. In the last few years, several interesting problems with potential quantum speedup have been brought forward in the domain of quantum physics, like eigenvalue-search using quantum phase estimation algorithms and evaluation of observables in quantum chemistry, e.g. by means of the hybrid variational quantum eigensolver (VQE) algorithm. The simulation of the electronic structure of molecular and condensed matter systems is a challenging computational task as the cost of resources increases exponentially with the number of electrons when accurate solutions are required. With the deeper understanding of complex quantum systems acquired over the last decades this exponential barrier bottleneck may be overcome by the use of quantum computing hardware. To achieve this goal, new quantum algorithms need to be develop that are able to best exploit the potential of quantum speed-up. While this effort should target the design of quantum algorithms for the future fault-tolerant quantum hardware, there is pressing need to develop algorithms that can be implemented in present-day NISQ (noisy intermediate scale quantum) devices with limited coherence times. In this talk, I will introduce the basics of quantum computing using superconducting qubits, focusing on those aspects that are crucial for the implementation of quantum chemistry/physics algorithms.

Invited Talk TT 11.5 Mon 17:15 HSZ 03

Randomized measurements: A toolbox for probing quantum simulators and quantum computers — •Benoit Vermersch[1,2,8], Andreas Elben[1,2], Jinlong Yu[1,2], Lukas Sieberer[1,2], Guanyu Zhu[3], Marcello Dalmonte[4], Frank Pollmann[5], Mohammad Hafezi[3], Norman Yao[6], Ignacio Cirac[7], Peter Zoller[1,2], Tiff Brydges[1,2], Manoj Joshi[1,2], Christine Maier[1,2], Petar Jurcevic[1,2], Ben Lanyon[1,2], Christian Roos[1,2], and Rainer Blatt[1,2] — [1]Center for Quantum Physics and Institute for Experimental Physics, University of Innsbruck, Austria — [2]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck, Austria — [3]JQI - University of Maryland, USA — [4]ICTP, Trieste, Italy — [5]TU Munich, Garching, Germany — [6]LBL - University of California, Berkley, USA — [7]Max-Planck-Institut fur Quantenoptik, Garching, Germany — [8]LPMMC CNRS/Universite Grenoble Alpes, Grenoble, France

Randomized measurements have emerged as a new tool to probe the properties of quantum simulators and quantum computers beyond standard observables. In the talk I will present our recent results including randomized measurement protocols to measure entanglement [1], out-of-time-ordered correlations [2], and many-body topological invariants [3]. I will also show some experimental results [4,5] obtained in collaboration with the group of Rainer Blatt (IQOQI Innsbruck).

[1] Phys. Rev. Lett. 120 (2018) 050406
[2] Phys. Rev. X 9 (2019) 021061
[3] arXiv:1906.05011
[4] Science 364.6437 (2019), pp. 260-263
[5] M. Joshi et al., in preparation

TT 11.6 Mon 17:45 HSZ 03

Crossing a topological phase transition with a quantum computer — •Bernhard Jobst[1], Adam Smith[1,2], Andrew Green[3], and Frank Pollmann[1,4] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom — [3]London Centre for Nanotechnology, University College London, Gordon St., London WC1H 0AH, United Kingdom — [4]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, D-80799 München, Germany

Quantum computers promise to perform computations beyond the reach of modern computers with profound implications for scientific research. Due to remarkable technological advances, small scale devices are now becoming available for use. One of the most apparent applications for such a device is the study of complex many-body quantum systems, where classical computers are unable to deal with the generic exponential complexity of quantum states. Even zero-temperature equilibrium phases of matter and the transitions between them have yet to be fully classified, with topologically protected phases presenting major difficulties. We construct and measure a continuously parametrized family of states crossing a symmetry protected topological phase transition on the IBM Q quantum computers. The simulation that we perform is easily scalable and is a practical demonstration of the utility of near-term quantum computers for the study of quantum phases of matter and their transitions.

TT 11.7 Mon 18:00 HSZ 03

analysis of probabilistic error cancellation method on NISQ quantum computers — •Jiasheng Xie[1,2], Sebastian Zanker[1], and Michael Marthaler[1] — [1]HQS Quantum Simulations GmbH, Haid-und-Neu Straße 7, 76131 Kralsruhe, Germany — [2]Freie Universität Berlin, 14195 Berlin, Germany

Noisy Intermediate-Scale Quantum (NISQ) technologies are likely to be developed in the near future with the possibility of building devices with 50 to a few hundred physical qubits. NISQ devices are very useful in simulating quantum many body systems and may be able to perform tasks beyond the capability of classical computers. However, these devices are very noisy and lack fault tolerance. In order to reduce the noise level in the NISQ devices, it is useful to implement quantum error mitigation scheme. We have tested probabilistic error cancellation (PEC) method, a quantum error mitigation protocol that utilizes gate set tomography and quasiprobability decomposition. We have benchmarked the noiseless system and noisy systems with basic types of decoherences for 4 qubit case and will compare them with the noise mitigated circuit using Richardson linear extrapolation and PEC method from simulation. This will provide us a good understanding of the usefulness of this particular error mitigation protocol for the NISQ quantum computer algorithms.

TT 12: Topological Insulators 2 (joint session TT/HL)

Time: Monday 15:00–16:45 Location: HSZ 103

TT 12.1 Mon 15:00 HSZ 103

Simulating Floquet topological phases in static systems — •Selma Franca[1], Fabian Hassler[2], and Ion Cosma Fulga[1] — [1]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstr. 20, 01069 Dresden, Germany — [2]JARA-Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We show that the transport properties of static, higher-order topological insulators (HOTIs) can be used to simulate the behavior of time-periodic (Floquet) topological insulators, without the need for external driving. We consider D-dimensional HOTIs with gapless corner states, which are weakly probed by means of a transport measurement. The unitary reflection matrix describing back-scattering from the HOTI boundary is topologically equivalent to a $(D-1)$-dimensional nontrivial Floquet operator. To characterize the topology of the resulting unitary, we introduce the concept of "nested" scattering matrices, showing that they correctly determine its topological invariants. Our results provide a route to engineer topological unitaries in the lab, using HOTIs and measurement techniques that have already been demonstrated in experiment. Unlike previous methods used to simulate Floquet systems, the resulting phase is expected to be robust against decoherence, since it occurs in the absence of any external driving field.

TT 12.2 Mon 15:15 HSZ 103

Boundary State Engineering and Topological Charge Pumps in non-Hermitian Floquet systems — •Bastian Höckendorf, Andreas Alvermann, and Holger Fehske — Institut für Physik, Universität Greifswald, Greifswald, Germany

In Hermitian topological systems, the bulk-boundary correspondence strictly constraints boundary transport to values determined by the topological properties of the bulk. We demonstrate that this constraint can be lifted in non-Hermitian Floquet insulators. Provided that the insulator supports an anomalous topological phase, non-Hermiticity allows us to modify the boundary states independently of the bulk, without sacrificing their topological nature. Non-Hermitian boundary state engineering specifically enables the enhancement of boundary transport relative to bulk motion, helical transport with a preferred direction, and chiral transport in the same direction on opposite boundaries [1]. Through dimensional reduction, the Floquet insulator reduces to a one-dimensional Floquet chain which possesses a topological phase with unidirectional transport. The topological signature of this phase are non-contractible loops in the spectrum of the Floquet propagator that are separated by an imaginary gap. We define the corresponding topological invariant as the winding number of the Floquet propagator relative to the imaginary gap and then establish that the charge transferred over one period equals the winding number. In fundamental difference to the situation for static or Hermitian chains, the chain acts as a topological charge pump [2].

[1] Phys. Rev. Lett. **123**, 190403 (2019)
[2] arXiv:1911.11413

TT 12.3 Mon 15:30 HSZ 103

Experimental evidence for spin-momentum locking in topological insulator nanoribbons — •Jonas Kölzer[1], Abdur Rehman Jalil[1], Daniel Rosenbach[1], Kristof Moors[1,2], Dennis Heffels[1], Peter Schüffelgen[1], Tobias W. Schmitt[1,3], Gregor Mussler[1], Thomas L. Schmidt[2], Detlev Grützmacher[1], Hans Lüth[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA Jülich-Aachen Research Alliance, 52425 Jülich, Germany — [2]University of Luxembourg, Physics and Materials Science Research Unit,Avenue de la Faïencerie 162a, 1511 Luxembourg, Luxembourg — [3]JARA-FIT Institute Green IT, RWTH Aachen University, 52056 Aachen, Germany

Crosses and triple junctions of nanoribbons are at the center of most of the Majorana braiding schemes proposed, since a minimum of three leads is geometrically required for braiding. Topological insulators are a promising class of materials for realizing Majorana states when combined with a superconductor. Making use of these states in a braiding scheme would allow fault tolerant quantum computing. An experimental realization of a Bi_2Te_3 nanoribbon triple junction which is grown selectively using molecular beam epitaxy is presented. The magnetotransport characteristics of the topological insulator triple junctions at low temperatures are analyzed and compared to the theoretical prediction derived from tight binding transport simulations. The experimental data not only suggests the contribution of surface state transport, but it also provides evidence for spin-momentum locking in topological insulators.

TT 12.4 Mon 15:45 HSZ 103

Meta-magnetism of weakly-coupled antiferromagnetic topological insulators — •Aoyu Tan[1,3], Valentin Labracherie[1,3], Narayan Kunchur[1], Anja Wolter[1], Joseph Dufouleur[1], Bernd Buechner[1,2], Anna Isaeva[1,2], and Romain Giraud[1,3] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, 01069 Dresden, Germany — [2]Faculty of Physics, TU Dresden, 01062 Dresden, Germany — [3]Univ. Grenoble Alpes, CEA, CNRS, Spintec, 38000 Grenoble, France

The magnetic properties of van der Waals magnetic topological insulators $MnBi_2Te_4$ and $MnBi_4Te_7$ are investigated by magneto-transport measurements. We evidence that the relative strength of the inter-layer exchange coupling J to the uniaxial anisotropy K controls a transition from an A-type antiferromagnetic order to a ferromagnetic-like metamagnetic state. A bi-layer Stoner-Wohlfarth model allows us to describe this evolution, as well as the typical angular dependence of specific signatures, such as the spin-flop transition of the uniaxial antiferromagnet and the switching field of the metamagnet. In micron-size magnets, the single-domain switching-field astroid are however partly truncated by the nucleation of domain walls along the easy-axis direction.

TT 12.5 Mon 16:00 HSZ 103

Analytic continuation of Bloch states and the significance for universal boundary physics — Mikhail Pletyukhov[1], Dante Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and •Herbert Schoeller[1] — [1]RWTH Aachen University, Germany — [2]University of Basel, Switzerland

For generic tight-binding models in one dimension with non-degenerate bands we present an analytic continuation of Bloch states to complex quasimomentum [1], useful for an understanding of boundary physics in half-infinite systems. We show that the pole positions provide the oscillation frequency and localization length of edge states and the branching points define the corresponding quantities for the total density. Each edge state is shown to have a fingerprint in the bulk density which cancels exactly the edge state density. The remaining part of the density is shown to have a pre-exponential power-law with universal exponent -1/2. Introducing a phase variable which continuously shifts the boundary, we derive topological constraints for the edge modes and show that the pole positions oscillate around the branch cuts. We find that the phase dependence of the model parameters can always be chosen such that no edge mode crosses the chemical potential when shifting the boundary by one lattice site. This provides a rigorous proof for universal properties of the boundary charge found in Ref.[2].

[1] M. Pletyukhov et al., arXiv:1911.06886.
[2] M. Pletyukhov et al., arXiv:1911.06890.

TT 12.6 Mon 16:15 HSZ 103

Strong topology and Dirac semimetal phase in cubic half-Heusler under strain — •Sanjib Kumar Das[1], Jorge Facio[1], Ion Cosma Fulga[1], and Jeroen van den Brink[1,2] — [1]IFW Dresden, Helmholtzstrasse 20, 01069 Dresden — [2]Department of Physics, Technical University Dresden, 01062 Dresden, Germany

Theoretically, many half-Heusler compounds exhibit topological phases under strain. Depending on sign of the strain, they can host either a Dirac semimetal or a topological insulating phase. Strain along a suitable direction can split the quadratic band crossing of the bulk band structure, and hence open up a topological gap in these materials. By combining density functional theory(DFT) and tight-binding model calculations, we show that one such cubic half-Heusler material hosts strong topological and Dirac semimetallic phases under compressive or tensile strain, respectively. We hope that our work will motivate further experiments in this direction.

TT 12.7 Mon 16:30 HSZ 103

Fractional corner charges in a 2D super-lattice Bose-Hubbard model — •Julian Bibo[1,4], Izabella Lovas[1,4], Yizhi You[3], Fabian Grusdt[1,2,4,5], and Frank Pollmann[1,4] — [1]Technische Universität München — [2]Ludwig-Maximilians-Universität München — [3]Princeton Center for Theoretical Science — [4]Munich Center for Quantum Science and Technology — [5]Department of Physics and Institute for Advanced Study, Technical University of Munich

Higher order topological insulators (HOTIs) represent a novel class of topological phases protected by a combination of spatial and internal symmetries. While many non-interacting system have been introduced and studied, it is unclear to which extend the results obtained in non-interacting systems transfer to their strongly-interacting counter parts. In our work, we introduce an experimentally accessible model, a 2D super-lattice Bose-Hubbard model on a square lattice at half-filling, that realizes a robust higher order topological phase protected by charge conservation and fourfold rotation symmetry. Excitingly, our model predicts the presence of symmetry protected fractional charges e/2 to occur at the corners. The presence and robustness of the predicted fractional corner charges is confirmed using the Density Renormalisation Group Ansatz (DMRG). Finally, we propose a way to measure the characteristic fractional corner charges and also provide simulations for the measurement.

TT 13: Graphene (joint session TT/DY/HL)

Time: Monday 15:00–18:30 Location: HSZ 201

TT 13.1 Mon 15:00 HSZ 201

Edge state crossing behaviour in a multi-band tight-binding model of graphene — •Thorben Schmirander, Marta Prada, and Daniela Pfannkuche — I. Institut für theoretische Physik Universität Hamburg, Hamburg, Deutschland

The description of Dirac electrons in the band structure of graphene is commonly performed using effective tight binding models [1]. These effective models use single-orbital Hamiltonians with modified hopping parameters in order to account for the influence of the higher energy orbitals in graphene. We go beyond such effective models by including d-orbitals in an atomistic tight-binding model. The inclusion of the d-orbitals results in a breaking of electron-hole symmetry which in turn changes the dispersion of the states around the Fermi energy. When considering a finite graphene sample, edge states occur, which cross the band gap and connect the Dirac cones at the K and K' point. These edge states are the key to the topological properties of graphene, because they may exhibit the Spin Hall effect [3]. The band gap crossing is discussed by comparing different expectation values computed from the edge states. These expectation values change under different influences, such as strain or an external electric field. Apart from qualitatively treating these influences on the crossing of the band gap, electron-electron interactions are included via a self-consistent mean-field approach.

[1] van Miert, G., Juricic, V. and Morais Smith, C. Phys. Rev. B 90 195414 (2014)
[2] van Gelderen, R. and Morais Smith, C., Phys. Rev. B 81 125435 (2010)
[3] Kane, C. L . and Mele, E. J., Phys. Rev. Lett. 95, 226801 (2005)

TT 13.2 Mon 15:15 HSZ 201

Graphene grain boundaries for strain sensing: a computational study — •Delwin Perera and Jochen Rohrer — Institut für Materialwissenschaft, Technische Universität Darmstadt, Germany

Graphene has been celebrated as a material with exceptional properties at various fronts of electronics. In this contribution we investigate the strain sensing capabilities of graphene containing grain boundaries by using the non-equilibrium Green function formalism. Our work is inspired by an enhanced piezoresistivity of nanocrystalline graphene found experimentally in 2015 [1]. We investigate how different structural realizations of the grain boundary impact the transport properties. In particular, we compute strain gauge factors solely from *ab initio* electronic structure calculations as a function of the grain boundary topology. Thereby, we can compare this popular figure of merit for strain gauges with experimental values.

[1] Riaz *et al.*, Nanotechnology **26**, 325202 (2015)

TT 13.3 Mon 15:30 HSZ 201

Virtual experiments on negative refraction across graphene pn junctions — •Wun-Hao Kang and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Graphene is a promising 2D material exhibiting optics-like properties due to its relativistic electronic structure linear in momentum. When charge carriers pass through a bipolar junction, the group velocity component parallel to the interface changes sign, leading to a negative refraction angle and hence effectively a negative refraction index in Snell's law. Many groups have been working on negative refraction in graphene, both theoretically and experimentally. However, most studies focus on the design of Veselago lensing. Here, we revisit a recent experiment [1] and perform quantum transport simulations for the same device geometry, based on the scalable tight-binding model [2]. Under ideal conditions, our result shows clear conductance peaks due to electron focusing, which is a combined effect of Klein tunneling and negative refraction. To single out the effect of negative refraction, we have further proposed a simpler design for future experiments.

[1] G.-H. Lee et al., Nat. Phys. **11**, 925–929 (2015)
[2] M.-H. Liu et al., Phys. Rev. Lett. **114**, 036601 (2015)

TT 13.4 Mon 15:45 HSZ 201

Electronic properties in a Bernal bilayer graphene monitored by selective functionalization — •Ahmed Missaoui[1,3], Jouda khabthani[1], Didier Mayou[2], and Guy Trambly de Laissardière[3] — [1]Laboratoire de la Physique de la Matière Condensée, Faculté des Sciences de Tunis, Université de Tunis El Manar, Tunis, Tunisia — [2]Institut Néel, CNRS, Univ. Grenoble Alpes, France — [3]Laboratoire de Physique théorique et Modélisation, CNRS , Univ. de Cergy- Pontoise, France

The absence of a band gap in the monolayer graphene presents a great limitation of the fields of application. In a Bernal bilayer of graphene we can exceed its limits with induce a tunable band gap here by applying a gate voltage. In this context, we study the electronic properties of bilayer graphene in the presence of adsorbates such as hydrogene.

We used a tight binding modelisation and DFT calculations for our study. We analyze [1] the effects of a selective distribution of adosrbats between the two sublattices A and B [2] on band structure and the microscopic conductivity with Kubo formalisim. The results show that in some cases depending on Fermi energy value and specific adsorbate distribution a gap appears, and in others cases, a linear dispersion with an increase in conductivity with the concentrations is reported.

[1] Jyoti. Katoch et al., Phys. Rev. Lett. 121, 136801 (2018)
[2] A. Missaoui et al., J. Phys. : Condens. Matter 30, 195701 (2018)

TT 13.5 Mon 16:00 HSZ 201

Zero-magnetic-field Hall effects in artificially corrugated bilayer graphene — •Sheng-Chin Ho[1], Ching-Hao Chang[1,2], Yu-Chiang Heish[1], Shun-Tsung Lo[1], Botsz Huang[1], Carmine Ortix[3,4], and Tse-Ming Chen[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [3]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University, Princetonplein 5, NL-3584 CC Utrecht, Netherlands — [4]Dipartimento di Fisica E. R. Caianiello, Universita di Salerno, IT-84084 Fisciano, Italy

We propose a new scheme that uses a lithographically-defined strain technology to modify the interlayer coupling and intralayer interaction of bilayer graphene (BLG). In this deformed BLG system, we demonstrate an unusual pseudo-magnetoresistance anisotropy and the so-called nonlinear Hall effect. These observations are the consequence of the Fermi surface anisotropy and tilted mini-Dirac cones, which originate from the non-zero first-order moments of the pseudo-magnetic field in both real- and momentum-spaces, i.e., the pseudo-magnetic field dipole and Berry curvature dipole. This new approach enables us to turn a simple bilayer graphene into an exotic phase of matter with nontrivial band dispersion generated by the strain engineering, on par with the creation of metamaterials or state-of-art twistronics engineering.

TT 13.6 Mon 16:15 HSZ 201

Spin-caloritronic transport in hexagonal graphene nanodots — Thi Thu Phùng[1], Robert Peters[2], •Andreas Honecker[1], Guy Trambly de Laissardière[1], and Javad Vahedi[1,3] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France — [2]Department of Physics, Kyoto University, Japan — [3]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

First, we investigate magnetism in the Hubbard model for hexagonal graphene dots. Employing static respectively dynamic mean-field theory (DMFT) we show that magnetism can be generated at the zigzag edges beyond a critical interaction of the on-site Coulomb interaction U that decreases with increasing dot size. Building on these results, we apply the Landauer formalism in the framework of the non-equilibrium Green function method to calculate the spin and charge currents through these dots as a function of temperature. We show that in the "*meta*" configuration of a hexagonal dot subject to weak Coulomb interactions, a pure spin current can be driven just by a temperature gradient in a temperature range that is promising for device applications.

15 min. break.

TT 13.7 Mon 16:45 HSZ 201

Lévy flights and Hydrodynamic Superdiffusion on the Dirac Cone of Graphene — •Egor Kiselev[1] and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We show that the hydrodynamic collision processes of graphene electrons at the neutrality point can be described in terms of a Fokker-Planck equation with a fractional derivative, corresponding to a Lévy flight in momentum space. Thus, electron-electron collisions give rise to frequent small-angle scattering processes that are interrupted by rare large-angle events. The latter give rise to superdiffusive dynamics of collective excitations. We discuss the relevance of our results to experiments with injected electron beams, and show how the superdiffusive behavior makes it possible to obtain analytical results for transport coefficients relevant to the hydrodynamics of graphene electrons.

TT 13.8 Mon 17:00 HSZ 201

Gate-controllable graphene superlattices: Numerical aspects — •Szu-Chao Chen, Wun-Hao Kang, and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

We study transport properties of gate-controllable graphene superlattices by performing quantum transport simulations based on the scalable tight-binding model and calculations of miniband structures within the continuum method [1]. Good agreement between transport simulations and the corresponding miniband structures confirms the reliability of our calculations for electrostatic superlattices in graphene. Combined with realistic potential profiles obtained from finite-element-based electrostatic simulations, our transport simulations agree well with recent transport experiments for gate-controllable square superlattices. This work therefore paves the way toward exploring gate-controllable graphene superlattices of arbitrary lattices, such as honeycomb or Lieb.

[1] S.-C. Chen et al., arXiv:1907.03288 (2019).

TT 13.9 Mon 17:15 HSZ 201

Localization at the Van Hove singularity — •Peter Silvestrov[1] and Jakub Tworzydlo[2] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Institute of Theoretical Physics, Warsaw University, Hoża 69, 00–681 Warsaw, Poland

Van Hove singularities are found in the electron spectrum of many 2-dimensional materials of current interest, including graphene systems (twisted bilayer and monolayer on a substrate), transitional dichalcogenides, and 2-dimensional superconductors. They appear due to saddle points in the energy bands at certain momenta. Even though the effective kinetic energy corresponding to such saddle point is unbounded from both above and below, we show that exponentially localized electronic states generically appear here in the presence of a smooth potential $U(x, y)$ with sufficiently diverse landscape. We also consider high order Van Hove singularities, where we predict a discrete spectrum of non-exponentially localized states.

TT 13.10 Mon 17:30 HSZ 201

The optical conductivity of strongly interacting Dirac fermions: a bosonization approach to the Kadanoff-Baym self-consistent resummation — •Sebastián Mantilla and Inti Sodemann — Max Planck Institute for the Physics of Complex Systems

The optical conductivity of 2D Dirac fermions at low energies is controlled by fundamental constants of nature $\sigma_0 = e^2/16\hbar$. However, Coulomb interactions produce a non-trivial dependence of the conductivity with the frequency. We use a bosonization approach to implement exactly a self-consistent Kadanoff-Baym resummation of the electron-hole propagator by mapping the momentum space lattice onto a Heisenberg-type model of interacting spins and employ this approach to determine the frequency dependence of the optical conductivity for Coulomb repulsions. We recover the perturbative renormalization group results at small coupling and extend its predictions to strong coupling. We discuss the relevance of our results to Dirac materials such as graphene and 3D topological insulator surface states.

TT 13.11 Mon 17:45 HSZ 201

Geometric-dissipative origin of the light-induced Hall current in graphene I — •Marlon Nuske[1,3], Lukas Broers[1], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

We determine the origin of the light-induced Hall current in graphene recently reported by J. McIver, et al., Nature Physics (2019). The Hall current derives from the total Berry curvature of the occupied states of the light-induced Floquet bands, in addition to the kinetic contribution deriving from the band velocities. The occupation of these states of the light-driven material emerges as a steady state that is determined by dissipative processes balancing out the optical driving force. For low electric field strength we propose an intuitive explanation of the Hall current within a two-level Rabi picture.

TT 13.12 Mon 18:00 HSZ 201

Geometric-dissipative origin of the light-induced Hall current

in graphene II — •Lukas Broers[1], Marlon Nuske[1,3], and Ludwig Mathey[1,2,3] — [1]Zentrum für optische Quantentechnologien, Universität Hamburg, 22761 Hamburg, Germany — [2]Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [3]CUI: Advanced Imaging of Matter, 22761 Hamburg, Germany

Inspired by the recent experiments by J. McIver, et al., Nature Physics (2019), we investigate the light-induced Hall current in graphene. We show that this Hall current derives from the Berry curvature and band velocity contributions of the occupied Floquet-states. To support this proposal we determine the energy and momentum resolved single particle correlation function. The resulting steady state momentum and energy distribution supports the interpretation as a Floquet induced mechanism. We find that for low driving intensity the main contribution to the Hall current emerges from the resonantly driven electron states of the Dirac cone. With increasing driving intensity, additional higher order resonances contribute, giving rise to the full Floquet-driven effect. We demonstrate this within a Master equation formalism, and obtain good quantitative agreement with the experimentally measured Hall current.

TT 13.13 Mon 18:15 HSZ 201

Lightwave valleytronics in graphene — •Hamed Koochaki Kelardeh[1], Alexandra Landsman[2], and Takashi Oka[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Ohio State University, Columbus, USA

We propose a valley-selective device based on graphene at a few-femtosecond timescale with charge separation at different sublattices, and correspondingly at nonequivalent valleys. We characterize the maximality condition of valley polarization and investigate the parameters and condition upon which we can coherently control the carriers and store data via valley degree of freedom. The valley polarization is controlled by the amplitude as well as the carrier-envelope phase of the pulse - one cycle optical field - and the curvature of the electron trajectory in the reciprocal space. We believe the results of our study will step forward the Valleytronics and shed light on ultrafast data storage and processing with uttermost reliability and robustness.

TT 14: Superconductivity: Theory 1

Time: Monday 15:00–18:15 Location: HSZ 204

Invited Talk TT 14.1 Mon 15:00 HSZ 204

Magnetotransport and 2D Superconductivity in Heterostructures of $BaBiO_3$ and $BaPbO_3$ — •German Hammerl — Experimental Physics VI, Center for Electronic Correlations an Magnetism, Institute of Physics, University of Augsburg, Germany

Perowskite-related $BaBiO_3$ is fascinating as it acts like a charge-density wave ordered insulator which becomes superconducing if homogeneously doped by, e. g., lead or potassium [1]. Furthermore it is theoretically predicted to be a topological insulator if electron or hole doped [2]. In this talk I will give an overview on this material and especially show that heterostructures of $BaBiO_3$ and $BaPbO_3$ show 2D superconductivity in agreement with a Berezinskiĭ-Kosterlitz-Thouless transition [3]. Temperature- and magnetic field-dependent sheet resistances are strongly affected by 2D quantum effects. Our analysis decodes the interplay of spin-orbit coupling, disorder and electron-electron interaction in this material [4].

[1] A. W. Sleight, *Phys. C* **514**, 152 (2015).
[2] B. Yan, M. Jansen, and C. Felser, *Nat. Phys.* **9**, 709 (2013).
[3] B. Meir, S. Gorol, T. Kopp, and G. Hammerl, *Phys. Rev. B.* **96**, 100507(R) (2017).
[4] P. Seiler, R. Bartel, T. Kopp, and G. Hammerl, *Phys. Rev. B* **100**, 165402 (2019).

TT 14.2 Mon 15:30 HSZ 204

Electron-lattice coupling and the superconductivity in hydrogen-rich systems — •Andrzej P. Kadzielawa[1,2], Andrzej Biborski[3], and Jozef Spalek[2] — [1]IT4Innovations, Vysoka skola banska - Technicka univerzita Ostrava, Ostrava, 17. listopadu 15/2172, 708 33 Ostrava-Poruba, Czech Republic — [2]Instyut Fizyki im. Mariana Smoluchowskiego, Uniwersytet Jagielloński, ulica Łojasiewicza 11, 30-348 Kraków, Poland — [3]Akademickie Centrum Materiałów i Nanotechnologii, AGH Akademia Górniczo-Hutnicza, Al. Mickiewicza 30, 30-059 Kraków, Poland

Recent development in the high-pressure physics provides us with a new class of the superconducting materials, namely with the hydrogen-rich materials, such as hydrogen sulphide ($T_c = 203\ K$ @ $150\ GPa$) or hydrogen lanthanide ($T_c = 274 - 286\ K$ @ $210\ GPa$).

We will discuss the versatility of the molecular-to-atomic transitions in one-, two-, and quasi-three-dimensional hydrogen systems, using our own original approach - the Exact Diagonalization Ab-Initio (EDABI) method. Starting from the extended Hubbard model, we examine an electron-correlation-driven conductivity connected with the creation of high-symmetry hydrogen molecular and atomic planes, as well as a series of both structural and electronic-in-nature quantum phase transitions. We obtain an effective electron-phonon Hamiltonian for which we estimate both the zero-point motion of the lattice ions, as well as of the electron-lattice coupling. Next, by using the McMillan formula we estimate the superconducting transition temperature versus the effective pressure (external and/or chemical).

TT 14.3 Mon 15:45 HSZ 204

Size of the Cooper pair in the Dynes superconductor — •Frantisek Herman — ETH, Zurich, Switzerland

After focusing on thermodynamic and spectroscopic properties considering role of the impurities on BCS superconductors within the Dynes phenomenology framework, here we turn to microscopic description of the underlying superconductive state. Within this talk, we provide detail analysis of the size of the Cooper pair as well as its underlying wave-function. We show that this length scale remains constant even at the critical disorder scattering, meanwhile the coherence length provided by the Ginzburg-Landau theory diverges, which shows that superconductor-metal transition driven by pair-breaking disorder occurs due to long-distance decoherence even when the Cooper pairs are locally stable. This mechanism is therefore very similar to the superconductor-metal transition driven by temperature. Presented analysis might be useful also from the point of view of preparing entangled state of electrons, since it deals with the pair-breaking as well as pair-conserving scattering rates effecting the size of the Cooper pair in different way.

TT 14.4 Mon 16:00 HSZ 204

The superconducting gap of the disordered NbAu compound from the Bogoliubov–de Gennes equations — •Bendegúz Nyári[1], Láaszló Szunyogh[1,2], and Balázs Újfalussy[3] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]MTA-BME Condensed Matter Research Group, Budapest, Hungary — [3]Wigner-MTA, Budapest, Hungary

The screened Korringa–Kohn–Rostoker (SKKR) method provides a possible solution of the Bogoliubov–de Gennes equations for superconducting heterostructures and alloys. We discuss the case of the disordered NbAu compound within the coherent potential approximation (CPA). The limit of low Nb concentration can be interpreted as a model of isolated (superconducting) Nb impurities in a (non-superconducting) Au host. We calculate the local density of states (LDOS) for the components and we investigate the formation of the superconducting gap in the Nb DOS and spectral function as we increase the concentration of the Nb doping. We study the appearance of the gap and its evolution throughout the entire concentration range.We also compare the result with the calculation of a single Nb impurity embedded into Au.

TT 14.5 Mon 16:15 HSZ 204

Full-bandwidth Eliashberg theory of superconductivity beyond Migdal's approximation — •Fabian Schrodi, Alex Aperis, and Peter M. Oppeneer — Department for Physics and Astronomy, Uppsala University

We solve the anisotropic, full-bandwidth and non-adiabatic Eliashberg equations for electron-phonon mediated superconductivity by fully including the first vertex correction in the electronic self-energy. The non-adiabatic equations are solved numerically here without further approximations, for a one-band model system. We compare the results to those that we obtain by adiabatic full-bandwidth, as well as

Fermi-surface restricted Eliashberg-theory calculations. We find that non-adiabatic contributions to the superconducting gap can be positive, negative or negligible, depending on the dimensionality of the considered system, the degree of non-adiabaticity, and the coupling strength. We further examine non-adiabatic effects on the transition temperature and the electron-phonon coupling constant. Our treatment opens a pathway to systematically study vertex correction effects in systems such as high-T_c, flat band and low-carrier density superconductors.

[1] arXiv:1911.12872.

TT 14.6 Mon 16:30 HSZ 204

Odd-frequency spin-triplet instability in disordered electron liquid — •Vladimir Zyuzin[1] and Alexander Finkel'stein[2] — [1]Texas A&M University, Nordita — [2]Texas A&M University

We theoretically consider a two-dimensional disordered conductor in the vicinity to the superconducting phase destroyed by a magnetic field. We find that a point of ending the superconductivity is a quantum critical point separating the conventional superconducting phase from a state with the odd-frequency spin-triplet superconducting pairing instability. We speculate that this could shed light onto a rather mysterious insulating state observed in the strongly disordered superconducting films in a broad region of magnetic fields.

15 min. break.

TT 14.7 Mon 17:00 HSZ 204

Quantitative Theory of Triplet Pairing in an Unconventional Superconductor — •Gabor Csire[1], Sudeep Ghosh[2], Balazs Ujfalussy[4], Martin Gradhand[3], James Annett[3], and Jorge Quintanilla[2] — [1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC, BIST, Campus UAB, Bellaterra, Barcelona, 08193, Spain — [2]SEPnet and Hubbard Theory Consortium, School of Physical Sciences, University of Kent, Canterbury CT2 7NH, United Kingdom — [3]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, United Kingdom — [4]Institute for Solid State Physics and Optics, Wigner Research Centre for Physics, Hungarian Academy of Sciences, PO Box 49, H-1525 Budapest, Hungary

We report a first-principles based semiphenomenological approach to study the superconductivity in the centrosymmetric superconductor $LaNiGa_2$ which shows spontaneous magnetism in the superconducting state. Based on symmetry considerations it was already shown that the breaking of time-reversal symmetry is only compatible with nonunitary triplet pairing states in these crystals. We study different internally antisymmetric equal-spin triplet pairing models involving the first-principle band structure. We compare our predictions for the temperature dependence of the specific heat and it is found that it can be described by an interorbital equal-spin pairing on the nickel which breaks the time-reversal symmetry. It is shown that this pairing induces nodeless, two-gapped quasiparticle spectrum which resolves in spin space and leads to finite magnetisation due to the redistribution of Cooper pairs in spin space.

TT 14.8 Mon 17:15 HSZ 204

Triplet superconductivity in the frustrated Mott insulator Sn/Si(111) — Sebastian Wolf and •Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

Two-dimensional atom lattices on semiconductor substrates have been established as tailored realizations of the extended Hubbard model. They feature charge ordered and antiferromagnetic ground states. Most recently, the onset of superconductivity at 4.3 K has been reported in the hole-doped triangular lattice of tin atoms on a silicon substrate. Here we investigate the nature of the superconducting instability in hole-doped Sn/Si(111) by virtue of the weak-coupling renormalization group. While hexagonal lattices are known to prefer chiral d-wave pairing for their unconventional superconducting ground state, this is not the case for the particular band structure of Sn/Si(111) leading to a competition of the chiral d-wave and spin-triplet pairings. We show that – by taking into account non-local Coulomb interactions – the chiral d-wave is strongly suppressed resulting in odd-parity f-wave pairing for moderate hole-doping. For stronger hole-doping around 10%, as feasible in current experiments, the archetypal chiral p-wave superconductor is stabilized.

TT 14.9 Mon 17:30 HSZ 204

Unconventional superconductivity in non-centrosymmetric structures — •Tilman Schwemmer, Michael Klett, Domenico di Sante, Werner Hanke, and Ronny Thomale — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

The pursuit of novel phases in correlated electron systems, such as possibly topological instances of unconventional superconductivity, must consider multiple energy scales including interaction strength, electronic band width, and, in particular, spin-orbit coupling (SOC). Furthermore the underlying crystal symmetries of a given system constrain the types of order that can be realized. While density functional theory and related ab initio techniques can provide a detailed description of a materials electronic structure that carefully accounts for the effects of SOC, it is necessary to additionally refine quantum many body techniques to study Fermi surface instabilities in the presence of SOC. Starting from a picture of itinerant electrons, we compute the effect of electronic correlations on the Fermi surface via renormalization group techniques. This allows us to study unconventional superconductivity arising from the interplay of SOC, Fermi surface topology, electronic correlations and crystal symmetries in real materials.

TT 14.10 Mon 17:45 HSZ 204

Eliashberg equations for an electron-phonon version of the Sachdev-Ye-Kitaev model: Pair Breaking in non-Fermi liquid superconductors — •Daniel Hauck[1], Markus Klug[1], Ilya Esterlis[2], and Jörg Schmalian[1,3] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, Karlsruhe 76131, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA — [3]Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe 76021, Germany

We present a theory that is a non-Fermi-liquid counterpart of the Abrikosov-Gor'kov pair-breaking theory due to paramagnetic impurities in superconductors. To this end we analyze a model of interacting electrons and phonons that is a natural generalization of the Sachdev-Ye-Kitaev-model. In the limit of large numbers of degrees of freedom, the Eliashberg equations of superconductivity become exact and emerge as saddle-point equations of a field theory with fluctuating pairing fields. In its normal state the model is governed by two non-Fermi liquid fixed points, characterized by distinct universal exponents. At low temperatures a superconducting state emerges from the critical normal state. We study the role of pair-breaking on T_c, where we allow for disorder that breaks time-reversal symmetry. For small Bogoliubov quasi-particle weight, relevant for systems with strongly incoherent normal state, T_c drops rapidly as function of the pair breaking strength before it vanishes at a critical pair-breaking strength via an essential singularity. The latter signals a breakdown of the emergent conformal symmetry of the non-Fermi liquid normal state.

TT 14.11 Mon 18:00 HSZ 204

Electron trimer states in conventional superconductors — •Ali Sanayei[1], Pascal Naidon[2], and Ludwig Mathey[1,3] — [1]Centre for Optical Quantum Technologies, Institute for Laser Physics, University of Hamburg — [2]RIKEN Nishina Centre, RIKEN — [3]The Hamburg Centre for Ultrafast Imaging, University of Hamburg

We expand the Cooper problem in a conventional superconductor by including a third electron in a higher empty band. This electron interacts with the other two electrons that are immersed in a Fermi sea of the lower band. We demonstrate that for sufficiently strong interband interactions the three electrons form a trimer state. We also show physical systems in which more than one trimer state can be formed.

TT 15: Frustrated Magnets - General 2 (joint session TT/MA)

Time: Monday 15:00–16:00 Location: HSZ 304

TT 15.1 Mon 15:00 HSZ 304

Quantum domain wall induced incommensurate magnetic phase in frustrated Ising model — •Zheng Zhou[1], Zheng Yan[1,2], Dong-Xu Liu[3], Yan Chen[1,4], and Xue-Feng Zhang[5] — [1]Department of Physics and State Key Laboratory of Surface Physics, Fudan University, Shanghai 200438, China — [2]Department of Physics, The University of Hong Kong, Hong Kong, China — [3]Department of Physics, Chongqing University, Chongqing, 401331, China — [4]Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China — [5]Department of Physics, and Center of Quantum Materials and Devices, Chongqing University, Chongqing, 401331, China

We study the AFM Ising model with transverse field h and NNN Ising interaction J' on triangular lattice, which describes the magnet $TmMgGaO_4$. Between the known clock and stripe phase at weak and moderate J', an incommensurate order may emerge due to the interplay between quantum fluctuation and geometrical frustration. In particular, the proliferation of quantum domain walls (DW) may stabilize such a novel phase. Numerical calculation of DW density and peaks of structure factor at certain positions provides evidence for this phase. Furthermore, we study its dynamical spectrum, which can be measured by neutron refraction. At a low h, we found a low-lying mode which agrees well with the behavior of DWs. At the h level of $TmMgGaO_4$, this mode merges with a high-lying mode corresponding to KT physics. We suggest that in materials with smaller splitting, distinct DW modes as strong evidence of this phase may be observed.

TT 15.2 Mon 15:15 HSZ 304

Non-Hermitian Topology of Spontaneous Magnon Decay — •Paul McClarty[1] and Jeff Rau[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Windsor, Ontario, Canada

I will briefly review recent progress on topological magnons placing particular emphasis on the effects of magnon-magnon interactions on the bulk and the boundary magnons. We show that the effects of interactions on single magnon states can often be recast in terms of an energy-independent non-Hermitian Hamiltonian. The spectral function has a characteristic anisotropy, in the vicinity of magnon touching points, arising from topologically protected exceptional points or lines in the non-Hermitian spectrum. This is, in principle, detectable using inelastic neutron scattering.

[1] P.A. McClarty and J. G. Rau, Phys. Rev. B 100, 100405(R) (2019)

TT 15.3 Mon 15:30 HSZ 304

Tuning the two-step melting of magnetic order in dipolar kagome ice by quantum fluctuations — Yao Wang[1,2], •Stephan Humeniuk[1], and Yuan Wan[1,2] — [1]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [2]University of Chinese Academy of Sciences, Beijing 100049, China

Complex magnetic orders in frustrated magnets may exhibit rich melting processes when the magnet is heated toward the paramagnetic phase. We show that one may tune such melting processes by quantum fluctuations. We consider a kagome lattice dipolar Ising model subject to transverse field and focus on the thermal transitions out of its magnetic ground state, which features a $\sqrt{3}\times\sqrt{3}$ magnetic unit cell. Our quantum Monte Carlo simulations suggest that, at weak transverse field, the $\sqrt{3}\times\sqrt{3}$ magnetic order melts by way of an intervening, magnetically charge ordered phase where the lattice translation symmetry is restored whilst the time reversal symmetry remains broken. By contrast, at strong transverse field, quantum Monte Carlo simulations suggest the $\sqrt{3}\times\sqrt{3}$ order melts through a floating Kosterlitz-Thouless phase. The two distinct melting processes are likely separated by a multicritical point.

TT 15.4 Mon 15:45 HSZ 304

Nematic correlations in the coupled J1-J2 chains — •Clio Efthimia Agrapidis[1], Stefan-Ludwig Drechsler[2], and Satoshi Nishimoto[1,3] — [1]Faculty of Physics, University of Warsaw — [2]Institute for theoretical solid state physics, IFW Dresden — [3]Department of Physics, Technical University Dresden

It is known that the ferromagnetic frustrated J_1-J_2 chain is a good minimal model for several cuprate chain materials. Moreover, this model exhibits multipolar physics in magnetic field. Motivated by this, we study antiferromagnetically coupled J_1-J_2 chains: the interchain coupling J' is considered to vary from pure Ising to Heisenberg exchange by varying the XXZ anisotropy parameter Δ. In general, the interchain coupling can act as an effective magnetic field. When J' is Ising-like, the system exhibits a fully magnetised state for $J'/|J_1| > 1$. This magnetisation might be related to the existence of a nematic state. Remarkably, the system shows finite magnetisation also in the limit of Heisenberg interchain coupling.

TT 16: Poster Session Superconductivity, Cryogenic Particle Detectors, Cryotechnique

Time: Monday 15:00–19:00 Location: P2/EG

TT 16.1 Mon 15:00 P2/EG

Superconducting granular aluminum films grown at cryogenic condition — •Alessandro D'Arnese, Martin Dressel, and Marc Scheffler — 1.Physikalisches Institut, Universität Stuttgart, Germany

Superconducting domes have been observed in many superconductors, raising questions of the driving mechanisms influencing T_c. One such material is granular aluminum, which is composed of aluminum nanograins coupled through thin insulating oxide layers. Granular aluminum has two decisive microscopic length scales: the grain size and the barrier thickness. These govern the fundamental energy scales for superconductivity, namely the superconducting energy gap and the superfluid stiffness, which can be determined with low-frequency optical spectroscopy [1].

In this work we developed a new evaporation setup for the growth of thin granular aluminum films at cryogenic temperatures. Controlling substrate temperature and oxygen pressure allows us to tune grain size and barrier thickness. Towards this goal, we implemented a bath cryostat to reach liquid-helium temperatures for the substrate. This project focuses on growth, characterization, and optimization of granular aluminum films. We also present DC and microwave data as a way of characterizing films and their superconducting energy scales.

[1] Uwe S. Pracht *et al.*, Phys. Rev. B **93**, 100503 (2016).

TT 16.2 Mon 15:00 P2/EG

Terahertz electrodynamics of low-temperature-grown granular aluminum — •Mehmet Ali Nebioglu, Alessandro D'Arnese, Martin Dressel, and Marc Scheffler — 1.Physikalisches Institut, Universität Stuttgart, Germany

Granular aluminum exhibits superconducting properties that can be tuned by its microscopic structure, in particular the size of the aluminum grains and the thickness of the aluminum-oxide barriers that separate the grains. This makes granular aluminum interesting for both fundamental studies of relevant superconducting energy scales and for applications. Terahertz (THz) spectroscopy is a powerful tool to study these energies via the frequency-dependent response of superconducting films that can be probed in transmission measurements, and it also gives access to superconducting collective modes [1, 2].

We study the THz response of granular aluminum films that are grown at cryogenic temperatures (down to the ^{4}He regime) and thus can exhibit substantial enhancement of T_c compared to room-temperature-grown films. We present the complex optical conductivity and we determine superconducting energy gap and superfluid stiffness. We compare these results to BCS predictions and to previous studies on granular aluminum films grown at higher temperatures [1, 3].

[1] Uwe S. Pracht *et al.*, Phys. Rev. B **93**, 100503 (2016).
[2] Uwe S. Pracht *et al.*, Phys. Rev. B **96**, 094514 (2017).
[3] Aviv Glezer Moshe *et al.*, Phys. Rev. B **99**, 224503 (2019).

TT 16.3 Mon 15:00 P2/EG

Scanning tunneling spectroscopy on disordered superconductors — •Martina Trahms[1], Idan Tamir[1], Franzisca Gorniaczyk[2], Marc Westig[1], Karl Jacobs[3], Dan Shahar[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany. — [2]Department of Condensed Matter Physics, The Weizmann Institute of Science, Rehovot 7610001, Israel. — [3]I. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany.

In some materials superconductivity co-exists with a certain amount of disorder. The true microscopic nature of disordered superconductors remains unknown [1]. These systems have mainly been investigated in transport experiments which average over the macroscopic sample area. More recently, scanning tunneling microscopy/spectroscopy (STM/STS) measurements revealed large spatial fluctuations of the superconducting gap, indicating a local modification of the ground-state [2]. Here, we will present preliminary results of high resolution STM measurements enabled by utilizing superconducting tips. We study thin films of amorphous InO and polycrystalline NbN as well as a 400 nm TiN sample. We observe local gap variations on the nanometer length scale and resolve a number of in-gap states showing high fluctuations both in energy and spatial distribution.

[1] P. W. Anderson, J. Phys. Chem. Solids **11**, 26-30 (1959).
[2] B. Sacépé *et al.*, Phys. Rev. Lett. **101**, 157006 (2008).

TT 16.4 Mon 15:00 P2/EG

Probing the dielectric properties of disordered thin-films with microwave resonators — •Nikolaj Ebensperger[1], Benjamin Sacépé[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Institut Néel, CNRS Grenoble, France

Weakly superconducting materials are of high interest for a multitude of recent studies. Yet probing the fundamental properties of these often highly disordered or granular materials is challenging and experiments are not easily performed. Specifically the insulating state terminating superconductivity in highly disordered amorphous indium oxide poses various theoretical and experimental challenges. A body of work indeed showed that the charge carriers in it are localized Cooper pairs. The electrodynamic response in this regime can offer important insight, but it is difficult to probe. In this study we present measurements of the dielectric properties of very highly disordered, insulating indium oxide films. We detail the experimental design of our microwave-resonator device as a discrete frequency probe in the GHz-range up to 20 GHz in an operable temperature range down to mK temperatures. Additionally we apply this method to a variety of different insulating/dielectric films with varying thickness and compare to simulations and theory [1].

[1] Rev. Sci. Instr. **90**, 114701 (2019)

TT 16.5 Mon 15:00 P2/EG

High-Pressure Magnetic Measurements of 2H-NbSe$_2$ — •Israel Osmond and Sven Friedemann — HH Wills Laboratory, University of Bristol, UK

With superconductivity often found in the vicinity of ordered states such as charge density waves (CDW) and antiferromagnetism, the ability to tune materials through these states serves as a vital tool in exploring the interplay of these phases with superconductivity. For characterizing a given superconductor, magnetic measurements provide a non-invasive method of studying vortex dynamics and measuring critical temperatures and fields.

Likewise, pressure measurements serve as a continuous tuning parameter across many of these phases. As such, the application of pressure provides a method to both access novel structures not available at ambient pressure, and to explore the competition between phases such as the CDW and superconducting order. This work develops current pressure cell technology compatible with commercial SQUID magnetometers, with both piston cylinder and gemstone anvil type cells.

Previous research into 2H-NbSe$_2$ has shown multiband superconductivity, CDW ordering, and the existence of a quantum critical point beneath the superconducting state. Here, we use the aforementioned pressure cells for magnetic susceptibility measurements, mapping the behaviour of the lower critical field and T_c with pressure and temperature. These provide insight into the multiband nature of superconductivity in this material, and provide evidence for a competition between the CDW and superconducting phases.

TT 16.6 Mon 15:00 P2/EG

Superconductivity in $[(\mathrm{SnSe})_{1+\delta}]_m[\mathrm{NbSe}_2]_n$ ferecrystals — •Olivio Chiatti[1], Klara Mihov[1], Martina Trahms[1], Theodor Griffin[1], Corinna Grosse[1], Danielle Hamann[2], Kyle Hite[2], Matty B. Alemayehu[2], David C. Johnson[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Solid State Chemistry, Inorganic Chemistry, Electrochemistry and Materials Science, University of Oregon, Eugene, OR 97403-1253, U.S.A.

The electrical properties of layered superconducting thin films have recently received a lot of attention. The ferecrystals are multilayers grown with atomic layer precision, but without an epitaxial relationship between the layers in growth direction. In this work, the ferecrystals are composed of a superconducting transition metal dichalgonide (NbSe$_2$) stacked repeatedly with a metal monochalgogenide (SnSe), which provides a model system for layered superconductors [1]. We examine ferecrystals with $n = 1$ and varying m, which show a superconducting phase below a critical temperature. The Ginzburg-Landau coherence lengths are determined from the critical magnetic fields and give information about the coupling between the superconducting NbSe$_2$ monolayers [2]. In addition, we discuss the conductivity corrections above the critical temperature due to quantum effects and superconducting fluctuations.

[1] C. Grosse *et al.*, Cryst. Res. Technol. **52**, 1700126 (2017)
[2] M. Trahms *et al.*, Supercond. Sci. Technol. **31**, 065006 (2018)

TT 16.7 Mon 15:00 P2/EG

Universal behavior of the IMS domain formation in superconducting niobium: Neutron scattering and molecular dynamics simulations — •Abdel Al-Falou[1,2], Alexander Backs[1,2], Michael Schulz[1,2], Alexei Vagov[3], Peter Böni[2], and Sebastian Mühlbauer[2] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Physikalisches Institut, Universität Bayreuth, Germany

In the intermediate mixed state (IMS) of type-II/1 superconductors, vortex lattice and Meissner state domains coexist due to a partial vortex attraction. Recently, we performed a systematic study on the domain formation in the IMS for Nb samples of varying purity [1,2]. Due to the wide range of length scales in the IMS, we combined several neutron based techniques with bulk magnetization measurements. We find a preferred vortex spacing a_{VL} in the IMS, independent of the external magnetic field. The temperature dependence of a_{VL} shows a universal behavior, related to the superconducting penetration depth and the sample purity. An elusive key feature so far is the domain morphology in bulk samples. Hence, we use molecular dynamics simulations on a 2D system of vortices as a complementary method, where the vortex interaction is given by extended Ginzburg-Landau theory [3]. In the simulations, we follow a field cooling path analogous to our experiments. The resulting morphology of the IMS depends on several parameters, e.g. the cooling rate or pinning strength. The results can be directly compared to neutron scattering data by Fourier transformation.

TT 16.8 Mon 15:00 P2/EG

Nernst Effect and Thermal Conductivity in Nd doped $\mathrm{La}_{1.81}\mathrm{Sr}_{0.19}$ CuO_4 — •Sanaz Shokri[1], Christoph Wuttke[1], Federico Caglieris[1], Koushik Karmakar[1], Andrey Malyuk[1], Silvia Seiro[1], Christian Hess[1,2], and Bernd Büchner[1,2,3] — [1]IFW , Dresden, Germany — [2]Centre for Transport and Devices, TU dresden, Germany — [3]Institut für Festkörper Physik, TU Dresden, Germany

The interrelation of superconductivity, stripe correlations, and pseudogap in cuprate superconductors is an unresolved issue for rationalizing the physics of these materials. Here we focus on the thermal conductivity κ and the Nernst coefficient ν of $\mathrm{La}_{2-y-x}\mathrm{Nd}_y\mathrm{Sr}_x\mathrm{CuO}_4$ at x=0.19, which is a prototype cuprate superconductor with a hole concentration close to p ≈ 0.18, below which pseudogap are considered to emerge in various physical properties [1]. Additionally, the Nd doping is understood to play an essential role for the appearance of stripe correlations [2]. Our data reveal a striking non-monotonic evolution of both ν and κ as a function of y. The data will be discussed in terms of the impact of Nd-doping on the buckling of the CuO$_2$ planes.

[1] O. Cyr-Choiniere et al., PRL 97, 064502(2017)
[2] J. Tranquada et al., Nature, 375, 561 (1994)

TT 16.9 Mon 15:00 P2/EG

Pump–probe spectroscopy of iron pnictides under high pressures — •Ivan Fotev[1,2], Harald Schneider[1], Manfred

Helm[1,2], Bernd Büchner[2,3], Saicharan Aswartham[3], and Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, Dresden, Germany

Iron pnictides are very susceptible to external pressure and can become superconducting (SC) at several GPa. Their rich temperature-pressure phase diagram contains a spin-density wave (SDW) phase next to the superconducting dome. Furthermore, it is thought that in iron pnictides the SDW and SC phases may even coexist, and they exhibit a quantum phase transition close to absolute zero.

We investigate the ultrafast quasiparticle dynamics of parental iron pnictides, like $BaFe_2As_2$, at low temperatures and high pressures, by combining optical pump–probe spectroscopy with a diamond anvil cell. This approach potentially enables us to identify SDW, SC or metallic state through their characteristic quasiparticle lifetimes and, therefore, scan the phase diagram of the material and explore the coexistence/competition between of SDW and SC phases.

TT 16.10 Mon 15:00 P2/EG

Analysis of Electronic Properties from Magnetotransport Measurements on $Ba(Fe_{1-x}Ni_x)_2As_2$ Thin Films — •Ilia Shipulin[1], Aleena Anna Thomas[1,2], Stefan Richter[1,2], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]Leibniz IFW Dresden, Institute for Metallic Materials, Dresden, Germany — [2]2 School of Sciences, TU Dresden, Dresden, Germany

Within the last years, significant progress was made in the field of single crystal growth of 122 based materials with isovalent, hole or electron doping, which made it possible to study the thermodynamic and transport properties of these compounds. At the same time, the preparation of high-quality epitaxial thin films of 122 materials resulted at least for the $BaFe_2As2_2$ based compounds in properties comparable to single crystals. Such films are of particular interest for the study of both fundamental and applied questions. Therefore, we focused our research on the two tasks: growing epitaxial thin films of $Ba(Fe_{1-x}Ni_x)_2As_2$ with different nickel concentrations by PLD method and studying the main electronic characteristics of the obtained Ba(Fe1-xNix)2As2 thin films. Based on the results of magnetotransport studies we estimated the density of electronic states at the Fermi level, the coefficient of electronic heat capacity and other electronic parameters of this compound and their dependence on the dopant concentration within the framework of the Ginzburg-Landau-Abrikosov-Gorkov theory. The comparison of the determined parameters with the measurement data of similar $Ba(Fe_{1-x}Ni_x)_2As_2$single crystals demonstrates a good agreement, which confirms the high quality of the obtained films.

TT 16.11 Mon 15:00 P2/EG

Superconductivity and quasi two dimensional magnetism in $EuRbFe_4As_4$ — •Noah Winterhalter-Stocker[1], Stefan Gorol[1], Stevan Arsenijevic[2], Yurii Skourski[2], Hans-Albrecht Krug von Nidda[3], Mamoun Hemmida[3], Dieter Ehlers[3], Anton Jesche[1], Veronika Fritsch[1], and Philipp Gegenwart[1] — [1]EP VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]EP V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

$EuRbFe_4As_4$ is a member of the new 1144 structure type of IBSCs, which contains parmagnetic Eu 4f moments. This structure is highly related to half doped 122 IBSCs. In contrast to the latter $EuRbFe_4As_4$ shows a superstructure with distinct Eu and Rb positions. The material shows a superconducting transition at $T_c = 36.8\,K$ and an onset of magnetic order of the Eu moments at $T_m = 15\,K$ [1]. We study the magnetic order and superconductivity by magnetization, magnetotransport and ESR measurements. Our analysis reveals the temperature dependence of the lower and upper critical fields. The ESR-measurements along with the magnetization data indicate the quasi two dimensional nature of the Eu magnetism. This becomes manifest in a Berezinsky-Kosterlitz-Thouless transition of the Eu, which was proposed by [2] and is confirmed by the ESR data.

[1] M. P. Smylie *et al.*, Phys. Rev. B **98**, 104503 (2018)
[2] K. Willa *et al.*, Phys. Rev. B **99**, 180502 (2019)

TT 16.12 Mon 15:00 P2/EG

Growth and characterisation of substitution variants of LaOFeAs single crystals — •Felix Anger[1], Anja Wolter-Giraud[1], Sebastian Gass[1], Hans-Joachim Grafe[1], Saicharan Aswartham[1], Sabine Wurmehl[1,2], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research, IFW, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Dresden, Germany

Facetted LaOFeAs single crystals with considerably growth in the crystallographic c direction were first prepared by R. Kappenberger et al. The growth process takes place via diffusion in solid state, the so-called Solid State Crystal Growth (SSCG) method. The single crystals are grown from a polycrystalline matrix by the introduction of NaAs as a liquid phase to aid the crystallization process.[1] Here, we present some additional experimental findings on the role of NaAs for the growth. Furthermore, we are aiming to grow novel series of crystals of substitution variants as, e.g., Co-doped SmOFeAs and $LaO_{1-x}F_xFeAs$. The crystals were characterized regarding their composition, structure and magnetic properties.

[1] R. Kappenberger et al., *Journal of Crystal Growth* **483**, 9-15 (2018).

TT 16.13 Mon 15:00 P2/EG

Charge density wave in Li doped NaFeAs — Jose M. Guevara[1], •Sven Hoffmann[1], Zhixiang Sun[1], Steffen Sykora[1], Yevhen Kushnirenko[1], Alexander Fedorov[1], Chanhee Kim[2], Aga Shahee[2], Dilipkumar Bhoi[2], Kee Hoon Kim[2], Saicharan Aswartham[1], Sergei Borisenko[1], 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

The hierarchy between superconductivity, magnetism and charge order remains as an indecipherable and breathtaking puzzle in solid state physics. Clarifying the role of these interaction is immensely important to understand the pairing mechanism of superconductivity in Iron-based superconductors. Here, we use SI-STS to visualize the atomic-scale electronic structure of $Na_{0.96}Li_{0.04}FeAs$. We find short range electronic order in the LDOS with a periodicity $\sim$ 8 nm. We use q-selective STS and angle-resolved photoemission to find a gap with value $2\Delta = 15$ meV and an appropriate nesting vector of $q_{2k_F} \sim 0.05\frac{\pi}{a_{Fe}}$ in the d_{yz} band at the Γ point, respectively. These observations are a clear signature of a band-selective charge density wave (CDW). We conjecture that the band-selective CDW is responsible for the change in the spin-fluctuations and therefore resulted in a different nematic state. We compared these findings with results for the parent compound NaFeAs.

TT 16.14 Mon 15:00 P2/EG

Electronic nematicity and thermal expansion in $FeSe_{1-x}S_x$ — •Liran Wang[1], Sven Sauerland[1], Dmitriy Chareev[2], Alexandre Vassiliev[2], Michael Merz[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]NRC Kurchatov institute, Moscow, Russie — [3]Institute for Solid State Physics, Karlsruhe Institute of Technology, Germany

We report the study on electronic nematicity in pure and sulfer doped FeSe high quality single crystals by means of thermal expansion and shear modulus measurements. Clear anomalies in the thermal expansivity are observed at both the magneto-structural and superconducting transition. By means of the three-point bending technique in the capacitance dilatometer, we obtain the nematic susceptibility from the shear modulus response. The shear modulus softens well above T_s implying a Curie-Weiss-like behaviour of the nematic susceptibility. Sulfur-doping suppresses T_s but no clear effect on T_c can be found. The evolution of the nematic phase as well as of nematic fluctuations is mapped out towards the superconducting regime. The relation between the nematic susceptibility and spin, structure and orbital degrees of freedom is discussed.

TT 16.15 Mon 15:00 P2/EG

Towards the study of uniaxial strain in epitaxial $FeSe_xTe_{1-x}$ films — •Aleena Anna Thomas[1,2], Thomas Doert[2], Kornelius Nielsch[1,2], and Ruben Hühne[1] — [1]Leibniz Institute for Metallic Materials, IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany

The discovery of high temperature superconductivity in layered iron-based material has ignited significant scientific interest in basic studies of their properties as well as for technological applications. Among them, iron selenide has the simplest crystal structure, in which superconductivity can be tuned either by strain or by doping. In particular, it has been reported in literature that the transition temperature can be increased by compressive substrate-induced biaxial strain in thin film. Our aim is to extend these investigations in order to study the correlation between uniaxial strain and critical temperature in thin films. In order to study such thin film in a uniaxial strain cell, we grew iron selenides on ultra-thin single crystalline substrates. Therefore, a thin Fe(Se,Te) seed layer was deposited on these substrates at 400 °C using pulsed laser deposition, followed by a homo-epitaxially grown Fe(Se,Te) film at 300 °C. All films are highly textured and show a maximum superconducting transition temperature of 21 K, 19 K and 17 K on CaF_2, $SrTiO_3$ and MgO, respectively. These thin films will be studied to infer the influence of uniaxial strain on the superconducting transition in FeSe materials using the aid of uniaxial strain cell.

TT 16.16 Mon 15:00 P2/EG

FIB-Fabricated Micro-Resonators to Probe Symmetry Breaking in Unconventional Superconductors — •Amelia Estry[1], Carsten Putzke[1], Chunyu Guo[1], Markus König[2], and Philip J. W. Moll[1] — [1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Determining the broken symmetries in the strongly correlated states of unconventional superconductors is critical to their understanding. I will present a measurement technique currently being developed to probe symmetry breaking by examining the elastic moduli in crystalline micro-resonators in their competing ground states. We use Focused Ion Beam (FIB) micro-machining to cut cantilevers with well-defined geometry and crystallographic direction directly out of high-quality single crystals. The hundred-nanometer resolution of FIB fabrication leads to well-defined boundary conditions for the simulation of the elastic problem. We propose to explore symmetries by studying the resonance frequencies of cantilevers with different crystallographic orientations and complex shapes. The proximity of the pseudogap in cuprates and nematicity in pnictides to superconductivity raises the question of their interplay and possible common origin. Particularly, the pseudogap is debated to be either a crossover of energy scales or a distinct thermodynamic phase. With this novel approach we aim to identify the symmetries in the pseudogap, probing current theoretical predictions.

TT 16.17 Mon 15:00 P2/EG

Angular-dependent specific heat of the organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ — •T. Reimann[1], H. Kühne[1], J. A. Schlueter[2], and J. Wosnitza[1,3] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Division of Materials Research, National Science Foundation, Alexandria, VA 22314, USA — [3]Institut für Festkörper- und Materialphysik, TU Dresden, D-01062 Dresden, Germany

The layered organic superconductor κ-(BEDT-TTF)$_2$Cu(NCS)$_2$ ($T_c \approx$ 9.4 K) has recently gained strong interest because macroscopic, such as specific heat and magnetic torque, as well as microscopic NMR studies indicate the formation of a Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state above the Pauli-limit of $B_P \approx 21$ T (For a recent review, see [1]). However, details about the nature of the phase transition remained controversial, since already a small off-alignment α of the superconducting layers to the magnetic field gives rise to orbital effects and reduces T_c considerably. Here, we present angular-resolved specific heat measurements in fields ranging from 0 to 22 T, covering the conventional superconducting as well as the FFLO state. For strictly parallel alignment, a sharpening of the superconducting transition accompanied by an upturn of $T_c(B)$ clearly hallmarks the FFLO state above B_P. However, for $0.5 \leq \alpha \leq 3.5$, pronounced first-order transitions appear slightly below T_c possibly indicating melting of the vortex lattice.

[1] J. Wosnitza, *Ann. Phys.* **530**, 1700282 (2018)

TT 16.18 Mon 15:00 P2/EG

Implementation of the full-potential relativistic KKR-BdG method — •Philipp Rüssmann[1], Phivos Mavropoulos[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Physics Department, National and Kapodistrian University of Athens, Greece

The realization of Majorana fermions in superconductor (SC)/topological insulator (TI) hybrid structures is a major international research challenge. Prerequisite is the understanding and optimization of SC/TI interface, which can in principle be achieved through the predictive power of density functional theory. However, treating superconductivity on this footing in complex systems, including defects, surfaces and interfaces, remains a major challenge. The Bogoliubov-de Gennes (BdG) method allows to combine the strengths of *ab initio* electronic structure calculations for the normal state with a simple description of the superconducting pairing interaction [1]. While taking care of the complexity of the normal state band structure, a material-specific semiphenomenological parameter can be introduced to allow the calculation of the BdG quasiparticle spectrum in the superconducting state. – Here, we present the implementation of the BdG method into our full-potential relativistic Korringa-Kohn-Rostoker Green function method [https://jukkr.fz-juelich.de], following Csire et al. [1]. We acknowledge financial support from DFG-Excellence Cluster ML4Q.

[1] G. Csire *et al.*, Phys. Rev. B **91**, 165142 (2015).

TT 16.19 Mon 15:00 P2/EG

Exact Diagonalization study of large Hubbard clusters — •Michael Danilov[1], Sergei Iskakov[2], Andrei Bagrov[3], Alexander Lichtenstein[1], and Mikhail Katsnelson[3] — [1]I. Institut für Theoretische Physik, Jungiusstr. 9, 20355 Hamburg, Germany — [2]Department of Physics, University of Michigan, Ann Arbor, Michigan 48109, USA — [3]Institute for Molecules and Materials, Radboud University, 6525AJ Nijmengen, The Netherlands

Using efficient exact diagonalization scheme, we study electronic structure of 4x4 doped Hubbard cluster with realistic hopping parameters including next nearest neighbour hopping $t' = -0.3t$, which is optimal for superconducting cuprates.

To find possible candidates for superconducting regime we calculate the spectral function and network entanglement measures for different doping and Coulomb interaction.

TT 16.20 Mon 15:00 P2/EG

Josephson inductance of epitaxial Al-InAs-based Josephson junction arrays — •Christian Baumgartner[1], Linus Fresz[1], Lorenz Fuchs[1], Geoffrey Gardner[2,3], Michael Manfra[2,3], Nicola Paradiso[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, Germany — [2]Station Q Purdue, Purdue University, West Lafayette, Indiana 47907, USA — [3]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907,USA

We study one-dimensional Josephson junction arrays (JJAs) in epitaxial Al/InAs/InGaAs heterostructures. Our measurement circuit allows us to measure simultaneously the Josephson inductance and the DC transport characteristics. Both are measured as a function of the magnetic field vector, temperature, gate voltage or direct current. We find that the critical current determined at the equilibrium from the Josephson inductance is significantly larger than the transport critical current. This latter is, in fact, determined by the weakest link, whereas the Josephson inductance is insensitive to defects in the JJA. Interestingly, the measurement of the Josephson inductance makes it possible to directly reconstruct part of the current-phase relation, and therefore deviations from the sinusoidal dependence. The present method offers a new approach to investigate the nature of topological Josephson junctions.

TT 16.21 Mon 15:00 P2/EG

Controllable Josephson Junctions by ferromagnetic Proximity Effect — •Lukas Kammermeier, Maik Kerstingskötter, Marcel Thalmann, Elke Scheer, and Torsten Pietsch — Universität Konstanz

Josephson junctions (JJ) belong to the most important superconducting devices in terms of applications. Thereby an active tuneability of the JJ's properties is highly desirable. Creating the JJ through local suppression of superconductivity due to the inverse proximity effect with ferromagnets, offers versatile control possibilities. The presented project aims at controlling the JJ by tayloring the ferromagnetic interface and its repsonse to magnetic fields and high frequency radiation to lay the ground for further control via spin pumping and spin injection. We show preliminary experimental results on the transport properties and the observation of fractional Shapiro steps in these types of junctions.

TT 16.22 Mon 15:00 P2/EG

Transport and ferromagnetic resonance in superconductor-ferromagnet junctions — •Andreas Bloch, Marcel Thalmann, Marcel Rudolf, Elke Scheer, and Torsten Pietsch — Physics Department, University of Konstanz, 78457 Konstanz, Germany

Hybrid superconductor nanostructures have the potential to overcome the limitations of conventional, dissipative electronic devices. We investigate novel spin and charge transport phenomena in superconductor (S) - ferromagnet (F) hybrid nanostructures under non-equilibrium conditions. We focus on ferromagnetic Josephson junctions (fJJs), where two S are separated by a F barrier. Theory predicts the possibility to generate long range triplet pairing in SF hybrid systems via a dynamic coupling of the electron spin to the magnetic resonance of the ferromagnet (FMR) [1]. We present here the first results of our project aiming at investigating experimentally this novel phenomenon. The samples under study are realized by electron beam and photo lithography. We use Al as S and Co or Py as F metal. A pre-patterned coplanar waveguide introduces microwaves (frequency up to 40 GHz) to the integrated SF contact to drive the FMR. The local and non-local current-voltage characteristics under irradiation will be discussed.

[1] S. Hikino et al., Supercond. Sci. Technol. **24**, 024008 (2011)

TT 16.23 Mon 15:00 P2/EG

Development of a fabrication process for nanoSQUIDs with three independent Nb layers — •Silke Wolter[1], Oliver Kieler[1], Thomas Weimann[1], Josepha Altmann[2], Sylke Bechstein[2], Jörn Beyer[2], Julian Linek[3], Reinhold Kleiner[3], and Dieter Koelle[3] — [1]Fachbereich Quantenelektronik, Physikalisch-Technische Bundesanstalt (PTB), Braunschweig — [2]Fachbereich Kryosensorik, Physikalisch-Technische Bundesanstalt (PTB), Berlin — [3]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen

Nanometer-sized superconducting quantum interference devices, nanoSQUIDs (nSQs), offer high spatial resolution und high spin sensitivity approaching the order of $1\,\mu_B/\mathrm{Hz}^{1/2}$ (μ_B is the Bohr magneton), making them suitable for the detection of the magnetic states of magnetic nanoparticles. Our fabrication technology for nSQs with overdamped SNS (S: superconductor, N: normal conductor) trilayer Nb-HfTi-Nb Josephson junctions is based on the combination of electron beam lithography with chemical-mechanical polishing and magnetron sputtering on thermally oxidized Si wafers to produce dc nSQs with 100-nm-dimensions for Nb lines and junctions (down to $80\,\mathrm{nm}\times 80\,\mathrm{nm}$). We extended the process from originally two to three independent Nb layers. This extension offers the possibility to increase the density of structures on the wafer and to realize superconducting vias to all Nb layers without the HfTi barrier. We present results on the yield of this process and measurements of nSQs characteristics.

This work was supported by the DFG (KI 698/3-2).

TT 16.24 Mon 15:00 P2/EG

Towards direct on-chip spectroscopy of the Bloch oscillations in a small Josephson junction — •Sergey Lotkhov — Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

In our presentation, we address an experimental design which should make it possible to directly detect and to measure the linewidth of Bloch oscillations in a small Josephson junction. A dual experiment has been recently reported by our group [1] in respect to the Josephson radiation transmitted via a SQUID-tunable coplanar waveguide (CPW) to a photon-assisted tunneling (PAT) detector fabricated on the same on-chip. Single-photon-state readout has been demonstrated for the microwave frequencies around 80 GHz. In the new design, the source of oscillations is realized as a Bloch junction embedded into reactive high-impedance environment. The oscillations are coupled weakly to a sharp CPW resonant mode within the Bloch frequency range of 15-30 GHz. We discuss the experimental challenges and the promising solutions which we are about to deal with in the new experiments. In particular, we address our recent progress towards lower-threshold PAT detectors and highly transparent Bloch junctions. Furthermore, we will briefly overview the expected impact of the known stray mechanisms, like Landau-Zener tunneling or electron heating, on the oscillations linewidth for the scope of feasible parameters.

[1] S. V. Lotkhov et al., Appl. Phys. Lett. 115, 192601 (2019)

TT 16.25 Mon 15:00 P2/EG

Characterization of Nb/Al-AlO$_x$/Nb Josephson tunnel junctions suited for SQUID applications — •Fabienne Bauer, Dominik Zehender, Felix Herrmann, Constantin Schuster, Christian Enss, and Sebastian Kempf — 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 qubits, Josephson voltage standards or superconducting quantum interference devices (SQUIDs). Since many recent applications strongly demand for circuits involving a large number of Josephson junctions, a reliable wafer-scale fabrication process yielding JJs with a reproducible and uniform high quality as well as a small parameter spread is required. To potentially readjust critical fabrication parameters, the quality of the fabricated JJs has to be continuously monitored.

In this contribution, we present our methods and approaches to characterize our home-made Nb/Al-AlO$_x$/Nb junctions which are utilized for SQUID applications. Current-voltage characteristics are recorded to check for the scaling of junction parameters like the critical current I_c with respect to the junction area and to extract different figures of merit such as the ratio of subgap to normal state resistance R_{sg}/R_N or the I_cR_N-product. To further check for the quality of the tunnel barrier, we measure the magnetic field dependence of I_c. In addition, we use unshunted SQUIDs to determine the intrinsic junction capacitance.

TT 16.26 Mon 15:00 P2/EG

Reducing the influence of SQUID Joule heating in dc-SQUIDs on the performance of cryogenic detectors — •Felix Herrmann, Matthäus Krantz, Anna Ferring-Siebert, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Metallic magnetic calorimeters (MMCs) are energy dispersive single particle detectors that are usually operated at temperatures below 50 mK. By making use of a paramagnetic temperature sensor absorbed energy is converted into a magnetic flux change which is measured by a dc-SQUID using a superconducting flux transformer.

In order to reduce parasitic inductances within the flux transformer, detector and SQUID should be placed in close vicinity. However, the Joule heat dissipated by the SQUID might negatively effect the detector temperature, thereby degrading the energy resolution. The energy dissipation of the SQUID is even more important in MMCs with direct sensor readout, a highly promising readout scheme to push the energy resolution in the sub-eV range. There, the paramagnetic sensor is placed directly on top of the SQUID loop, maximizing signal coupling while minimizing stray inductances.

In this contribution we discuss our recent efforts to reduce the influence of SQUID Joule heating on the performance of MMCs. In particular, we present a setup allowing to operate large detector arrays read out by conventional dc-SQUIDs, several means to reduce SQUID Joule heating e.g. by changing the shunt resistor geometry, as well as advanced heat sinking techniques using on-chip membranes.

TT 16.27 Mon 15:00 P2/EG

Metallic Magnetic Calorimeters for High Resolution X-Ray Spectroscopy of Highly Charged Ions — •M. Friedrich[1], S. Allgeier[1], M. Arndt[1], J. Geist[1], D. Hengstler[1], C. Schötz[1], S. Kempf[1], L. Gastaldo[1], A. Fleischmann[1], C. Enss[1], Ph. Pfäfflein[2], S. Trotsenko[2,3], T. Morgenroth[3], M.O. Herdrich[2], G. Weber[2], R. Märtin[2], and Th. Stöhlker[2,3,4] — [1]KIP, Heidelberg University — [2]HI Jena — [3]GSI Darmstadt — [4]IOQ, Jena University

Heavy Highly Charged Ions (HCIs) are promising candidates to test QED in extreme electromagnetic fields. Due to the high nuclear charge of such ions the electronic transitions are shifted to the X-ray regime, while the Lamb-Shift amounts to more than 0.1 % of the transition energies. Metallic magnetic calorimeters are energy dispersive X-ray detectors, which provide an extremely high energy resolution over a wide energy range as well as an excellent energy calibration. Thus, they are perfectly suited for high precision X-ray spectroscopy on HCIs in ion storage rings where photon flux is small and beam time is limited.

For an upcoming measurement on H-like U^{91+} at CRYRING@ESR we report on our newly developed, fabricated and characterised two-dimensional detector array maXs100 consisting of 64 pixels with a total detection area of $10\mathrm{x}10\,\mathrm{mm}^2$. An absorber thickness of $100\,\mu$m ($50\,\mu$m) results in an expected energy resolution of $\Delta E_{\mathrm{FWHM}} \sim 38\,\mathrm{eV}(27\,\mathrm{eV})$. This detector is mounted on a side arm of a dilution refrigerator and will enable the determination of the 1s Lamb-Shift with sub-eV precision.

TT 16.28 Mon 15:00 P2/EG

Low Temperature MMC Detector Arrays for IAXO — •Daniel Unger, Andreas Abeln, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, and Daniel Hengstler —

Kirchhoff Institute for Physics, Heidelberg University

The International Axion Observatory (IAXO) is searching for evidence of axions or axion-like particles generated in the Sun. A large magnet inside a helioscope pointing towards the Sun is used to generate the required magnetic field to convert solar axions into photons via the Primakoff effect. The expected photon spectrum considering only axion-photon coupling has a black body shape with its maximum at around 4 keV. Hence, X-ray detectors with high efficiency and low intrinsic background are necessary. Low temperature detectors based on metallic magnetic calorimeters (MMCs) fulfill these requirements.

We present the characterization of the first MMC detector setup developed for IAXO. This system consists of a two dimensional 64 pixel MMC array covering a detection area of 16 mm^2. Together with the SQUIDs necessary for the readout, the detector is mounted on a structure designed to be suitable for even larger MMC arrays. The performance of the detector array was investigated over a period of two months and will be discussed in terms of energy resolution, stability over time and background rate. To cope for different X-ray optics, a larger array covering an area of 1 cm^2 is at present under development.

The results, in particular the achieved low intrinsic background, demonstrate that two dimensional MMC arrays are a promising technology for IAXO.

TT 16.29 Mon 15:00 P2/EG

Large x-ray detector design for Baby-IAXO — •Andreas Abeln, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, Daniel Hengstler, and Daniel Unger — Kirchhoff-Institute for Physics, Heidelberg University

Axions are promising candidates for cold Dark Matter as well as for solving the strong CP problem, their detection could shine light onto two important open questions in particle physics. The International AXion Observatory (IAXO) is an experiment designed for the validation of the existence of axion or axion-like particles (ALPs) produced in the Sun. IAXO is a fourth generation helioscope and will consist of a 20 m long magnet with field up to 6 T filling eight bores with diameter 60 cm. In this volume axion can be converted back to photons. Solar axions would produce a black body spectrum picking between 4 keV and 6 keV. The photons produced in the conversion volume are then focused onto high resolution and low background x-ray detectors. Metallic magnetic calorimeters (MMCs) have shown extremely good energy resolution and mainly unit quantum efficiency in the energy range of interest. First investigations have shown the possibility to reach very low level of undesired events.
We present the development of a new 2D MMC array characterized by 64 pixels covering an active surface of 1 cm^2. This absorber area perfectly contains the focal area of the x-ray optics foreseen to be used in Baby-IAXO, an intermediate stage of IAXO. The pixels are optimized to have high efficiency up to 10 keV. The expected energy resolution is 12 eV FWHM. We discuss the chip design and expected performance.

TT 16.30 Mon 15:00 P2/EG

dc-SQUID readout with intrinsic frequency-division multiplexing capability and high dynamic range — •Ludwig Hoibl, Daniel Richter, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

Direct-current superconducting quantum interference devices (dc-SQUIDs) are extraordinarily sensitive flux-to-voltage converters. Due to their periodic flux-to-voltage characteristic, the linear flux range is rather small. For this reason, a flux locked loop (FLL) circuit is typically used to linearize the output signal. However, FLL operation often sets a practical limit for the realization of multi-channel SQUID systems since feedback wires have to be routed to each SQUID. There is hence a great need for SQUID based multi-channel readout techniques, providing a linear input-output signal relation.
In this contribution, we present a frequency-division multiplexing (FDM) readout technique with linear input-output signal relation and simultaneously a large dynamic range. It is based on flux-ramp modulation and hence relies on converting the input signal into a phase shift of the flux-to-voltage SQUID characteristic which is continuously measured by applying a periodic, sawtooth-shaped flux signal to the SQUID. We introduce the basic concept of our multiplexing technique and discuss the performance of a home-made four channel multiplexer device. Moreover, we present the status and performance of a custom-made readout electronics as well as potential applications in detector readout.

TT 16.31 Mon 15:00 P2/EG

Microwave SQUID multiplexer based on lumped element resonators — •Constantin Schuster, Mathias Wegner, Felix Ahrens, Daniel Richter, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

To our present knowledge, microwave SQUID multiplexing is the most promising technique for reading out large detector arrays consisting of hundreds or even thousands of metallic magnetic calorimeters. Here, a non-hysteretic rf-SQUID is used to convert the detector signal into a phase or amplitude change of a superconducting microwave resonator for frequency encoding. So far, quarterwave transmission line resonators have been used exclusively, which somehow suffer from rather large lateral dimensions, severe sensitivity to frequency noise due to atomic tunneling systems as well as a challenging frequency control considering fabrication inaccuracies.

In this contribution we will present a microwave SQUID multiplexer (LEMUX) which is based on lumped element resonators and allows for a significantly increased channel density on the chip as well as the possibility for trimming the resonance frequency. We introduce our LEMUX design with a new generation of optimised rf-SQUIDs, discuss the achieved device performance and compare it to existing microwave SQUID multiplexers based on transmission line resonators.

TT 16.32 Mon 15:00 P2/EG

Investigation of the influence of nuclear spins and hydrogen absorbates on low-frequency excess flux noise — •Fabian Kaap, Anna Ferring-Siebert, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

The performance of superconducting quantum devices (SQDs) such as SQUIDs or qubits often suffers from low frequency excess flux noise (LFEFN). It is widely accepted that spin fluctuations at the surface of the superconductor, e.g. caused by adsorbed oxygen or hydrogen, is one of many sources of LFEFN. Recent works also suggest that spin fluctuations inside the bulk superconductor, e.g. due to nuclear spins, could give rise to LFEFN. However, there have been no experimental proofs or hints confirming or excluding these predictions so far.

In this contribution, we first present a chemical method to load hydrogen inside Nb layers in a controllable manner. We then discuss if and how LFEFN depends on hydrogen loading present in the bulk of the SQUID loop. Finally, we discuss our experimental approach to investigate the influence of device material on the LFEFN to ultimately reveal whether or not nuclear spins is another source of LFEFN. Within this context, we compare measurements on dc-SQUIDs with SQUID-washer made of Al to our conventional Nb-based SQUIDs.

TT 16.33 Mon 15:00 P2/EG

Spatially resolved SQUID-NMR measurement instrumentation for investigation of superfluid ^{3}He-thin-films — •Josepha Altmann[1], Sylke Bechstein[1], Joern Beyer[1], Oliver Kieler[2], Silke Wolter[2], Andrew Casey[3], and John Saunders[3] — [1]7.6 Kryosensorik, Physikalisch-Technische Bundesanstalt Berlin — [2]2.4 Quantenelektronik, Physikalisch-Technische Bundesanstalt Braunschweig — [3]Department of Physics, Royal Holloway University of London

Superfluid ^{3}He stands out as an unique and sophisticated condensed matter system. At the Royal Holloway University of London the different phases of ^{3}He-thin-films with heights varying from 100 nm up to 1100 nm are investigated to study the topological effects of the superfluid. To measure the phase diagram nuclear magnetic resonance (NMR) spectroscopy is used. In our setup, a Superconducting Quantum Interference Device (SQUID), designed as a current sensor, measures the NMR signal. To specify the location of the NMR signal, spatially resolving pick-up-coils are employed with dimensions ranging from 10 μm to 400 μm. Concurrently, coil inductances from about 20 nH up to 20 μH are needed to match well to the input circuit of SQUID current sensors. Electron beam lithography (EBL) enables the fabrication of superconducting planar structures with sub-μm-dimensions and thus a high ratio of inductance to coil size. We present the design, EBL-based fabrication and characterization of fine-pitch superconducting Nb-coils with line widths of 200 nm and their foreseen application in spatially resolved NMR on superfluid ^{3}He-thin-films.

TT 16.34 Mon 15:00 P2/EG

Optimized geometry for a compact 3D quantum memory — •Julia Lamprich[1,2], Stephan Trattnig[1,2], Yuki Nojiri[1,2,3], Qiming Chen[1,2,3], Stephan Pogozarek[1,2], Michael Renger[1,2,3], Kirill Fedorov[1,2,3], Achim Marx[1,2,3], Matti Partanen[1,3], Frank Deppe[1,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Quantum memories are of high relevance in the context of quantum computing and quantum communication. In view of the tremendous publicly-funded and commercial efforts to build scalable architectures based on superconducting quantum circuits, 3D cavities are promising candidates for a quantum memory. Recently, a compact layout exploiting the multimode structure of a rectangular 3D cavity has been demonstrated [1]. As an alternative to an improved operation mode of this device with optimal control strategies [2], we discuss an optimization of the cavity geometry here. Our results are promising with respect to key properties such as storage time and scalability.

We acknowledge support by the Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No. 820505).

[1] E. Xie et al., Appl. Phys. Lett. 112, 202601 (2018).
[2] Sh. Machnes et al., Phys. Rev. Lett. 120, 150401 (2018)

TT 16.35 Mon 15:00 P2/EG

Quantum key distribution with squeezed displaced microwave states — •Florian. Fesquet[1,2], Kirill.G. Fedorov[1,2], Stefan. Pogorzalek[1,2], Michael. Renger[1,2], Qi-Ming. Chen[1,2], Yuki. Nojiri[1,2], Matti. Partanen[1], 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]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Quantum key distribution (QKD) is a technique to secretly communicate a key string between two parties. For continuous variables, the security can be achieved using properties of quantum mechanics, notably the non-commutativity of variables. We investigate a prepare-and-measure continuous-variables QKD protocol based on single-mode squeezed displaced microwave states to communicate a Gaussian modulated key. We theoretically investigate the secrecy and secret key rate of the protocol with an eavesdropper. It is shown that depending on the additional noise induced by the eavesdropper, the protocol is proven to be secure at the cost of an increased signal-to-noise ratio. Additionally, we show preliminary experimental results of the protocol in the microwave regime.

We acknowledge support by the Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (GrantNo.820505).

TT 16.36 Mon 15:00 P2/EG

Optimized superconducting NbN resonators for hybrid quantum systems in strong magnetic field — •Thomas Koch[1], Kiril Borisov[1,2], Dennis Rieger[1], Christoph Sürgers[1], Patrick Winkel[1], Ioan Pop[1,2], and Wolfgang Wernsdorfer[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe — [2]Institute of Nanotechnology, Karlsruher Institut für Technologie, Karlsruhe

Superconductors are utilized as highly precise detectors for magnetometry, superconducting qubits and other hybrid quantum systems. Our goal is superconducting NbN microwave resonators with high magnetic field stability and high quality factors at single photon regime. Therefore, we optimized deposition conditions and patterning geometries and achieved high critical temperature ($\approx$ 15 K), high critical fields ($>$ 9 T), reduced susceptibility to vortex dynamics and high kinetic inductance (L $\approx$ 80 pH/square) in thin (10 nm) NbN films. We extracted quality factor and resonance frequency of stripline NbN resonators by microwave reflection in parallel and perpendicular field up to 1 T at 20 mK. Initial results on the realization of a hybrid quantum system with a NbN resonator as a read-out sensor will be presented as well.

TT 16.37 Mon 15:00 P2/EG

Low temperature suppression of the critical current in nanoscale Josephson junction parallel arrays — •Konrad Dapper[1], Lukas Powalla[1,2], Yannick Schön[1], Micha Wildermuth[1], Hannes Rotzinger[1,3], and Alexey V. Ustinov[1,4] — [1]Institue of physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institut für Festköperphysik, Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia

We investigate the dynamics of fluxoids in parallel arrays of discrete, nanoscale Josephson junctions (JJPA) in the quantum regime where both charging and Josephson energy exceed the thermal energy. One mayor problem of these circuits is the confinement of current vortices in the array, since the small size of the Josephson junctions also leads to a vortex size typically much larger than the array length. To overcome this issue, we place additional Josephson junctions as kinetic inductance elements to each individual plaquette. Special care has also been taken to ensure a homogeneous biasing scheme of the array and a high impedance environment. The arrays are analyzed with transport measurements, in particular, we perform switching current measurements at various milli-Kelvin temperatures. We present data, which show a critical current suppression below temperatures of 600 mK, which indicates an influence of non-thermal quasiparticles and / or quantum phase slips.

TT 16.38 Mon 15:00 P2/EG

Microwave environment design for compact arrays of granular aluminum fluxonium qubits — •Patrick Paluch[1,2], Martin Spiecker[2], Daria Gusenkova[2], Ivan Takmakov[2], Francesco Valenti[2], Patrick Winkel[2], Dennis Rieger[2], and Ioan Pop[1,2] — [1]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, 76137 Karlsruhe, Germany

Fluxonium qubits employing the high kinetic inductance of granular aluminum (grAl) have recently been implemented, demonstrating state-of-the-art coherence time [1]. In superconducting qubit design, the use of 3D waveguides is generally advantageous in reducing dielectric losses; however, it can limit the availability of in-situ magnetic flux lines. Moreover, given the localized nature of the fluxonium qubit mode, with the junction capacitance dominating, the advantages of 3D waveguides can be debated. Here we present a fast-flux tunable grAl fluxonium design in a coplanar waveguide geometry, surrounded by a normal metal ground plane, potentially decreasing the number of quasiparticles in the system [2] and avoiding flux trapping.

[1] Grünhaupt and Spiecker et al., Nat. Mater. 18, 816-819 (2019)
[2] Henriques and Valenti et al., Appl. Phys. Lett. 115, 212601 (2019)

TT 16.39 Mon 15:00 P2/EG

Two-level-systems spectroscopy in Transmon qubits. — •Serhii Volosheniuk[1], Alexander Bilmes[1], Alexey V. Ustinov[1,2], and Jürgen Lisenfeld[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe 76131, Germany — [2]Russian Quantum Center, National University of science and Technology MISIS, Moscow 1190449, Russia

Despite the announcement of achieving quantum supremacy, we are still far away from a superconducting quantum processor. One of the principal causes is low qubit fidelity due to parasitic material defects. These act like two-level-systems (TLS) which limit qubit coherence and create environmental fluctuations.

To understand how TLS are forming during sample fabrication, we seek information on their location in a given qubit circuit. For this, TLS are tuned with applied elastic strain and dc electric fields, allowing us to distinguish defects in Josephson junction tunnel barriers from those at film interfaces[1,2].

Here we present our latest results and ideas on TLS spectroscopy with E-field tuning in qubits. One goal is to obtain two-dimensional maps of defect locations in the vicinity of the qubits Josephson junctions to elucidate and mitigate the role of junction lithography on defect formation.

[1] J. Lisenfeld et al., npj Quantum Inf 5, 105 (2019)
[2] A. Bilmes et al., arXiv:1911.08246 (2019)

TT 16.40 Mon 15:00 P2/EG

Dielectric Low Temperature Properties of Printed Circuit Boards made of FR4 — •Andreas Rall, Benedikt Frey, Andreas Schaller, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, D-69120 Heidelberg

Printed circuit boards (PCB) are commonly used in electronic devices and are increasingly utilized in various low temperature applications.

In many cases standard FR4 is used, which is a laminate of glass-fibers (alumino-borosilicate glass) and brominated epoxy resin. Little is known about its low temperature properties. We present dielectric measurements of FR4 down to a few millikelvin temperatures, where we use the material as dielectric sample of a plate capacitor in a superconducting LC-resonator at MHz frequencies.

The observed behavior can be well understood in terms of atomic two-level tunneling systems, that are known to dominate the low temperature properties of amorphous solids. The material shows a good thermalisation with the cryogenic environment even at the lowest measured temperatures. Measurements of the sample's temperature with a thermometer directly mounted on the sample can confirm this good thermalisation.

TT 16.41 Mon 15:00 P2/EG

Investigating the Non-equilibrium Dynamics of two-level systems at Low Temperatures — •Marcel Haas, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University, 69120 Heidelberg

The dielectric loss of amorphous materials along with noise and decoherence is the major limiting factor in many applications like superconducting circuits, Josephson junctions and quantum computing. It is mainly determined by atomic tunneling systems described by quantum mechanical two-level systems (TLS) leading to a broad distribution of low-energy excitations in the sample. The spontaneous phonon emission of an excited TLS gives rise to a relaxation time T_1 and the interaction between TLSs with their thermally excited surrounding induces a dephasing timescale T_2. These effects mainly determine the measurable dielectric loss in the observed material, which we ascertain by measuring the quality factor of a bridge type superconducting LC-resonator. The dielectric medium in between the capacitor plates is a sputter deposited a-SiO_2 film. A variation of the Rabi-frequency through the electric field strength of the drive can thereby change the transition probability of the TLSs and thus the influence of loss generating effects. The experimental setup additionally allows the application of a DC to AC electric bias field across the capacitance. This enables us to manipulate the occupation difference of the TLSs by shoving new unexcited TLSs through resonance which restores the influence of decoherence. We present first measurements at a frequency of 1 GHz performed with a microfabricated superconducting resonator.

TT 16.42 Mon 15:00 P2/EG

Machine learning for quantum chemistry with quantum computers — •Tomislav Piskor[1,2], Sebastian Zanker[1], Thilo Mast[1], Peter Schmitteckert[1], Frank Wilhelm-Mauch[2], and Michael Marthaler[1] — [1]HQS Quantum Simulations GmbH, Haid-und-Neu-Straße 7, 76131 Karlsruhe — [2]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Simulating chemical systems is a major field of interest not only for the pharma and chemistry, but also for the automotive industry. One such example is the simulation of functional groups of a large molecule or proteine, which can be useful for QM/MM methods. In order to get the exact ground state of the functional group, we can use quantum computers in the future. However, every call to a quantum computer will be relatively expensive, making high-throughput simulations with quantum computers unfeasible.

To bypass this, we propose the following scheme: a few single point calculations are determined with the quantum computer and then extended to more conformations with machine learning methods. We use sGDML (symmetric gradient domain machine learning), where the atomic coordinates of the molecules are given as the input and the corresponding forces as the output. A modified Gaussian kernel is then used in order to obtain the trained force fields and by performing an integration with respect to the atomic coordinates one gets the potential energy surface. This routine was tested on molecules such as enediyne and malonaldehyde, where we observe very good results not only for the force field, but also energy predictions.

TT 16.43 Mon 15:00 P2/EG

Influence of the nuclear quadrupolar interactions in periodically driven quantum dots — •Iris Kleinjohann and Frithjof Anders — Lehrstuhl für Theoretische Physik II, Technische Universität Dortmund, 44227 Dortmund

Periodic optical driving of the electron spin in singly charged semiconductor quantum dots generates a spin polarization and induces a synchronization of the spin dynamics with the driving frequency. An external magnetic field perpendicular to the optical axis results in the Larmor precession of electron and nuclear spins of the quantum dot ensemble. While the electron spin precession adjusts to the periodicity of optical pumping, the synchronization is transmitted to the surrounding nuclear spins via hyperfine interaction generating a non-equilibrium distribution of the Overhauser field. We describe the spin dynamics by a central spin model and employ a Lindblad equation for the time evolution between optical pulses. Due to the growth process of the quantum dot sample a strain occurs in the quantum dots entailing quadrupolar interactions in the nuclear spin bath. We extend the central spin model to include these interactions and show that the influence on the synchronization with the periodic driving depends strongly on the parameters of the quadrupolar interactions.

TT 16.44 Mon 15:00 P2/EG

Effect of an RKKY interaction between electron spins in different quantum dots on their spin dynamics — •Kira Deltenre and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

Two-colored pump-probe experiments on self-assembled InGaAs quantum dots with spectrally narrow pump pulses allow to excite disjunct subsets of quantum dots. The observed correlations between the spin polarizations of the subsets suggest an interaction between the electron spins in the different quantum dots (Spatzek et al., Phys. Rev. Lett. **107**, 137402 (2011)). The observed phase shift between the measured ellipticities depends on the time delay between the two differently colored pump pulses. For our simulation, we assume an RKKY interaction transmitted via the wetting layer of the sample. The calculations of the spin dynamics are based on the central spin model. A semiclassical approach enables a simulation of a large number of quantum dots ($Q > 1000$). The extracted time dependent phase shifts are qualitatively similar to the experimental data for a specific set of parameters entering the distance dependent RKKY interaction strength.

TT 16.45 Mon 15:00 P2/EG

Bose condensation of squeezed light — •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

Light with an effective chemical potential and no mass is shown to possess a general phase-transition curve to Bose-Einstein condensation. This limiting density and temperature range is found by the diverging in-medium potential range of effective interaction. While usually the absorption and emission with Dye molecules is considered, here it is proposed that squeezing can create also such an effective chemical potential. The equivalence of squeezed light with a complex Bogoliubov transformation of interacting Bose system with finite lifetime is established with the help of which an effective gap is deduced. This gap phase creates a finite condensate in agreement with the general limiting density and temperature range. The phase diagram for condensation is presented due to squeezing and the appearance of two gaps is discussed. Phys. Rev. B 99 (2019) 205124

TT 16.46 Mon 15:00 P2/EG

A sustainable sub-Kelvin cooling technology for quantum electronics — •Klaus Eibensteiner[1,2], Jan Spallek[1], Alexander Regnat[1], Tomek Schulz[1], Felix Rucker[1], Nico Huber[1,2], Carolina Burger[1,2], Anh Tong[1,2], and Christian Pfleiderer[2] — [1]kiutra GmbH, München, Germany — [2]Physik-Department, Technische Universität München, Germany

Cooling devices providing temperatures well below 1 K are a key prerequisite for basic research and quantum technologies. Commercially available cooling solutions typically require either the rare and costly helium isotope helium-3 or provide cooling only for a limited period of time. Here we present a compact demagnetization refrigerator for the cryogen-free, continuous generation of sub-Kelvin temperatures based on prevalent and affordable solid-state cooling media.

TT 16.47 Mon 15:00 P2/EG

Development and characterization of a small scale two-stage pulse tube cryocooler — •Bernd Schmidt[1,2], Jack-André Schmidt[1,2], Jens Falter[2], Günter Thummes[1,2], and André Schirmeisen[1,2] — [1]Justus-Liebig Universität Gießen, Germany — [2]TransMIT GmbH, Gießen, Germany

Small scale pulse tube cryocoolers with input powers < 2 kW are a valuable alternative for liquid Helium cryostats, especially for long time measurements. In this input power regime, Helium compressors with air cooling and single phase power supply are commercially available, lowering the requirements for the measuring environment. Also, since pulse tube cryocoolers are closed cycle systems, the refilling of cryogen is not needed, leading to long running intervals of up to several years and less usage of Helium gas, which is consistently suffering of shortages [1].

In this poster, we present the development process of a new 4 K two-stage pulse tube cryocooler with an input power of about 1 kW [2]. The cryocooler reaches temperatures of < 2.5 K and provides a cooling power of > 70 mW at liquid Helium temperature. The cryocooler was simulated using Sage and Regen simulation environments. Afterwards it was fabricated, tested and optimized using a SHI CNA-11 Helium compressor with about 1 kW input power. A cooling load map was measured to characterize the system.

[1] Halperin, William P., Nature Physics 10.7 (2014): 467.
[2] Schmidt, B., et al., Cryogenics 88 (2017): 129-131.

TT 16.48 Mon 15:00 P2/EG

Construction of mK-scanning tunneling microscope combined with electron spin resonance technique — •Won-Jun Jang[1,2], Jinkyung Kim[1,2], Thi Hong Hong[1,2], Denis Krylov[1,2], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea

For a well-defined energy resolution of STM combined with electron spin resonance (ESR) technique, the lowering the effective temperature is necessary. Here we present technical efforts for the construction of mK-STM with the lowest effective temperature under ESR measurement. To reduce the effective temperature, we need to be lower a base temperature of inner conductor of RF signal lines, RF noises and the eddy current effect by external vibration. We achieved 10 mK using the dilution refrigerator (Janis research) with STM supporting structures made by SiPCu. We applied the thermal anchoring structure for RF signal lines. To reduce RF noises, we are planning to use RF filter at each signal line. To prevent the external vibration, we designed the pendulum structure for the circulation line for mixture gas and two vibration isolation stages. And also, we applied the slit structure to reduce the eddy current. Finally, we will introduce our effective temperature by the measurement of superconducting gap.

TT 17: Poster Session Correlated Electrons 1

Time: Monday 15:00–19:00 Location: P2/EG

TT 17.1 Mon 15:00 P2/EG

RMn_2Ge_2 (R = Nd, Sm, Dy): Single crystal growth and characterization — •Michelle Ocker, Robert Möller, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

The compounds RMn_2Ge_2, where R is a rare earth element, crystallize in the body centered tetragonal $ThCr_2Si_2$ structure type and exhibit a complex magnetic behaviour. At high temperature, the magnetism is determined by the ordering of the Mn-Mn layer, while at low temperatures it is dominated by the ordering of the rare earths local moments [1, 2]. There are many studies of polycrystalline samples or small single crystals, but large and pure single crystals suitable for spectroscopic studies are missing. In this contribution, we present the details of the growth by Czochralski method from a levitating melt of RMn_2Ge_2 (R=Nd, Sm, Dy) single crystals and their structural, chemical and physical characterization.

[1] G. Guanghua, M.V. Eremin, A. Kirste, N.P. Kolmakava, A.S. Lagutin, R.Z. Lebitin, M von Ortenberg and A.A. Sidorenko, Journal of Experimental and Theoretical Physics, **93**, 796 (2001)
[2] N. P. Kolmakova, A. A. Sidorenko, and R. Z. Levitin, Low Temperature Physics 28, 653 (2002).

TT 17.2 Mon 15:00 P2/EG

Crystal growth and characterization of materials with the $ThCr_2Si_2$ structure type — •Susanna Rongstock, Ali Scherzad, Alexej Kraiker, Doan-My Tran, Sebastian Witt, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe University Frankfurt, Germany

We present the single crystal growth of different intermetallic compounds within the LnT_2Si_2 family (with Ln = lanthanides and T = Rh, Ir), by employing a high-temperature metal-flux technique. The habitus of the obtained crystals is platelet like with the crystallographic *c* direction perpendicular to the surface [1]. The magnetic properties of these crystals were characterized by magnetization, heat-capacity, thermopower and resistivity measurements. These crystals form the materials basis for a thorough study of exciting surface properties by angle-resolved photoemission spectroscopy [2,3].

[1] K. Kliemt *et al.*, Cryst. Res. Technol., 1900116 (2019).
[2] A. Chikina *et al.*, Phys. Rev. B. 95, 155127 (2017).
[3] A. Generalov *et al.*, Phys. Rev. B. 98, 115157 (2018).

TT 17.3 Mon 15:00 P2/EG

Crystal growth and characterization of $CeCo_2P_2$ and $EuFe_2P_2$ — •Thanh Duc Nguyen, Johannes Hellwig, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The ternary phosphides $CeCo_2P_2$ and $EuFe_2P_2$ are compounds that belong to the '122'-systems crystallizing in the $ThCr_2Si_2$ structure type. $CeCo_2P_2$ is an antiferromagnet due to the ordering of cobalt atoms at $T_N = 440$ K [1]. $EuFe_2P_2$ is a ferromagnet due to the ordering of divalent europium atoms with a Curie temperature of $T_C = 27.5$ K [3]. We synthesized both compounds in tin-flux using either quartz or niobium ampoules [2]. In this way, large platelet-like $CeCo_2P_2$ single crystals of several mm lateral size were created. For the europium system the crystals are smaller. Electrical transport measurements and a magnetic characterization were done for both compounds. In addition, $CeCo_2P_2$ is a candidate for the investigation of its surface states by ARPES.

[1] Yong Tian et al., Physica B: Condensed Matter, 512, 75, (2017)
[2] Kliemt et al., Cryst. Res. Technol., 1900116, (2019)
[3] E. Mörsen et al., Journal of Physics and Chemistry of Solids, 49, 7, (1987)

TT 17.4 Mon 15:00 P2/EG

Scanning Tunneling Microscopy on $Eu_5In_2Sb_6$: a non-symmorphic antiferromagnetic insulator — •Maria Victoria Ale Crivillero[1], Sahana Roessler[1], Priscila F. S. Rosa[2], and Steffen Wirth[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany. — [2]Condensed Matter and Magnet Science Group, Los Alamos National Laboratory, Los Alamos, NM 87545, USA.

Motivated by theoretical predictions of non-trivial Fermi surface topology stabilized by the non-symmorphic symmetry in the Zintl phase $Ba_5In_2Sb_6$, we investigated the magnetic analogue $Eu_5In_2Sb_6$. The inclusion of Eu gives rise to a complex magnetic behavior. At low temperatures, two magnetic transitions ($T_{N_1} \approx 14\,\mathrm{K}$ and $T_{M_2} \approx 7\,\mathrm{K}$), revealed in our magnetization, heat-capacity and transport measurements, point to such an intricate magnetic structure. Interestingly, the emergence of colossal magnetoresistance (CMR) suggests the formation of magnetic polarons.

We performed complementary STM/STS measurements. To this end, we attempted to cleave the samples *in situ* in UHV and at low temperatures along the *a*, *b* and *c*-axis. $Eu_5In_2Sb_6$ crystallizes in an orthorhombic structure (*Pbam*), characterized by infinite $[In_2Sb_6]^{10-}$ double chains along the *c*-axis. In the (010) plane, we obtained striped patterns that can be correlated to the double-chains stacking. The attempted cleavage along the *a*-axis revealed a more complex pattern, which could be indicative of cleavage along the $(1\bar{1}0)$ plane. So far, no clear experimental evidence of surface states was observed.

TT 17.5 Mon 15:00 P2/EG

Evidence of fully-gapped superconductivity in the locally noncentrosymmetric heavy-fermion system $CeRh_2As_2$ — •Seunghyun Khim[1], Manuel Brando[1], Jacintha Banda[1], Oliver Stockert[1], Zurab Guguchia[2], Robert Scheuermann[2], and Christoph Geibel[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Villigen PSI, Switzerland

Recently, we have discovered unconventional superconducting behavior in $CeRh_2As_2$. The upper critical field (H_{c2}) which exceeds by far the Pauli limit indicates the Rashba-type spin-polarized electronic structure originating from the lack of local inversion symmetry. Coexistence of superconductivity with a possible quadrupolar order is suggestive of multipolar quantum criticality. Here, we present a study of the superconducting state of $CeRh_2As_2$ using muon spin rotation/relaxation (μSR) experiments. Results of transverse-field μSR experiments confirm bulk superconductivity and suggest a fully-gapped superconductivity order parameter. We discuss this finding together with the low-temperature specific-heat data.

TT 17.6 Mon 15:00 P2/EG

Optical Spectroscopy of $CeRh_2As_2$ and $LaRh_2As_2$ — Shinichi Kimura[1,2], Seunghyun Khim[3], and •Jörg Sichelschmidt[3] — [1]Graduate School of Frontier Biosciences, Osaka University, Suita 565-0871, Japan — [2]Department of Physics, Graduate School of Science, Osaka University, Toyonaka 560-0043, Japan — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$CeRh_2As_2$ is a new heavy-fermion superconductor ($T_C \simeq 0.25$ K) which crystallizes in the $CaBe_2Ge_2$-type structure where inversion symmetry is locally broken at the Ce site. It is discussed to be a model system to investigate the influence of Rashba-type interactions on heavy-fermion superconductivity. We present results of optical reflectivity on $CeRh_2As_2$ and $LaRh_2As_2$ for temperatures down to 10 K. In the far-infrared energy region $CeRh_2As_2$ shows a strong spectral weight redistribution with decreasing temperature which is a typical feature found in heavy-fermion materials. The spectra of $LaRh_2As_2$ show an unexpected strong temperature dependence which has not been observed in other counterparts of heavy-fermion materials. The phonon peaks of both compounds show unusually strong softening. Furthermore, the phonon frequency is higher in the Ce-system than in the La-system, in contrast to expectation. We discuss these observations in terms of the lack of local inversion symmetry in the crystal structure.

TT 17.7 Mon 15:00 P2/EG

Monte Carlo Study of Field-Induced Multipolar Phases in the Kondo Material $PrTi_2Al_{20}$ — •Frederic Freyer[1], Simon Trebst[1], SungBin Lee[2], Yong Baek Kim[3], and Arun Paramekanti[3] — [1]University of Cologne, 50937, Germany — [2]Korea Advanced Institute of Science and Technology, Daejeon, 34141, Korea — [3]University of Toronto, Toronto, Ontario, Canada M5S 1A7

Multispin interactions have long been appreciated as a possible microscopic driver for the formation of spin liquids or other forms of unconventional magnetic ordering, e.g. in the proximity of the Mott transition. Here we discuss the role of such multispin interactions in the Kondo material $PrTi_2Al_{20}$, which exhibits a rich phase phase diagram including intertwined quadrupolar orders, superconductivity and non-Fermi-liquid behavior. Our focus is on magnetic-field induced phase transitions in the quadrupolar ordered state, which have recently been experimentally probed by the Nakatsuji group. Via extensive Monte Carlo simulations we demonstrate that three-spin interactions between the local moments play an important role to explain the observed field dependence of the quadrupolar regime, in the context of a relatively simple O(2) spin model.

TT 17.8 Mon 15:00 P2/EG

Carrier relaxation dynamics in Kondo insulator YbB_{12} — •Amrit R Pokharel[1], Steinn Y Agustsson[1], Fumitoshi Iga[2], Toshiro Takabatake[2], Hidekazu Okamura[3], and Jure Demsar[1] — [1]Johannes Gutenberg University Mainz, Germany — [2]Graduate School of Advanced Sciences of Matter, Hiroshima University, Japan — [3]Graduate School of Advanced Technology and Science, Tokushima University, Japan

We investigate the photoexcited quasiparticle relaxation dynamics in Kondo insulator YbB_{12} by means of time resolved all-optical pump-probe spectroscopy. In particular, we focus on temperature and excitation density dependent studies to address the temperature dependent changes in the low energy electron structure associated with the interplay/hybridization between the Yb 4f-levels and the conduction band electrons. At low temperatures, both the rise-time and recovery of the photoinduced reflectivity changes show dramatic temperature and excitation density dependence. The results are well accounted by the presence of the 15 meV indirect hybridization gap. While the static optical conductivity studies suggest the fully opening of gap around 20 K, our data implies its presence to much higher temperatures of the order of 150 K. Both, the dependence of build-up and its recovery on excitation density can be in detail accounted for by the phenomenological Rothwarf-Taylor model, describing the carrier relaxation across the narrow electronic gap, bottlenecked by the re-absorption of emitted phonons with energy larger than the gap.

TT 17.9 Mon 15:00 P2/EG

Interplay of spin-orbit coupling and spin-orbital superexchange — •Pascal Strobel and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart, 70550 Stuttgart, Germany

In strongly correlated materials with a t_{2g}^4 electron configuration the interplay of superexchange, tetragonal crystal field splitting, and spin-orbit coupling is supposed to support a superposition of singlet and triplet states from the spin-orbit coupling Hamiltonian. This property is often referred to as excitonic magnetism. Ca_2RuO_4 is argued to be a promising candidate for hosting this excitonic magnetism by Raman scattering data [1] as well as numerical results from the variational cluster approach [2]. In order to get a comparison to neutron scattering data [3], we derive an effective hopping Hamiltonian via second order perturbation theory which gives rise to a Kugel-Khomskii type model. Using exact diagonalization we obtain spectra of the magnetic structure factor which show a high agreement with the experiment. With this model it is possible for us to investigate the influence of the parameters appearing in the Kugel-Khomskii type Hamiltonian in the regime of non zero spin-orbit coupling.

[1] Phys. Rev. Lett.119, 067201 (2017)
[2] arXiv:1910.13977v2 (2019)
[3] Phys. Rev. Lett.115, 247201 (2015)

TT 17.10 Mon 15:00 P2/EG

Crystal growth and characterization of the frustrated spinsystems $(Cs_{2-x}Rb_x)CuCl_4$ — •Sarah Krebber, Christian Klein, and Cornelius Krellner — Goethe-Universität Frankfurt am Main, Max-von-Laue-Straße 1, D-60438 Frankfurt am Main

Crystals of the antiferromagnetic insulator Cs2CuCl4 and the substitution series $(Cs_{2-x}Rb_x)CuCl_4$ (x = 0, 0.1, 0.2) were grown by vertical Bridgman method. The controlled substitution of cesium atoms with the smaller rubidium, causes chemical pressure on the crystal lattice [1]. The magnetic properties are caused by Jahn-Teller distorted $(CuCl_4)$ tetrahedra, which are arranged in layers separated by the alkali atoms. In these layers the localized Cu^{2+} spins form a triangular lattice, where the spins interact through exchange couplings. The resulting geometric frustration leads to quantum spin liquid properties at low temperatures. In addition to the growth and characterization of $(Cs_{2-x}Rb_x)CuCl_4$, we discuss the structural changes in the lattice parameters and the magnetic behavior of the substituted system in comparison to the well-known parent compound Cs_2CuCl_4. Furthermore we report an experimental study of the low-temperature specific heat and magnetic susceptibility of the substitution series $Cs_2CuCl_{4-x}Br_x$ (x = 0, 1, 2, 4) [2].

[1] H.T. Witteveen et al., Mater. Res. Bull. 9, 345 (1974)
[2] U.Tutsch et al., PRL 123, 147202 (2019)

TT 17.11 Mon 15:00 P2/EG

Multiple Spin-Orbit Excitons and the Electronic Structure of α-$RuCl_3$ — •Philipp Warzanowski[1], Nick Borgwardt[1], Karolin Hopfer[1], Thomas Koethe[1], Petra Becker[2], Vladimir Tsurkan[3,4], Alois Loidl[3], Maria Hermanns[5], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]Inst. of Physics II, University of Cologne — [2]Sect. Crystallography, Inst. of Geology and Mineralogy, University of Cologne — [3]Exp. Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [4]Inst. of Applied Physics, Chisinau, Moldova — [5]Dept. of Physics, Stockholm University, AlbaNova University Center, Sweden

α-$RuCl_3$ is widely discussed as a proximate Kitaev spin-liquid material. This scenario builds upon spin-orbit entangled $j = 1/2$ moments which arise in a t_{2g}^5 electron configuration with strong spin-orbit coupling λ and a large cubic crystal field. Despite the keen interest in α-$RuCl_3$, the low-energy electronic structure is still puzzling. In particular the origin of infrared absorption features at 0.30, 0.53, and 0.75 eV is still a matter of debate. Also the energy of the spin-orbit exciton, the excitation from $j = 1/2$ to $j = 3/2$, and thus λ are controversial. Combining infrared absorption and Raman data, we attribute the infrared features to single, double, and triple spin-orbit excitons, yielding $\lambda = 0.16$ eV and a non-cubic crystal field splitting $\Delta = 42$ meV. These results support the $j = 1/2$ picture despite of the crystal field distortion. The

strength of the double excitation can be understood by the same hopping interactions that also establish dominant Kitaev exchange [1].
[1] P. Warzanowski *et al.*, arXiv:1911.09337

TT 17.12 Mon 15:00 P2/EG

Magnetic field effects on Kitaev spin liquids — •Christoph Berke, Ciaran Hickey, and Simon Trebst — University of Cologne

Frustrated quantum magnets can give rise to unconventional spin-liquid ground states. Paradigmatic examples are two- and three-dimensional Kitaev systems. The characteristic bond-directional interactions are realized in a number of spin-orbit entangled Mott insulators that, in the presence of magnetic fields, show no indications of long-range order. Here, we study quantum phase transitions in the Kitaev model on different lattices under a magnetic field with an emphasis on the topological nature of Majorana excitations. Our interest is particularly in the emergence of intermediate phases, expected to appear for *AFM* couplings between the Kitaev spin liquid and the field polarized phase.

TT 17.13 Mon 15:00 P2/EG

Heat transport in the Kitaev spin-liquid candidate α-$RuCl_3$ — •Matthias Gillig[1], Richard Hentrich[1], Xiaochen Hong[1], Maria Roslova[2], Anna Isaeva[1,2], Thomas Doert[2], Bernd Büchner[1,3], and Christian Hess[1,3] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [3]Center for Transport and Devices, TU Dresden, Germany

α-$RuCl_3$ is a prime candidate to be close to the realization of the Kitaev model in a real material. The model is of interest due to its exact solution with a spin-liquid ground state and emerging Majorana excitations. Additional Heisenberg and off-diagonal terms in the Hamiltonian of α-$RuCl_3$ distinguish it from a pure Kitaev system which leads to an antiferromagnetically ordered ground state below T = 7 K. By applying a magnetic field above 8 T parallel to the honeycomb plane the ordered phase can be suppressed and a new phase emerges which is predicted to have spin-liquid character. We have performed detailed studies on the longitudinal and transverse heat transport in α-$RuCl_3$ for magnetic fields applied parallel and perpendicular to the honeycomb plane to explore the field-induced phase.

TT 17.14 Mon 15:00 P2/EG

Anisotropic field-induced ordering in the triangular-lattice quantum spin liquid $NaYbSe_2$ — •K. M. Ranjith[1], S. Luther[2,3], T. Reimann[2], B. Schmidt[1], Ph. Schlender[4], J. Sichelschmidt[1], H. Yasuoka[1], A. M. Strydom[5], Y. Skourski[2], J. Wosnitza[2,3], H. Kühne[2], Th. Doert[4], and M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [5]Highly Correlated Matter Research Group, University of Johannesburg, South Africa

High-quality single crystals of $NaYbSe_2$, which resembles a perfect triangular-lattice antiferromagnet without intrinsic disorder, are investigated by magnetization and specific-heat, as well as the local probe techniques nuclear magnetic resonance and electron spin resonance. The low-field measurements confirm the absence of any spin freezing or long-range magnetic order down to 50 mK, which suggests a quantum spin liquid ground (QSL) state with gapless excitations. An instability of the QSL state is observed upon applying magnetic fields. The absence of magnetic long-range order at zero fields is assigned to the effect of strong bond-frustration, arising from the complex spin-orbit entangled $4f$ ground state. Finally, we derive the highly anisotropic magnetic phase diagram, which is discussed in comparison with the existing theoretical models for spin-$\frac{1}{2}$ triangular-lattice antiferromagnets.

TT 17.15 Mon 15:00 P2/EG

Spin dynamics in the quasi-2D Honeycomb material $Na_2Co_2TeO_6$ probed by Electron Spin Resonance — •Christoph Wellm[1,2], Vladislav Kataev[1], Bernd Büchner[1,2], Weiliang Yao[3], and Yuan Li[3,4] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — [3]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — [4]Collaborative Innovation Center of Quantum Matter, Beijing 100871, China

We report an electron spin resonance (ESR) study on single crystals of $Na_2Co_2TeO_6$, a layered honeycomb material providing a possible realization of Kitaev physics [1]. Similar to previously conducted magnetization measurements [1], ESR data reveals magnetic anisotropy and interesting, complex angular and temperature dependent behavior. In addition, low-energy magnetic excitations can be examined. Our results contribute to a thorough understanding of the magnetic properties and spin correlations in the title compound.
[1] W. Yao and Y. Li, Proc. Natl. Acad. Sci., arXiv:1908.09427

TT 17.16 Mon 15:00 P2/EG

DFT calculations and spin dynamics of the quantum spin liquid candidate $Na_2BaCo(PO_4)_2$ — •Christoph Wellm[1,2], Willi Roscher[1], Vladislav Kataev[1], Oleg Janson[1], Bernd Büchner[1,2], Robert J. Cava[3], and Ruidan Zhong[3] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — [3]Department of Chemistry, Princeton University, Princeton, US-08544

The recently synthesized triangular lattice magnet $Na_2BaCo(PO_4)_2$ shows effective S = 1/2 behavior with strong quantum fluctuations persistent down to 50 mK in absence of long-range order, rendering it a promising candidate for the quantum spin liquid (QSL) ground state [1,2]. In this joined work, DFT calculations and ESR measurements provide a microscopic insight into the leading magnetic interactions and spin dynamics of the system. Using the full-potential code FPLO, the leading magnetic exchanges, the spin orbit coupling constant and the trigonal crystal field splitting are evaluated. ESR hints at a temperature-dependent magnetic moment in line with magnetization data, and shows enhanced spin-spin correlations at low-temperatures. The theoretical findings are compared to the new experimental results.

TT 17.17 Mon 15:00 P2/EG

The present understanding of anisotropic exchange interactions in linarite and other frustrated edge-sharing chain cuprates — •Stefan-Ludwig Drechsler[1], Satoshi Nishimoto[1,2], Helge Rosner[3], Alexander Tsirlin[4], Rolf Schumann[2], and Ullrich Roessler[1] — [1]IFW-Dresden, Dresden, Germany — [2]TU Dresden, Germany — [3]MPI-cPfS, Dresden, Germany — [4]Experimental Phys. IV, University of Augsburg, Germany

Based on various recent experimental data /1-3/ and novel DFT calculations we discuss the interplay of symmetric and antisymmetric exchange anisotropies in the context of the rich $B-T$ phase diagram, in particular, with the focus on the high-field region, the asymptotic saturation, and the possibility of sizable multipolar (nematic and higher order) fluctuations. Consequences of the XYZ-anisotropy and the presence of Dzyaloshinskii-Moriya (DM) interactions including DFT estimates are taken into account. In the vicinity of the magnetic ordering a phenonmenological Ginzburg-Landau analysis is applied, too.
[1] L. Heintze *et al.* Phys. Rev. B **99** , 094436 (2019)
[2] E. Cemal *et al.* Phys. Rev. Lett. **120**, 067203 (2018)
[3] S.K. Gotovko *et al.* Phys. Rev. B **100**, 174412 (2019)

TT 17.18 Mon 15:00 P2/EG

Dynamical Monte Carlo Simulations with Applications in Dipolar Spin Ice and Open Floquet Systems — •Martin Gembe, Jan Attig, and Simon Trebst — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Many-body systems subject to a periodic drive have triggered an enormous research interest, as fluctuations induced by this drive can lead to a variety of exotic phenomena such as time crystals or novel topological states. These phenomena are by definition not accessible within ordinary stationary quantum mechanics but require large-scale full dynamic quantum simulations. In this work, we present dynamical Monte Carlo simulations based on the classical single spin flip Metropolis algorithm in order to study such systems out of equilibrium in the classical limit. With this algorithm, we explore the dynamics of emerging magnetic monopoles in dipolar spin ice in an external magnetic AC field, which exhibits a critical speeding up near the monopole liquid-gas transition. Secondly, we study an open Floquet system, in which analytically it is found that rapid periodic oscillations of the couplings drive the system away from criticality.

TT 17.19 Mon 15:00 P2/EG

Thermodynamic classification of 3D Kitaev spin liquids — •Tim Eschmann[1], Petr A. Mishchenko[2], Kevin O'Brien[1], Troels A. Bojesen[2], Yasuyuki Kato[2], Maria Hermanns[3,4],

Yukitoshi Motome[2], and Simon Trebst[1] — [1]Institute for Theoretical Physics, University of Cologne — [2]Department of Applied Physics, University of Tokyo — [3]Department of Physics, Stockholm University — [4]Nordita, KTH Royal Institute of Technology and Stockholm University

Kitaev models are prototypical spin models in which the spins fractionalize, and the emergent spin liquid ground state is composed of Majorana fermions coupled to a $\mathbb{Z}_2$ gauge field. At low temperatures, the $\mathbb{Z}_2$ gauge field is generally assumed to exhibit an ordered ground state, characterized by the presence or absence of $\mathbb{Z}_2$ fluxes through the elementary lattice plaquettes. In 3D, this ground state is separated from the paramagnetic phase through a thermal phase transition, at which the (gapped) vison excitations proliferate. Here, we further the understanding of this "gauge physics" by a comprehensive classification of the thermodynamics of a family of elementary 3D Kitaev models. Based on large-scale, sign-free quantum Monte Carlo simulations, we verified that the ground state flux sectors of these systems are entirely determined by their elementary plaquette length - extending the applicability of Lieb's theorem to a number of lattice geometries beyond its original scope. As manifestation of the close interplay of vison-physics and gauge-ordering transition, we report a (linear) correlation between the critical temperature and the size of the vison gap.

TT 18: Skyrmions (joint session TT/MA)

Time: Monday 16:15–18:15 Location: HSZ 304

TT 18.1 Mon 16:15 HSZ 304

Quantum skyrmions in a triangular frustrated ferromagnet

— •Vivek Lohani[1], Ciarán Hickey[1], Jan Masell[1,2], and Achim Rosch[1,3] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]RIKEN Center for Emergent Matter Science, Japan — [3]Department of Physics, Harvard University, USA

Classically, skyrmions are described as tiny whirls of magnetization possessing a topological winding number. Their dynamics is similar to that of a charge, proportional to the winding number, that is coupled to an effective magnetic field. However, in the limit of small skyrmion size, quantum effects become important. Frustration stabilized skyrmion models − which exhibit degeneracy between classical skyrmions and antiskyrmions, and an additional zero mode, the *helicity* − provide a natural playground to study these quantum effects.

This begs the question − what is a quantum skyrmion? We argue that, in the quantum sector, a skyrmion is defined through the stable bound states of the Hamiltonian. By performing a numerical study, via exact diagonalization, we first demonstrate the existence of quantum skyrmions and identify the associated quantum selection rules. Furthermore, we explore their dynamics through a low energy, phenomenological Hamiltonian spanned by the translational and the helicity modes, wherein the coupling between translations and helicity leads to a rich dynamics. Most interestingly, we incorporate quantum tunneling, and how it breaks the degeneracy in the classical model and allows effective skyrmion charge to flip, thereby leading to a non-trivial bandstructure that is quite sensitive to the spin quantum number.

TT 18.2 Mon 16:30 HSZ 304

Quantum skyrmion state

— •Evgeny A. Stepanov[1], Mikhail I. Katsnelson[2], and Vladimir V. Mazurenko[3] — [1]Institute of Theoretical Physics, University of Hamburg, Germany — [2]Radboud University, Institute for Molecules and Materials, Nijmegen, Netherlands — [3]Theoretical Physics and Applied Mathematics Department, Ural Federal University, Ekaterinburg, Russia

Skyrmions in physics of magnetism appear as classical spin structures that are formed in the systems as the result of a competition between different magnetic interactions. Such nontrivial magnetic textures can be observed in materials with the use of a spin-polarized scanning tunneling and Lorenz microscopy, or in X-ray and neutron scattering experiments. Theoretically, a skyrmion state can be described by solving a classical spin lattice problem or a corresponding continuous micromagnetic model. Here, we find that the classical skyrmion can be considered as a particular projection of a more general quantum skyrmion state. To perform a complete characterization of this novel state, we introduce a quantum analog for a classical skyrmion number that can be calculated as a scalar triple product of spin operators. We show that this quantity allows for a clear distinction of the quantum skyrmion state, which is characterized by a nontrivial correlation of spins in all three space directions, from other more simple spin orderings. On a basis of an exact numerical solution for supercells with up to 25 spins we demonstrate that the quantum skyrmion state can be obtained for a much broader range of magnetic fields than the corresponding classical skyrmion solution of the problem.

TT 18.3 Mon 16:45 HSZ 304

Vortex-Phase in Non-Centrosymetric Antiferromagnets

— •Benjamin Wolba[1], Sebastian Mühlbauer[2], and Markus Garst[1] — [1]Institut für Theoretische Festkörperphysik (TFP), Karlsruhe Institut für Technologie (KIT), 76131 Karlsruhe — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85748 Garching, Germany

In this work we consider two-dimensional, non-centrosymmetric antiferromagnets, for which the competition between exchange and Dyzaloshinskii-Moriya interaction leads to the formation of spatially modulated phases of the staggered order parameter. Within the framework of Ginzburg-Landau theory we show that by applying a magnetic field parallel to the c-axis, which thus induces easy-plane anisotropy, one can stabilize a square lattice of vortices close to Neel temperature. Upon decreasing temperature, this vortex phase undergoes spontaneous symmetry breaking into a rectangular phase, which was not anticipated before. We discuss the relevance of our results for the chiral antiferromagnet $Ba_2CuGe_2O_7$.

TT 18.4 Mon 17:00 HSZ 304

Weak Crystallization of Fluctuating Skyrmion Textures in MnSi

— Jonas Kindervater[1], Ioannis Stasinopoulos[1], Andreas Bauer[1], •Franz Xaver Haslbeck[1], Felix Rucker[1], Alfonso Chacon[1], Sebastian Mühlbauer[1], Christian Franz[1], Markus Garst[2,3], Dirk Grundler[1,4], and Christian Pfleiderer[1] — [1]TU München, Garching, Germany — [2]TU Dresden, Dresden, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany — [4]Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland

We report an experimental study of the emergence of nontrivial topological winding and long-range order across the paramagnetic to skyrmion lattice (SkL) transition in the transition metal helimagnet MnSi. Combining measurements of the susceptibility with small-angle neutron scattering, neutron-resonance spin-echo spectroscopy, and all-electrical microwave spectroscopy, we find evidence of skyrmion textures in the paramagnetic state exceeding 10^3 Å with lifetimes above several 10^{-9} s. Our experimental findings establish that the paramagnetic to SkL transition in MnSi is well described by the Landau soft-mode mechanism of weak crystallization, originally proposed in the context of the liquid-to-crystal transition. As a key aspect of this theoretical model, the modulation vectors of periodic small-amplitude components of the magnetization form triangles that add to zero. In excellent agreement with our experimental findings, these triangles of the modulation vectors entail the presence of the nontrivial topological winding of skyrmions already in the paramagnetic state of MnSi when approaching the SkL transition.

TT 18.5 Mon 17:15 HSZ 304

Tuning of the critical temperature of a superconducting thin film in proximity of a chiral magnet

— •Julius Grefe, Marvin Sach, Bastian Rubrecht, Jannis Willwater, Stefan Süllow, and Dirk Menzel — Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany

Theory has suggested a possibility to control the critical temperature T_C of a superconductor via the proximity effect with a magnetic system exhibiting a non-collinear spin structure [1]. MnSi being an archetype of the B20 structure shows helimagnetic behavior below $T_N = 29.5$ K and $B_{C1} = 100$ mT. The related pseudobinary compound $Fe_{1-x}Co_xSi$ with a tunable Néel-temperature from 0 K to 55 K even expands the accessible temperature range.

Superconducting Nb thin films have been deposited by molecular beam epitaxy on substrates prepared from Triarc-Czochralski grown single crystals. We investigate a shift of T_C in the Nb film upon reorientation of the spin helices in the substrate.

This proximity effect is suggested for usage in superconducting spin valves consisting only of a single magnetic layer and a thin superconducting film promising more simple and compact devices.

[1] N. G. Pugach et al., Appl. Phys. Lett. **111**, 162601 (2017).

TT 18.6 Mon 17:30 HSZ 304

Distribution of energy barriers associated with magnetic skyrmion decay in $Fe_{0.5}Co_{0.5}Si$ — •Alfonso Chacon[1], Marco Halder[1], Jonas Kindervater[1], Andreas Bauer[1], Sebastian Mühlbauer[2], Achim Rosch[3], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany

We report comprehensive measurements of the magnetization and small-angle neutron scattering of the time-dependence of the decay of metastable skyrmion lattice order in $Fe_{0.5}Co_{0.5}Si$ after field cooling. Comparison of the SANS intensity pattern with the magnetization allows to identify contributions in the magnetization that are due to skyrmions only. Combining first-order reversal behaviour with the time dependence under carefully selected conditions, justifies the application of time versus temperature superposition and infer the distribution of energy barriers associated with the decay of magnetic skyrmions. The resulting distribution of energy barriers allows to discriminate between contributions due to the non-trivial topology and defect- and disorder-related pinning.

TT 18.7 Mon 17:45 HSZ 304

Helix reorientation at the transition between helical and conical phases of the chiral magnet Cu_2OSeO_3 — •Laura Köhler[1,4], Peter Milde[1], Erik Neuber[1], Philipp Ritzinger[1], Andreas Bauer[2], Christian Pfleiderer[2], Helmuth Berger[3], and Markus Garst[4] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]Technische Universität München, 85748 Garching, Germany — [3]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [4]Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

In chiral magnets, the Dzyaloshinskii-Moriya interaction stabilizes a magnetic helix which is a one-dimensional periodic magnetic texture. The exact orientation of this helical texture is determined by the competition between crystalline anisotropies and the applied magnetic field. We study the reorientation process of the helix as a function of field in the insulating chiral magnet Cu_2OSeO_3 using magnetic force microscopy. As a function of field, we determine the wavelength projected onto the sample surface as well as the electric polarization induced by the magnetoelectric coupling. Our experimental observations are well described by an effective Landau theory for the helix orientation as previously applied to MnSi [1].

[1] A. Bauer, A. Chacon, M. Wagner, M. Halder, R. Georgii, A. Rosch, C. Pfleiderer, M. Garst, PR B 95, 024429 (2017).

TT 18.8 Mon 18:00 HSZ 304

Skyrmion Lattice Magnet Gd_2PdSi_3 Studied by High-Resolution Dilatometry — •Sven Spachmann[1], Matthias Frontzek[2], Chongde Cao[3], Wolfgang Löser[4], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Oak Ridge National Laboratory, Oak Ridge, USA — [3]Northwestern Polytechnical University, Xi'an, China — [4]Leibniz Institute for Solid State and Materials Research (IFW), Dresden, Germany

A Bloch-type skyrmion state emerging in low magnetic fields has recently been reported for the frustrated centrosymmetric triangular-lattice magnet Gd_2PdSi_3 [1]. Here, we present high-resolution thermal expansion and magnetostriction measurements on single crystals of this material in order to study the phase diagram and in particular the transitions to the skyrmion phase. In zero magnetic field, a single peak in the thermal expansion coefficient indicates the onset of long-range antiferromagnetic order at $T_N = 19.7$ K, which exhibits uniaxial pressure dependencies of opposite sign along the *a*- and *c*-axis, respectively. Up to $B = 4$ T, four known phases are confirmed, including the skyrmion phase for $B||c$ which appears in a discontinuous transition. In addition, a previously non-reported phase is observed. The anomalies in thermal expansion and magnetostriction at the different phase boundaries as well as the respective uniaxial pressure dependencies imply significant changes in the spin-lattice coupling for different fields.

[1] T. Kurumaji et al., Science 10.1126/science.aau0968 (2019)

TT 19: Low Dimensional Systems: Other Topics

Time: Monday 17:00–18:30 Location: HSZ 103

TT 19.1 Mon 17:00 HSZ 103

Luttinger liquids with inhomogeneous interactions — Sebastian Huber[1] and •Marcus Kollar[2] — [1]Theoretical Solid State Physics, Ludwig- Maximilians-University, Munich, Germany — [2]Theoretical Physics III, University of Augsburg, Germany

We study a generalization of the two-flavor spinless Tomonaga-Luttinger model which includes inhomogeneous local interactions and scattering potentials. For a wide range of parameters we obtain the spectrum and Green function exactly using Kronig identities with momentum transfer [1]. While Green functions have a power-law form as in homogeneous Luttinger liquids, a sufficiently strong position dependence of the interaction breaks their translational invariance. Furthermore, the Luttinger-liquid interrelations between excitation velocities and Green function exponents are modified in such 'Luttinger droplets' [2].

[1] S. Huber, M. Kollar, Verhandl. DPG (VI) 52, 2/TT24.1 (2017)
[2] S. Huber, M. Kollar, arXiv:1911.03158

TT 19.2 Mon 17:15 HSZ 103

Drude weight increase by orbital and repulsive interactions in fermionic ladders — Andreas Haller[1], •Matteo Rizzi[2,3], and Michele Filippone[4] — [1]Institute of Physics, Johannes Gutenberg University, D-55099 Mainz, Germany — [2]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, D-52425 Jülich, Germany — [3]Institute for Theoretical Physics, University of Cologne, D-50937 Köln, Germany — [4]Department of Quantum Matter Physics, Ecole de Physique, University of Geneva, CH-1211 Geneva 4, Switzerland

In strictly one-dimensional systems, repulsive interactions tend to reduce particle mobility on a lattice. Therefore, the Drude weight, controlling the divergence at zero-frequency of optical conductivities in perfect conductors, is lower than in non-interacting cases. We show that this is not the case when extending to quasi one-dimensional ladder systems. Relying on bosonization, perturbative and matrix product states (MPS) calculations, we show that nearest-neighbor interactions and magnetic fluxes provide a bias between back- and forward-scattering processes, leading to linear corrections to the Drude weight in the interaction strength. As a consequence, Drude weights counter-intuitively increase (decrease) with repulsive (attractive) interactions. Our findings are relevant for the efficient tuning of Drude weights in the framework of ultracold atoms trapped in optical lattices and equally affect topological edge states in condensed matter systems.

[1] arXiv:1911.11160

TT 19.3 Mon 17:30 HSZ 103

Signature of isotropic electric dipole dynamics in $BaFe_2X_3$ (X = S/Se) — •yuk tai chan[1], seulki roh[1], soohyeon shin[2,3], tuson park[2,3], martin dressel[1], and ece uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Physics, Sungkyunkwan University, Suwon, Republic of Korea — [3]Center for Quantum Materials and Superconductivity (CQMS), Sungkyunkwan University, Suwon, Republic of Korea

$BaFe_2S_3$ (BFS) and $BaFe_2Se_3$ (BFSe) hold a rare and interesting quasi-1D Fe-ladder structure. Although they are isostructual, magnetic ground states of these are significantly different: BFSe possesses a block-type antiferromagnetic (AFM) order along the leg with $T_N \sim 200$ K, whereas BFS forms a stripe-type AFM order along the leg with $T_N \sim 100$ K. The block-type AFM in BFSe has the potential to generate ferroelectric polarization and hence raise hope for a realization of robust multiferroic order. In this study, polarization-dependent dielectric spectroscopy has been performed on single crystals BFS and BFSe. Counterintuitive to the highly anisotropic quasi-1D structure, nearly isotropic relaxor ferroelectric behaviors are observed for both compounds. The range of temperature for the relaxation in BFSe is $\sim$ 100 K above that in BFS, which follows their AFM order, T_N, and therefore suggests a shrouded relationship between the magnetism and electric dipole dynamics.

TT 19.4 Mon 17:45 HSZ 103

1D coordination polymers on metal surfaces with distinct structures defined by the choice of the transition metal — •Vijai Meena Santhini, Christian Wackerlin, Ales Cahlik, Oleksander Stetsovych, Pingo Mutombo, and Pavel Jelinek — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

2,5-diamino-1,4-benzoquinonediimines (QDIs)belong to one of the most important classes of π-conjugated molecules and are particularly interesting because of the unusual distribution of their overall 12-π electrons system which can be described as two nearly-independent 6-π electrons subunits chemically connected through two C-C single bonds.

In this context, we explore here the reaction between transition metal atoms (Cr, Fe, Co, Ni and Cu) and QDI directly at the solvent-free solid-vacuum interface. The metals are introduced as neutral metal atoms from an electron-beam evaporator (all except Cu) or they are provided by the substrate (Cu). QDI is introduced by sublimation, and is let to react on Au(111) and Cu(111) surfaces with the metal atoms. . The {Cr, Fe, Co, Ni}-based wires are built from a four-fold rectangular-planar coordination motif while with Cu the wires are based on two-fold linear coordination motifs. The reaction products are characterized by combined scanning tunneling microscopy (STM) non-contact atomic force microscopy (nc-AFM) and N K near edge X-ray absorption fine structure (NEXAFS) spectroscopy.

TT 19.5 Mon 18:00 HSZ 103

RKKY-coupled Co adatom spins on WS_2 monolayers — •Jan Honolka[1], Charlotte Sanders[3], Sergey Mankovsky[4], Brian Kiraly[2], Sanjoy Mahatha[3], Svetlana Polesya[4], Martin Vondracek[1], Ales Cahlik[1], Sarnjeet Dhesi[6], Jan Minar[5], Hubert Ebert[4], Philip Hofmann[3], and Alexander Khajetoorians[2] — [1]Inst. of Physics ASCR, Na Slovance 4, CZ-8000 Praha — [2]Radboud Univ. Nijmegen, Inst. Molecules & Mat., NL-6525 AJ Nijmegen — [3]Aarhus Univ., Dept. Physics and Astronomy, DK-8000 Aarhus — [4]Ludwig Maximilians Univ. Muenchen, Dept. Chem., D-81377 Munich — [5]Univ. West Bohemia, New Technol. Research Center, Univ. 2732, CZ-30614 Pilsen — [6]Diamond Light Source, UK-OX11 0DE Didcot

Antiferromagnetic order can potentially change fundamental symmetries in 2D materials. Here we report on magnetic and structural properties of cold-deposited Co atoms on single layer WS_2/Au(111), which are characterised by X-ray magnetic circular dichroism (XMCD) measurements and scanning tunneling microscopy (STM) and spectroscopy (STS), respectively. We observe a highly compensated magnetic state at intermediate Co coverages of 0.2 - 0.3 monolayers. Density functional theory shows that indirect RKKY coupling constants between Co adatoms are of the order of few meV and negative at Co-Co distances 0.5 - 1 nm, which creates a non-collinear magnetic structure. In the limit of 1 monolayer ferromagnetism sets in. Strain effects due to the substrate are discussed.

TT 19.6 Mon 18:15 HSZ 103

Preferential out-of-plane conduction and quasi-one-dimensional electronic states in layered van der Waals material 1T-TaS_2 — Edoardo Martino[1,2], Andrea Pisoni[1], Luka Ćirić[1], Alla Arakcheeva[1], Helmuth Berger[1], Ana Akrap[2], Carsten Putzke[1], Philip Moll[1], Ivo Batistić[3], Eduard Tutiš[4], László Forró[1], and •Konstantin Semeniuk[1] — [1]EPFL, Lausanne, Switzerland — [2]University of Fribourg, Fribourg, Switzerland — [3]University of Zagreb, Zagreb, Croatia — [4]Institute of Physics, Zagreb, Croatia

The prevailing strategy for functionalising layered crystals is manipulating coupling between atomic sheets to create novel exploitable electronic states. The responsible interactions can be sensitively gauged by the interlayer charge transport, which has remained largely unexplored. We conducted an unambiguous study of resistivity anisotropy of 1T-TaS_2 — a system known for its plethora of diverse phases and a metal-insulator transition of highly debated origin. We present an unprecedented case of drastically better electronic coherence in the out-of-plane direction than within the planes, resulting in the resistivity anisotropy of the order of 1. In the unique nano-composite phase, the complex aperiodic lattice structure suppresses the in-plane conduction. Simultaneously, the material exhibits a conventional metallicity along the c-axis, predicted to originate from the charge-density-wave-induced formation of quasi-one-dimensional orbital chains. The proposed behaviour favours the band-insulator nature of the low-temperature state of 1T-TaS_2, contrary to the long-standing Mott localisation picture.

TT 20: Focus Session: The Nickel Age of Superconductivity: Cuprates Reloaded or Something New?

Time: Tuesday 9:30–12:45 Location: HSZ 03

Invited Talk TT 20.1 Tue 9:30 HSZ 03

Superconductivity in infinite layer nickelates — •Harold Hwang — Stanford University and SLAC National Accelerator Laboratory

Ever since their discovery, superconductivity in cuprates has motivated the search for materials with analogous electronic or atomic structure. Here we present how soft chemistry approaches can be used to synthesize superconducting infinite layer nickelates from their perovskite precursor phase [1], using topotactic reactions. We will discuss our preliminary understanding of aspects that are similar and different from the cuprates, as well as initial exploration of the doping dependence of the phase diagram.

[1] D. F. Li, K. Lee, B. Y. Wang, M. Osada, S. Crossley, H. R. Lee, Y. Cui, Y. Hikita, and H. Y. Hwang, Nature 572, 624 (2019).

Invited Talk TT 20.2 Tue 10:00 HSZ 03

Materials design of dynamically stable d^9 layered nickelates — •Ryotaro Arita — Department of Applied Physics, University of Tokyo, Tokyo, Japan — RIKEN Center for Emergent Matter Science, Saitama, Japan

The recent discovery of superconductivity in the doped nickelate $Nd_{0.8}Sr_{0.2}NiO_2$ has stimulated renewed interest in unconventional superconductivity in layered correlated materials. Recently, we perform a systematic computational materials design of layered nickelates that are dynamically stable and whose electronic structure better mimics the electronic structure of high-T_c cuprates. While the Ni 3d orbitals are self-doped from the d^9 configuration in $NdNiO_2$ and the Nd-layer states form Fermi pockets, we find more than 10 promising compounds for which the self-doping is almost or even completely suppressed. We derive an effective single-band model for those materials and find that the system is in a strongly-correlated regime. We also investigate the possibility of palladate analogues of high-T_c cuprates. Once synthesized, these nickelates and palladates will provide a firm ground for studying superconductivity in the Mott-Hubbard regime of the Zaanen-Sawatzky-Allen classification, which will also help the understanding of the superconductivity in high-T_c cuprates realized in the charge-transfer regime.

Invited Talk TT 20.3 Tue 10:30 HSZ 03

Superconductivity in Nickelates: Similarities and Differences from Cuprates — •Michael Norman — Materials Science Division, Argonne National Laboratory, USA

The recent discovery of superconductivity in Sr-doped NdNiO2 has refocused attention on the relation of nickelates to cuprates. First, I review the experimental situation, including earlier work on trilayer nickelates, as well as the new work on infinite-layer nickelates. Next, I comment on various proposed models, including charge-transfer, Mott, and Kondo. Then, I relate these models to the electronic structure of nickelates, contrasting this with cuprates. Finally, I comment on relevant parameters in regards to the observation of superconductivity.

15 min. break.

Invited Talk TT 20.4 Tue 11:15 HSZ 03

Comparing the electronic structure and magnetism of hole doped Nickelate and Cuprate superconductorslate and Cuprate superconductors — •George Sawatzky, Mi Liang, Mona Berciu, Kateryna Foyevtsova, and Ilya Elfimov — Stuart Blusson Quantum Matter Institute Institute University of British Columbia Vancouver BC V6T1Z4,

Using the same theoretical methods used for the cuprates we investigate the electronic and magnetic structure and excitations of the new infinite layer $NdNiO_2$. We show that the nickelates are expected to be Mott Hubbard rather than charge transfer gap insulators provided that there are no other bands crossing the Fermi energy. In this case the much larger charge transfer energy will result in a strongly reduced superexchange interaction and also reduces the crystal field splittings of the d levels. This results in a near degeneracy of the triplet and singlet states for the hole doped nickelate . All these effects make the Nick=elates very different from the cuprates.

Invited Talk TT 20.5 Tue 11:45 HSZ 03

Doping infinite-layer nickelates: A superlattice approach — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recently, the observation of superconductivity in strontium-doped $NdNiO_2$ thin films has attracted a lot of attention [1]. We have been working on a different approach to dope the infinite-layer nickelates, where we considered layer-selective, topotactically reduced rare-earth nickelate layer stacks in a superlattice structure with the aim to control the doping level by the stack thickness. In my talk I will present our results from x-ray spectroscopy together with *ab-initio* calculations of the layer-resolved, local nickel electronic configuration in these artificial superlattices and discuss similarities and differences to the electronic structure of copper in high-temperature superconductors.

[1] D. Li, K. Lee, B. Y. Wang, M. Osada, S. Crossley, H. R. Lee, Y. Cui, Y. Hikita, and H. Y. Hwang, Nature 572 (2019) 624

TT 20.6 Tue 12:15 HSZ 03

Topotactic hydrogen in nickelate superconductors and akin infinite-layer oxides $AB\mathrm{O}_2$ — •Karsten Held[1], Liang Si[1,2], Wen Xiao[2], Josef Kaufmann[1], Yi Lu[3], Jan M. Tomczak[1], and Zhicheng Zhong[2] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]Chinese Academy of Science NIMTE, Ningbo, China — [3]Institute for Theoretical Physics, Heidelberg University, Germany

The seminal work by Li et al. [1] opens the door wide to the nickelate age of superconductivity. But it appears to be most difficult to reproduce. Since the chemical reduction of ABO_3 (A: rare earth; B transition metal) with CaH_2 may result in both, ABO_2 and ABO_2H, we calculate [2] the topotactic H binding energy by density functional theory (DFT). We find intercalating H to be energetically favorable for $LaNiO_2$ and $NdNiO_2$ but not for Sr-doped $NdNiO_2$.

This topotactical hydrogen turns the electronic structure upside down. Our DFT+dynamical mean field theory calculations show [2] that $3d^9$ $LaNiO_2$ is similar to (doped) cuprates, whereas $3d^8$ $LaNiO_2H$ is a two-orbital Mott insulator, similar to $LaNiO_3|LaAlO_3$ heterostructures prior to engineering their bandstructure to a cuprate-like one [3]. Topotactic H might hence explain why some nickelates are superconducting and others are not.

[1] D. Li et al., Nature 572, 624 (2019).
[2] L. Si, W. Xiao, J. Kaufmann, J.M. Tomczak, Y. Lu, Z. Zhong, K. Held, arXiv:1911.06917.
[3] P. Hansmann, X. Yang, A. Toschi, G. Khaliullin, O. K. Andersen, and K. Held, Phys. Rev. Lett. 103, 016401 (2009).

TT 20.7 Tue 12:30 HSZ 03

Role of interface polarity in the electronic reconstruction of infinite-layer vs. perovskite nickelate films on $\mathbf{SrTiO_3(001)}$ — •Benjamin Geisler and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg

Motivated by the recent observation of superconductivity in the infinite-layer nickelate $NdNiO_2$ on $SrTiO_3(001)$ by Li *et al.* [1], we explore the effect of interface polarity on the electronic properties of $NdNiO_n/SrTiO_3(001)$ and $LaNiO_n/SrTiO_3(001)$ thin films ($n = 2, 3$) by performing first-principles calculations including a Coulomb repulsion term. For infinite-layer nickelate films ($n = 2$), electronic reconstruction drives the emergence of a two-dimensional electron gas (2DEG) at the interface due to a strong occupation of the Ti $3d$ states. This effect is more pronounced than in the paradigmatic $LaAlO_3/SrTiO_3(001)$ system and accompanied by a substantial reconstruction of the Fermi surface. We contrast our findings with results for the perovskite compounds ($n = 3$). Moreover, we analyze the topotactic reaction from a perovskite to an infinite-layer heterostructure and show why the reduction is confined to the nickelate film, whereas the $SrTiO_3$ substrate remains intact.

Funding by the DFG within TRR 80 (G3) is acknowledged.

[1] D. Li *et al.*, Nature **572**, 624 (2019)

TT 21: Topological Semimetals 1

Time: Tuesday 9:30–13:00 Location: HSZ 103

TT 21.1 Tue 9:30 HSZ 103

Optical conductivity of generalized Weyl semimetals — •Lucky Z. Maulana[1], Ece Uykur[1], Seulki Roh[1], Yohei Saito[1], Motoharu Imai[2], Kaustuv Manna[3], Claudia Felser[3], Martin Dressel[1], and Artem V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0047, Japan — [3]MPI für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Generalizations of Weyl semimetals are realized in materials, where more than two non-degenerate electronic bands touch at a given point of Brillouin zone. We have optically studied two groups of such materials: the multifold semimetals RhSi, CoSi, and PdGa, where the higher-spin generalizations of Weyl points have been confirmed, and $SrSi_2$ – a material, where quadratic double-Weyl fermions are supposed to be realized. In the presentation, we report our results on broadband complex optical conductivity for all these materials, comparer their optical spectra, and conclude on the peculiarities of their low-energy band structure based on our experiments.

TT 21.2 Tue 9:45 HSZ 103

The chiral anomaly in Weyl semimetals as seen by optics — Ece Uykur[1], Lucky Z. Maulana[1], Shekhar Chandra[2], Claudia Felser[2], Martin Dressel[1], and •Artem V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]MPI für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The density imbalance between the electronic excitations with different chiralities in simultaneously applied parallel electric and magnetic fields, the chiral anomaly, is perhaps the most fascinating phenomenon occurring in Weyl semimetals. The existing experimental results reported on the chiral anomaly are mostly based on electrical-transport measurements using direct current, for example, on observations of the negative longitudinal magnetoresistance. However, it has been argued that dc transport may suffer from other effects, such as current jetting. Reports on detecting the chiral anomaly by other experimental methods are therefore of paramount importance. Here, we report on optical observations of the chiral anomaly in the Weyl semimetals TaAs and NbAs and also in GdPtPi, a triple-point semimetal, which becomes a Weyl semimetal upon application of a magnetic field.

TT 21.3 Tue 10:00 HSZ 103

Optical fingerprinting of magnetic reorientation in Weyl semimetals — •Ananya Biswas[1], Hechang Lei[2], Martin Dressel[1], and Ece Uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials & Micro-nano Devices, Renmin University of China, Beijing, China

Three dimensional magnetic Weyl semimetals are relatively new members of this topological realm, where the electron correlations are intertwined with flat bands and heavy fermions. They have been investigated extensively via transport and magneto-transport studies, while the optical investigations on these systems are scarce. Here, we focus on the optical characterization of the Fe_3Sn_2 single crystals that has shown to be one of the magnetic Weyl semimetal candidates. This material is a soft ferromagnet with distinguished flat bands and Weyl nodes, where the T_c=640 K and a spin reorientation takes place at $\sim$ 150 K. Our optical results demonstrate the typical signatures of the electron correlations together with the optical anomalies at the spin reorientation temperature indicating the close relation of the electronic and underlying magnetic structure in these new class of materials.

TT 21.4 Tue 10:15 HSZ 103

Resonance Raman scattering and magnetic-field tuning of the electronic band structure in the topological semimetal PdGa — Vladimir Gnezdilov[1,2,3], Dirk Wulferding[1,2], •Peter Lemmens[1,2], Florian Büscher[1], Yurii Pashkevich[4], Tanya Shevtsova[4], Claudia Felser[5], and Kaustuv Manna[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]ILTPE Kharkov, Ukraine — [4]Galkin DonFTI, Kyiv, Ukraine — [5]MPI Dresden, Germany

The novel chiral topological semimetal PdGa is the first known compound where electronic bands acquire a maximal Chern number of $C = \pm 4$ [1]. Using Raman spectroscopy, we uncover a strong and sharp electronic resonance around $E = 2.35$ eV that allow us to follow changes of electronic Raman scattering occurring in moderate magnetic fields as well as phonon anomalies. Both observations point to a possible modification of the electronic band structure in PdGa in magnetic fields.
Work supported by DFG LE967/16-1 and QUANOMET NL-4.
[1] Schröter et al., arXiv:1907.08723 (2019)

TT 21.5 Tue 10:30 HSZ 103

Semi-Dirac state revealed in black phosphorus via high-pressure studies — •D. Rodriguez[1], Q. Yan[2], M. Dressel[1], and E. Uykur[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569, Stuttgart, Germany — [2]Department of Chemistry, Tsinghua University, Beijing 100084, China

Semi-Dirac materials are a class of Dirac/Weyl semimetals that display a two-feature energy dispersion: linear (relativistic) along one momentum direction and quadratic (non-relativistic) in the other direction. The realization of this unique state in real materials is still pending. One promising system is the black phosphorus (BP). It has been theoretically predicted that hydrostatic pressure can close the band gap, driving the system through several electronic transitions from a gapped insulator with inverted bands to a Dirac semimetal state. An intermediate phase exists though, the semi-Dirac state characterized by a gapless anisotropic spectrum dispersing linearly along its armchair direction and parabolically along the zigzag. Here, we report high-pressure infrared measurements of BP tuned successfully through the insulator-to-metal transition. Our optical conductivity results present a highly anisotropic behavior for different light polarization in the low energy range consistent with the theoretical predictions of a semi-Dirac state. Moreover, results indicate that Dirac state in BP has a 3D character rather than 2D.

TT 21.6 Tue 10:45 HSZ 103

Surface Berry curvature dipole of Weyl semimetals — •Dennis Wawrzik[1], Jhih-Shih You[1], Inti Sodemann[2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Department of Physics, TU Dresden, Germany

In the absence of magnetic field, the Hall effect in the linear response regime vanishes due to time-reversal symmetry. However, a transverse charge current can still occur in second-order response to an external electric field, as a result of the Berry curvature dipole (BCD) in momentum space. While there has been much effort to understand nonlinear transport due to a BCD in bulk, here we show that for Weyl semimetals the surface Fermi arcs of a proper chosen surface give rise to a giant BCD. In particular, the surface BCD scales with the sample size. In our study, we employ a general k-dot-p model which covers a wide class of type-I Weyl materials.

TT 21.7 Tue 11:00 HSZ 103

$e/2$ and $e/4$ quantization of the boundary charge in one-dimensional Weyl semimetals — •Mikhail Pletyukhov[1], Dante Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and Herbert Schoeller[1] — [1]RWTH Aachen University, Germany — [2]University of Basel, Switzerland

Universal properties of the boundary charge Q_B for one-dimensional and one-channel insulators have been studied in the recent papers [1]. At half-filling, the gap can close under certain conditions, and in this talk we discuss the associated Weyl semimetal physics extending our previous study of the boundary charge. We find quantization of Q_B in two generic classes of charge $e/2$ or $e/4$ in the presence of nonlocal inversion/chiral symmetries. We make a generalization to the Weyl case of both the Diophantine equation [2] , which includes numbers of edge modes connecting adjacent Weyl points, and the universal phase-dependence of the boundary charge [1]. Its fluctuations are shown to be very small in the quantized regions and featuring a remarkable power-law behaviour close to the phase points where the boundary charge makes a jump.
[1] M. Pletyukhov et al, arXiv: 1911.06886; 1911.06890
[2] I. Dana et al, J. Phys. C 18, L679 (1985); M. Kohmoto, Phys. Rev. B 39, 11943 (1989); Y. Hatsugai, Phys. Rev. B 48, 11851 (1993)

15 min. break.

TT 21.8 Tue 11:30 HSZ 103

Non-Abelian anomalies in multi-Weyl semimetals — •Renato Miguel Alves Dantas, Francisco Peña-Benitez, Bitan Roy, and Piotr Surówka — Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

We construct the effective field theory for time-reversal symmetry breaking multi-Weyl semimetals (mWSMs), composed of a single pair of Weyl nodes of (anti-)monopole charge n, with $n = 1, 2, 3$ in crystalline environment. From both the continuum and lattice models, we show that a mWSM with $n > 1$ can be constructed by placing n flavors of linearly dispersing simple Weyl fermions (with $n = 1$) in a bath of an $SU(2)$ non-Abelian static background gauge field. Such an $SU(2)$ field preserves certain crystalline symmetry (four-fold rotational or C_4 in our construction), but breaks the Lorentz symmetry, resulting in nonlinear band spectra (namely, $E \sim (p_x^2 + p_y^2)^{n/2}$, but $E \sim |p_z|$, for example, where momenta $\mathbf{p}$ is measured from the Weyl nodes). Consequently, the effective field theory displays $U(1) \times SU(2)$ non-Abelian anomaly, yielding anomalous Hall effect, its non-Abelian generalization, and various chiral conductivities. The anomalous violation of conservation laws is determined by the monopole charge n and a specific algebraic property of the $SU(2)$ Lie group, which we further substantiate by numerically computing the regular and "isospin" densities from the lattice models of mWSMs. These predictions are also supported from a strongly coupled (holographic) description of mWSMs.

TT 21.9 Tue 11:45 HSZ 103

Spin and valley wave collective modes in metals with population imbalance — •Alexander Zyuzin — Aalto University, Finland

The effect of electron-electron exchange interaction in metals with non-equilibrium spin orientation will be first reviewed. It will be shown, that as a result of the interaction, there exists a spin wave mode, describing the spin precession in the absence of applied magnetic field. The dispersion relation of the mode is gapless, proportional to the square of the wave vector at small frequencies, and inversely proportional to the electron-electron exchange interaction energy. The valley wave analog will be then discussed for the case of metals with valley population imbalance. Doped graphene and three-dimensional Weyl-Dirac semimetals will be considered as particular material candidates. The spin and valley waves serve as the energy gain sources for the external field, that generates the spin or inter-valley transitions.

TT 21.10 Tue 12:00 HSZ 103

Temperature effects on the conductivity of strongly-correlated Dirac semimetals — •Niklas Wagner[1], Sergio Ciuchi[2], Björn Trauzettel[1], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physical and Chemical Sciences, University of L'Aquila, Italy

Dirac semimetals can be seen as the three-dimensional generalization of graphene, hosting linearly dispersing bands in the vicinity of a degeneracy point of the bandstructure. We investigate the effects of strong electronic correlations on various Dirac semimetal models by applying Dynamical Mean Field Theory (DMFT), focusing in particular on the finite-temperature crossover regions. By applying Iterated Perturbation Theory (IPT) we have the resolution on the real axis to calculate accurate transport properties. We calculate the conductivity as a function of the temperature and interaction strength and discuss the physical differences with respect to conventional metals.

TT 21.11 Tue 12:15 HSZ 103

Correlated phases from a three-dimensional pseudo-Landau flat band in a nodal-line semimetal — •Alexander Lau[1], Dmitry Pikulin[2], and Timo Hyart[1] — [1]International Research Centre MagTop, Warsaw, Poland — [2]Microsoft Station Q, Santa Barbara, USA

Nodal-line semimetals are a class of three-dimensional topological semimetals featuring two-fold degenerate band-crossing points that form closed loops in the Brillouin zone of the material. Based on an effective low-energy theory, we show how strain can be used to induce a set of three-dimensional pseudo-Landau levels in nodal-line semimetals. In particular, the zeroth Landau level realizes a three-dimensional flat band which gives rise to strong electron-electron interactions. We study magnetic and superconducting phases arising in this setup and discuss differences to similar phases in two dimensions.

TT 21.12 Tue 12:30 HSZ 103

Photoinduced Anomalous Hall Current in Nodal-Line Semimetals — •Andreas Leonhardt and Andreas P. Schnyder — Max Planck Institute for Solid State Research

Symmetry-protected nodal lines in three dimensions fall into the same topological category as graphene in two dimensions. The Berry curvature vanishes everywhere except for the nodal line, where it is divergent. This implies that the nodal line gives rise to an anomalous Hall conductivity. Like in the graphene case however, there are two valley currents from opposite sides of the nodal line that cancel exactly due to additional spatial symmetries. In candidate materials with a nodal line, spin-orbit coupling is non-negligible. Coupling the spin sub-spaces allows for the nodal line to gap out, turning the material into a topological insulator with a vanishing Berry curvature.

Driving the systems coherently with circular polarized light creates an imbalance between the two valley contributions. Using Floquet theory, we show that a net anomalous Hall current arises in the periodically driven nodal-loop semimetal. Depending on the polarization, the sign of the current can be switched, which is the distinguishing feature of this effect. We further investigate its stability upon gapping the nodal line via spin-orbit coupling or small symmetry breaking terms.

TT 21.13 Tue 12:45 HSZ 103

Strain engineered higher order topological phases for spin-3/2 Luttinger fermions — •Andras Szabo — MPIPKS Dresden

Higher order topological phases attracted a lot of attention in the recent years, and apart from elemental Bi have so far evaded experimental realization in electronic systems. I will present a potential path to use a Luttinger semimetal (LSM) in order to strain engineer a higher order topological Dirac semimetal (HOTDSM).

A Luttinger semimetal is constituted by effective spin-3/2 fermions and describes a bi-quadratic touching of Kramers degenerate valence and conduction bands. Several materials are believed to be sufficiently described by such model, including 227 pyrochlore iridates, half-Heuslers, HgTe and gray-Sn. Moreover, advances in experimental technology (piezoelectric-based apparatus, and growing samples on suitable substrates) present an infrastructure promising for the strain-engineering of such HOT phases.

I will show that certain nematic phases of a LSM, that can be induced by the application of external strain, describe a HOTDSM with topological hinge states along the strain direction. I will also argue that these phases are stable in the presence of sufficiently weak disorder, an inherent feature of real world material samples.

TT 22: Quantum Dots, Quantum Wires, Point Contacts

Time: Tuesday 9:30–13:15 Location: HSZ 201

TT 22.1 Tue 9:30 HSZ 201

Cross-correlation spin-noise spectra of interacting quantum dot ensembles — •Andreas Fischer and Frithjof Anders — Theoretische Physik 2, Technische Universität Dortmund, 44227 Dortmund

Two-color pump-probe experiments indicate interactions between the electron spins in ensembles of singly charged InGaAs quantum dot. The interaction strength is comparable to the strength of hyperfine fluctuations but the microscopic origin of the interaction is still unknown. Previously these inter-dot interactions where studied far from thermal equilibrium via periodic optical excitations. We propose the investigation of inter-dot interactions by spin cross-correlation functions accessible in non-invasive two-color spin-noise spectroscopy. For our calculations we use a semiclassical central spin model extended by a Heisenberg interaction between the electron spins. We demonstrate that the cross-correlation function is sensitive to inter-dot interactions and robust in a broad range of frequencies against disorder caused by nuclear quadrupolar interactions, spin-phonon interactions and ensemble inhomogeneities of the electron g-factor.

TT 22.2 Tue 9:45 HSZ 201

Asymmetry effects and spin dynamics in resonant transport through quantum-dot spin valves — •Simon Mundinar, Alfred Hucht, Jürgen König, and Stephan Weiss — Theoretische Physik, Universität Duisburg-Essen and CENIDE, Lotharstr. 1, 47048 Duisburg, Germany

We present results of a theoretical investigation of spin effects in resonant transport through an interacting quantum-dot spin valve. The system is built from a quantum dot tunnel-coupled to two ferromagnetic leads, that induce spin-dependent tunneling. In the regime of small to intermediate interaction strengths we study the current through the system as well as occupation number and spin components of the dot, using the method of iterative summation of path integrals (ISPI) to achieve numerical exact data. We find an asymmetry in the current with respect to the gate voltage, that manifests once a local Zeeman field is applied to the quantum dot. The asymmetry can be traced back to the spin-dependent hybridization between dot and leads, together with higher order exchange field effects. Additionaly, we report on the strong impact of resonant tunneling processes on the tunnel magnetoresistance (TMR) at low temperatures [1]. We find a strong response of the TMR to an externally applied Zeeman field, resulting in a change in the sign of the TMR.

[1] S. Mundinar, P. Stegmann, J. König, S. Weiss, Phys. Rev. B **99**, 195457 (2019)

TT 22.3 Tue 10:00 HSZ 201

Charge-Photon statistics and short-time correlation in a single quantum dot-resonator system — •Tineke L. van den Berg[1] and Peter Samuelsson[2] — [1]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [2]Physics Department, Lund University, Sweden

Electrical quantum conductors coupled to microwave resonators have in the last decade emerged as a versatile testbed for controllable light-matter interaction on the nanometer scale. Recent experimental progress with high impedance resonators has resulted in conductor-resonator systems with a large, dimensionless coupling parameter $\lambda \gtrsim 0.1$, well beyond the small coupling regime $\lambda \ll 1$. Motivated by this progress, we here analyse theoretically the joint statistics of transported electrons and emitted photons in a single level quantum dot coupled to a microwave resonator, for arbitrarily large λ. Describing the electron-photon dynamics via a number-resolved master equation, we evaluate the joint long-time probability distribution as well as joint short-time, $g^{(2)}(t)$, correlation functions.

[1] T. L. van den Berg and P. Samuelsson PRB **100**, 035408 (2019).

TT 22.4 Tue 10:15 HSZ 201

Transport geometric phases: breaking gauge symmetries — •Roman-Pascal Riwar[1] and Janine Splettstoesser[2] — [1]PGI-2, Forschungszentrum Jülich, Germany — [2]MC2, Chalmers University of Technology, Sweden

Geometric phases and their relation to topological phase transitions are by now well-established notions in closed quantum systems. The generalization to open quantum systems on the other hand is an actively considered problem. We here review some of our recent works on geometric phases defined in the charge transport statistics of small quantum systems, and explore possible relations. Namely, the geometric phase can either be defined along the time axis (time-dependently driven systems) or along the detector momentum (time-dependent measurements). We find that there are two important gauge degrees of freedom: one related to energy displacement currents, and the other to charge displacement currents. We show for driven quantum systems, that violation of energy conservation renders the geometric phase highly sensitive to whether or not many-body interactions are present in the system. We contrast these findings to time-dependent measurements schemes, where geometric phases along the detector momentum are important. Here, the presence of non-zero displacement currents allows to probe and analyse dynamical phase transitions, and the resulting fractional charges.

TT 22.5 Tue 10:30 HSZ 201

Interference and shot noise in a degenerate Anderson-Holstein model — Michael Niklas, •Andrea Donarini, and MIlena Grifoni — Institut für Theoretische Physik, Universität Regensburg, Germany

Mechanical degrees of freedom can leave clear signatures in the transport characteristics of a nanojunction. We study an Anderson-Holstein model with orbital degeneracies [1] and tunnelling phases that allow for the formation of dark states [2]. The resulting destructive interference yields a characteristic pattern of positive and negative differential conductance features with enhanced shot noise, without further asymmetry requirements in the coupling to the leads. Measurements on suspended carbon nanotubes showed analogous effects [3,4], which acquire in this framework a new interpretation, free of ad-hoc matching of vibrational and electronic energies. The Lamb-shift renormalization introduced by charge fluctuations is the key ingredient for the understanding of such transport characteristics.

[1] M. G. Schultz, Phys. Rev. B 82, 155408 (2010)
[2] A. Donarini et al., Nature Comm. 10, 381 (2019)
[3] S. Sapmaz et al., Phys. Rev. Lett. 96, 026801 (2006)
[4] R. Leturcq et al., Nat. Phys. 5, 327 (2009)

TT 22.6 Tue 10:45 HSZ 201

Spin interference effects in quantum rings in the presence of SU(2) fields — Alberto Hijano[1,2,3] and •Dario Bercioux[3,4] — [1]University of the Basque Country, UPV/EHU, Bilbao, Spain — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [3]Donostia International Physics Center, Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We present a theory for quantum transport in quantum networks that accounts for Rashba spin-orbit coupling (SOC) and an in-plane magnetic field, the theory is based on a generalization of previous works with only Rashba SOC [1,2]. We investigate the conductance of polygonal structures as square and rings with symmetric contacts so as studied experimentally in the group of Nitta at Tohoku University. For the case of rings our approach is in agreement with the experimental finding [3]. Additionally, for the case of the square [4], we find interesting results when the in-plane magnetic field is parallel to two of the links for the network. Specifically, along this direction, the magnetic field erases the spin-precession effect due to the Rashba spin-orbit coupling, similarly to the case of systems where the Rashba and the Dresselhaus SOCs have the same strengths.

[1] Bercioux *et al.*, Phys. Rev. Lett. **93**, 056802 (2004).
[2] Bercioux *et al.*, Phys. Rev. B **72**, 113310 (2005).
[3] Nagasawa *et al.*, Nat. Comm. **4**, 2526 (2013).
[4] Wang *et al.*, arXiv:1908:01825 (2019).

TT 22.7 Tue 11:00 HSZ 201

Spin-dependent scattering in a nanowire with spin-orbit coupling and an impurity — Alba Pascual[1], •Tineke L. van den Berg[1,2], Vitaly N. Golovach[1,2,3], Dario Bercioux[2,3], Juan José Sáenz[2,3], and Sebastián Bergeret[1,2] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU,E-20018 Donostia-San Sebastián, Spain — [2]Donostia International Physics Center (DIPC), E-20018 Donostia-San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation of Science, E-48011 Bilbao, Spain

We study a quasi-one-dimensional quantum wire with spin-orbit coupling (SOC), and containing a spinless impurity. We use a perturbative approach to leading order in SOC to obtain an effective Hamiltonian with decoupled sub-bands of size quantization. We calculate the scattering matrix using the Lippmann-Schwinger approach, accounting for the SU(2) gauge field generated by the SOC in the nanowire. The well-known dip in the conductance due to Fano interference is lifted from zero as a result of the spin scattering at the impurity. Going beyond the perturbative approach, we discuss numerical results of a tight-binding calculation in the continuous limit of fine discretization. We analyse the conductance dip behaviour as a function of the impurity and the SOC strength. We relate the numerical results to our toy-model calculation using an asymptotic-freedom approach.

15 min. break.

TT 22.8 Tue 11:30 HSZ 201

Pair-amplitude dynamics in superconductor-quantum dot hybrids — •Mathias Kamp and Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Electromagnetic pulses in the THz regime have recently been used to excite oscillations of the order parameter in bulk superconductors [1]. These oscillations can be understood as a collective precession of the Anderson pseudospin and are linked to the Higgs amplitude mode of the order parameter.
Here, we consider a superconductor-quantum dot hybrid driven out of equilibrium by a temperature and phase bias. We investigate the dynamics of the proximity-induced pair amplitude on the dot after both a quench and under periodic driving of system parameters. We find that the system can exhibit coherent oscillations of the pair amplitude and link them to the time- dependent charge and heat currents through the system.

[1] Matsunaga et al., Science **345**, 1145 (2014).

TT 22.9 Tue 11:45 HSZ 201

Single-photon pump by Cooper-pair splitting — Mattia Mantovani, Wolfgang Belzig, Gianluca Rastelli, and •Robert Hussein — Fachbereich Physik, Universität Konstanz, Germany

Cooper-pairs are a source of correlated electrons and their nonlocal breaking can be used in entanglement generation [1,2], thermoelectric transport [3], and spin-current-control [4]. Here, we consider a hybrid superconductor-double-quantum-dot system as a Cooper-pair splitter. By coupling each quantum dot to an electromagnetic or mechanical resonator, one can simultaneously cool down both resonators into their ground state [5]. We demonstrate that the process of cross-Andreev reflection can additionally be employed to coherently transfer single photons, and therewith heat, between these two distant resonators, realizing an efficient photon bus. The proposed scheme has further potential applications in quantum heat engines and refrigerators

[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).
[3] R. Hussein, M. Governale, S. Kohler, W. Belzig, F. Giazotto, and A. Braggio, Phys. Rev. B 99, 075429 (2019).
[4] A. Rezaei, R. Hussein, A. Kamra, and W. Belzig, arXiv:1908.09610.
[5] M. Mantovani, W. Belzig, G. Rastelli, and R. Hussein, Phys. Rev. Research 1, 033098 (2019).

TT 22.10 Tue 12:00 HSZ 201

Waiting time distribution and current cross-correlations in triple quantum dot-based Cooper pair splitters — •Kacper Wrześniewski and Ireneusz Weymann — Faculty of Physics, Adam Mickiewicz University in Poznań, Poland

We study the spin-resolved subgap transport in a triple quantum-dot system coupled to one superconducting and two ferromagnetic leads. The Andreev processes are examined in the parallel and antiparallel alignments of ferromagnets' magnetic moments in both linear and nonlinear response regimes. The emphasis is put on the analysis of the electron waiting time distributions and cross-correlations between the currents flowing through the left and right arms of the device. In particular, we consider various detuning schemes of the quantum dots' energy levels and find the optimal parameters for the efficient splitting and maximized Andreev current. We predict short waiting times for electrons tunneling through the distinct ferromagnetic contacts indicating fast splitting of emitted Cooper pairs and strong positive cross-correlations associated with the presence of tunneling processes enhancing the Cooper pair splitting efficiency.

TT 22.11 Tue 12:15 HSZ 201

Perturbation theory for superconducting double quantum

dot systems — •Vladislav Pokorný[1] and Martin Žonda[2] — [1]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Praha 8 CZ-182 21, Czech Republic — [2]Institute of Physics, Albert Ludwig University of Freiburg, Hermann-Herder-Strasse 3, Freiburg DE-791 04, Germany

We present an approach based on the second order perturbation theory in the Coulomb interaction to calculate properties of double quantum dots coupled to superconducting BCS leads. We map the system on a generalized two-impurity Anderson model and using this perturbative method we evaluate several single-particle quantities such as the on-dot induced gap and generalized occupation numbers together with the Andreev in-gap spectra and compare them with numerically exact results from the Numerical Renormalization Group and Quantum Monte Carlo finding a good correspondence for not too strongly correlated regimes. This method can offer an efficient and reliable alternative to the heavy numerical tools in a wide parameter range.

TT 22.12 Tue 12:30 HSZ 201

Pseudospin resonances in a double quantum dot — •Christoph Rohrmeier and Andrea Donarini — Institute of Theoretical Physics University of Regensburg, Regensburg, Germany

The interplay between interference and interaction produces several effects in degenerate quantum systems, including spin torques [1], all electrical spin control [2] and dark states formation [3]. In this context, a spin resonance without spin splitting has been first predicted for a single quantum dot spin valve [4]. We consider a spin-full double quantum dot with the orbital degree of freedom described by a pseudospin and predict a rich variety of pseudospin resonances. The latter are modulated with the system parameters, can be split up and even turned into a Fano-like resonance in the presence of ferromagnetic leads. This interplay of spin and pseudospin is understood in terms of spin dependent pseudo-exchange fields. The numerical results are obtained in the framework of a generalized master equation, calculated up to next to leading order in the tunnelling coupling.

[1] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[2] A. Donarini et al., Nano Lett. 9, 2897 (2009)
[3] A. Donarini et al., Nature Comm. 10, 381 (2019)
[4] M. Hell et al., Phys. Rev. B 91, 195404 (2015)

TT 22.13 Tue 12:45 HSZ 201

Colortronics in Triple Quantum Dots — •Martin Maurer[1], Jürgen König[2], and Herbert Schoeller[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen and JARA - Fundamentals of Future Information Technology — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE

We study coherence effects in a three-level spinless quantum dot with strong local Coulomb interaction coupled weakly to metallic reservoirs. Employing the generators of the SU(3), we decompose the reduced density matrix in the subspace of single occupation. It is then characterized by an eight-dimensional real vector that is the analogue to the vector of average (iso-)spin in a two-level setup. We call this vector the dot color. In the high-temperature limit we derive a kinetic equation for the dot color to first order in the dot-lead coupling. This equation can be decomposed into an accumulation, a relaxation, and a rotation component, providing intuitive insight into the dot dynamics. We discuss the inclusion of spin and a generalization to an arbitrary number of dot levels.

Regarding the three-level case, we propose an experimental setup that produces a complete current blockade in nonlinear response for degenerate levels. This blockade is based on the formation of a coherent superposition of dot levels and is broken when dot energies are detuned. The resulting current-detuning curve highlights the role of coherence between all three dot levels in the blockade.

TT 22.14 Tue 13:00 HSZ 201

Extended quasiparticle picture for quantum wires in the high-density limit — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [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]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab) - 144 011, India — [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 high-density limit of quantum wires are considered and an extended quasiparticle picture is developed. This allows to calculate the reduced density, the pair correlation function and the effective mass. A non-universal behaviour of the Tan constant is reported for the Coulomb limit. The structure factor is obtained analytically which provides the exact correlation energy. [Eur. Phys. J. B 91 (2018) 29, Phys. Rev. B 97 (2018) 155147, arXiv:1909.09331]

TT 23: Nonequilibrium Quantum Many-Body Systems 1 (joint session TT/DY)

Time: Tuesday 9:30–13:00 Location: HSZ 204

TT 23.1 Tue 9:30 HSZ 204

Exponential damping in perturbed quantum many-body systems — •Jonas Richter[1], Fengping Jin[2], Lars Knipschild[1], Hans De Raedt[3], Kristel Michielsen[2], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]Forschungszentrum Jülich, Germany — [3]University of Groningen, The Netherlands

Given a quantum many-body system and the expectation-value dynamics of some operator, we study how this reference dynamics is altered due to a perturbation of the system's Hamiltonian. Based on projection operator techniques, we unveil that if the perturbation exhibits a random-matrix structure in the eigenbasis of the unperturbed Hamiltonian, then this perturbation effectively leads to an exponential damping of the original dynamics. Employing a combination of dynamical quantum typicality and numerical linked cluster expansions, we demonstrate that our theoretical findings are relevant for the dynamics of realistic quantum many-body models. Specifically, we study the decay of current autocorrelation functions in spin-1/2 ladder systems, where the rungs of the ladder are treated as a perturbation to the otherwise uncoupled legs. We find a convincing agreement between the exact dynamics and the lowest-order prediction over a wide range of interchain couplings, even if the perturbation is not weak.

[1] J. Richter et al., arXiv:1906.09268.

TT 23.2 Tue 9:45 HSZ 204

Slow quantum thermalization and many body revivals from mixed phase space — •Alex Michailidis[1], Chris Turner[2], Dimitry Abanin[3], Zlatko Papic[2], and Maksym Serbyn[1] — [1]IST Austria, Klosterneuburg, Austria — [2]University of Leeds, Leeds, United Kingdom — [3]University of Geneva, Geneva, Switzerland

Isolated, interacting quantum systems thermalize when local measurements are distributed according to the Gibbs ensemble. The ability of an isolated quantum many body system to thermalize is tied to the absence of an extensive set of integrals of motion. The thermalization rate may, however, depend strongly on the initial state. A class of kinetically constraint systems [Nat. Phys. 14, 745 (2018)] displays such features, due to a set of quasi-eigenmodes, known as “quantum many body scars”, which form a slowly thermalizing subspace. The slow thermalization is also associated to an unstable periodic orbit in a slightly entangled manifold of matrix product states (MPS) [PRL 122, 040603 (2019)] .

First, by using tensor tree states (TTS) and ideas from standard mean field theory, we generalize the MPS ansatz to higher dimensions. We employ the time-dependent-variational-principle to analytically calculate the equations of motion for lattices of arbitrary connectivity. We find that the coherent oscillations in the quantum system are associated to stable periodic orbits in a mixed phase space. This method provides a new way to identify entangled states which display coherent dynamics. Finally, we associate slowly thermalizing states to regular “islands” in the mixed phase space.

TT 23.3 Tue 10:00 HSZ 204

Collective behavior of an excitonic insulator in the quantum electromagnetic field — •Katharina Lenk and Martin Eckstein — Department of Physics, University of Erlangen-Nuremnberg, 91058 Erlangen, Germany

The strong coupling of light and matter in cavity quantum electrodynamics provides new avenues to engineer properties of complex materials. In this talk, we investigate the behavior of a so-called excitonic insulator (EI) in a cavity. The EI is a phase driven by the Coulomb interaction, in which two bands of a semiconductor or semimetal spontaneously hybridize, leading to the opening of a gap. We consider the particular case in which the EI implies a breaking of the U(1) symmetry related to the conservation of charge in the individual bands. The coupling of a generic bosonic mode, such as the coordinate of a phonon, reduces the symmetry, adds a mass to the phase mode, and stabilizes the symmetry-broken phase. While this suggests that a similar mechanism may be at work for the coupling of the EI to a cavity mode, we show that the balancing of dipolar interactions and the dipolar light-matter coupling leaves the phase mode massless, in spite of the breaking of the U(1) symmetry.

TT 23.4 Tue 10:15 HSZ 204

A memory truncation scheme to investigate long-time dynamics in correlated systems — •Antonio Picano and Martin Eckstein — Friedrich-Alexander-Universität Erlangen-Nürnberg

We present an approach to follow the evolution of many-body systems up to previously unaccessible long time scales. Provided only that the system of interest shows a self-energy that is short-range in time, its time evolution can be determined by solving a simplified version of the full Kadanoff-Baym equations. The computational effort scales only linearly with the number of time-steps, and the computer memory is independent of the propagation time.

We have applied the method to investigate the dynamical phase transitions from antiferromagnetic to paramagnetic states driven by an interaction quench in the fermionic Hubbard model, using the nonequilibrium dynamical mean-field theory. We have observed the presence of two dynamical transition points: one is related to the thermal phase transition, the other is connected to the existence of a transient non-thermal antiferromagnetic order above the thermal critical temperature. The non-thermal order displays a slow decay, which is followed by a faster thermalization process, and thermalization is significantly delayed by the trapping of the system in the nonthermal state.

TT 23.5 Tue 10:30 HSZ 204

Critical quenches in the attractive Hubbard model — •Christopher Stahl and Martin Eckstein — Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg, Deutschland

We investigate critical quenches from a paramagnetic phase in a three dimensional attractive Hubbard model towards the ordered superconducting phase using a two-time Green's function formalism on the Keldysh contour and the fluctuation exchange approximation (FLEX). This self-consistent approach gives access to the coupled dynamics of single particle properties and collective fluctuations in the transient state, and allows to study the growth of order in the initially disordered system. By truncating the two-time self-energy with respect to relative time we set up a long-time multi-scale simulation which resolves the dynamics of both the fast electronic and slow bosonic degrees of freedom. This may help to close the gap between short time microscopic simulations and predictions for the long time behavior based on Ginzburg-Landau-theory and the theory of dynamic critical phenomena.

TT 23.6 Tue 10:45 HSZ 204

Thermalization of a two-species condensate — •Jan Louw[1], Michael Kastner[2], and Johannes Kriel[2] — [1]University of Goettingen, Goettingen, Germany — [2]Stellenbosch University, Stellenbosch, South Africa

Motivated by recent experiments, we study the time evolution of a two-species Bose-Einstein condensate which is coupled to a bosonic bath. For the particular condensate, unconventional thermodynamics have recently been predicted. To study these thermal properties we find the conditions under which this open quantum system thermalizes—equilibrates to the Gibbs state describing the canonical ensemble. We do this in a semi-classical picture with corrections scaling with the inverse system size.

TT 23.7 Tue 11:00 HSZ 204

Exceptional points and the topology of quantum many-body spectra — •David Luitz and Francesco Piazza — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We show that in a generic, ergodic quantum many-body system the interactions induce a nontrivial topology for an arbitrarily small non-Hermitian component of the Hamiltonian. This is due to an exponential-in-system-size proliferation of exceptional points which have the Hermitian limit as an accumulation (hyper)surface. The nearest-neighbor level repulsion characterizing Hermitian ergodic many-body systems is thus shown to be a projection of a richer phenomenology, where actually all the exponentially many eigenvalues are pairwise connected in a topologically robust fashion via exceptional points.

15 min. break.

TT 23.8 Tue 11:30 HSZ 204

η–paired hidden phase in photodoped Mott insulators — •Jiajun Li[1], Denis Golez[2], Philipp Werner[3], and Martin Eckstein[1] — [1]University of Erlangen-Nuremberg, Germany — [2]Flatiron Institute, New York, US — [3]University of Fribourg, Switzerland

We show that a metastable η–pairing superconducting phase can be induced by photodoping doublons and holes into a strongly repulsive fermionic Hubbard model. The doublon-hole condensate extends over a wide range of doublon densities and effective temperatures. Different non-equilibrium protocols to realize this state are proposed and numerically tested. We also study the optical conductivity in the superconducting phase, which exhibits ideal metallic behavior, i.e., a delta function at zero-frequency in the conductivity, in conjunction with negative conductivity at large frequencies. These characteristic optical properties can provide a fingerprint of the η-pairing phase in pump-probe experiments.

TT 23.9 Tue 11:45 HSZ 204

η-pairing in one-dimensional Mott insulators — •Satoshi Ejima[1], Tatsuya Kaneko[2], Florian Lange[1], Seiji Yunoki[3,4,5], and Holger Fehske[1] — [1]Institute of Physics, University Greifswald, Greifswald, Germany — [2]Department of Physics, Columbia University, New York NY, USA — [3]RIKEN Cluster for Pioneering Research, Wako, Japan — [4]RIKEN Center for Emergent Matter Science, Wako, Japan — [5]RIKEN Center for Computational Science, Kobe, Japan

Very recently, it was theoretically demonstrated that unconventional superconductivity correlation can be induced by pulse irradiation in the simple Mott insulator of the half-filled Hubbard model [1]. This superconducting-like state stems from the so-called η-pairing mechanism, characterized by staggered pair-density-wave oscillations of the off-diagonal correlations.

In this study, we first explore precisely under which conditions the η-pairing state appears most pronouncedly at zero temperature by means of the time-dependent density-matrix renormalization group (DMRG) method in the matrix-product-state representation. Carrying out temperature-dependent DMRG in combination with the purification technique, we furthermore prove whether this state can survive at finite temperatures, in order to check the possible experimental observation of the pairing state, e.g., in optical lattices.

[1] T. Kaneko, T. Shirakawa, S. Sorella and S. Yunoki, Phys. Rev. Lett. **122**, 077002 (2019).

TT 23.10 Tue 12:00 HSZ 204

Effect of dimensionality on the dynamics of optically excited Mott-Hubbard clusters — •Junichi Okamoto — Institute of Physics, University of Freiburg, Freiburg, Germany

Development of intense light sources and of various time-resolved spectroscopies has opened up a new avenue in condensed matter physics. In particular, optically excited nonequilibrium states of strongly correlated systems show nontrivial and intriguing phenomena such as light-induced superconductivity or ultrafast structural switching. An important step to understand these phenomena is to investigate the excitation spectrum of a system. To this end, we use an exact diagonalization method to study the effect of dimensionality on the dynamics of optically excited states in Mott-Hubbard clusters. We compare the excitation spectrum in one and two dimensions, and demonstrate the different transient dynamics induced by short optical pulses.

TT 23.11 Tue 12:15 HSZ 204

Disentangling sources of quantum entanglement in quench dynamics — •Lorenzo Pastori[1], Markus Heyl[2], and Jan Carl Budich[1] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max-Planck-Institut für Physik

komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany

Quantum entanglement may have various origins ranging from solely interaction-driven quantum correlations to single-particle effects. Here, we explore the dependence of entanglement on time-dependent single-particle basis transformations in fermionic quantum many-body systems, thus aiming at isolating single-particle sources of entanglement growth in quench dynamics. Using exact diagonalization methods, for paradigmatic nonintegrable models we compare to the standard real-space cut various physically motivated bipartitions. Moreover, we search for a minimal entanglement basis using local optimization algorithms, which at short to intermediate postquench times yields a significant reduction of entanglement beyond a dynamical Hartree-Fock solution. In the long-time limit, we identify an asymptotic universality of entanglement for weakly interacting systems, as well as a crossover from dominant real-space to momentum-space entanglement in Hubbard models undergoing an interaction quench. Finally, we discuss the relevance of our findings for the development of tensor-network based algorithms for quantum dynamics.

TT 23.12 Tue 12:30 HSZ 204

Statistical localization: from strong fragmentation to strong edge modes — •Tibor Rakovszky[1], Pablo Sala[1], Ruben Verresen[2], Michael Knap[1], and Frank Pollmann[1] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Certain disorder-free Hamiltonians can be non-ergodic due to a strong fragmentation of the Hilbert space into disconnected sectors. Here, we characterize such systems by introducing the notion of "statistically localized integrals of motion" (SLIOM), whose eigenvalues label the connected components of the Hilbert space. SLIOMs are not spatially localized in the operator sense, but appear localized to sub-extensive regions when their expectation value is taken in typical states with a finite density of particles. We illustrate this general concept on several Hamiltonians, both with and without dipole conservation. Furthermore, we demonstrate that there exist perturbations which destroy these integrals of motion in the bulk of the system, while keeping them on the boundary. This results in statistically localized strong zero modes, leading to infinitely long-lived edge magnetizations along with a thermalizing bulk, constituting the first example of such strong edge modes in a non-integrable model. We also show that in a particular example, these edge modes lead to the appearance of topological string order in a certain subset of highly excited eigenstates. Some of our suggested models can be realized in Rydberg quantum simulators.

TT 23.13 Tue 12:45 HSZ 204

Matrix product state investigations of time-dependent spectral functions after a photoexcitation — •Constantin Meyer and Salvatore R. Manmana — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We study the time-dependent dynamical structure factor after a photoexcitation of a variant of the 1d Hubbard model with a background staggered magnetic field using matrix product state (MPS) techniques. In particular, we use the time-dependent variational principle (TDVP) to investigate the time evolution of the band population, which is a quantity accessible to time-resolved ARPES experiments. Different scenarios for the photoexcitations are discussed, e.g., Peierls-substitution or direct excitation in k-space. Using MPS, we can study in detail the effect of the electron-electron interaction on the redistribution of the band populations in the various photoexcitation setups. An outlook to the relevance of electron-electron interactions on light-harvesting mechanisms in correlated materials is given.

We acknowledge financial support by SFB/CRC 1073 (project B03) of the DFG.

TT 24: Frustrated Magnets - Spin Liquids 1 (joint session TT/MA)

Time: Tuesday 9:30–13:00 Location: HSZ 304

TT 24.1 Tue 9:30 HSZ 304

Low temperature thermal transport studies on the kagome quantum spin liquid candidate herbertsmithite — Jan Bruin, •Ralf Claus, Yosuke Matsumoto, Jürgen Nuss, Masahiko Isobe, and Hidenori Takagi — Max Planck Institute for Solid State Research, Stuttgart, Germany

Quantum spin liquids (QSLs) are a novel state of matter that may host exotic excitations like itinerant charge-neutral spin-1/2 quasiparticles (spinons). The prototype for a QSL ground state is the spin-1/2 Heisenberg antiferromagnet on the kagome lattice. In terms of materials, herbertsmithite ($ZnCu_3(OH)_6C_{12}$) provides a perfect realization of this model. However, despite theoretical and experimental efforts the nature of its ground state remains under debate. An important question concerns the existence of an excitation gap.

To address this issue, we performed thermal transport measurements down to 80 mK. The measurement of the thermal conductivity (k) only captures mobile excitations in the material and is therefore a powerful tool to detect low-lying (gapless) spinons. In our measurements, we confirmed the absence of a finite k/T (spinon) term but observed a robust T-squared power-law behavior. I will discuss the possible QSL ground state scenarios in detail as well as an unusual field dependence.

TT 24.2 Tue 9:45 HSZ 304

Magnetic properties of the $NaYbO_2$ and $KYbO_2$ triangular antiferromagnets — •Franziska Grussler, Sebastian Bachus, Philipp Gegenwart, and Alexander A. Tsirlin — Centerfor Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany

$NaYbO_2$ and $KYbO_2$ feature the same space group $R\bar{3}m$ as the spin-liquid candidate $YbMgGaO_4$ but evade structural disorder pertinent to that compound. We report a comparative study of these triangular antiferromagnets including their structural characterization and thermodynamic properties in the milli-K temperature range. Both $NaYbO_2$ and $KYbO_2$ reveal magnetic interactions of about 4 K and no signs of magnetic order in zero field, but undergo field-induced magnetic order that in the Na case occurs between 3 T and 8 T. By studying specific heat of $NaYbO_2$ at milli-K temperatures, we conclude that between 0.5 T and 2 T, within the putative spin-liquid phase, magnetic specific heat follows quadratic behavior expected for the gapless Dirac spin liquid. In zero field, no simple power-law behavior can be observed, but the data clearly deviated from an activated behavior expected for a gapped ground state. Our observations establish gapless nature of the spin-liquid phase of triangular antiferromagnets.

TT 24.3 Tue 10:00 HSZ 304

NMR and bulk magnetometry investigations of the field-induced order in the frustrated triangular-lattice compound $NaYbSe_2$ — •S. Luther[1,2], K. M. Ranjith[3], T. Reimann[1], Ph. Schlender[4], B. Schmidt[3], J. Sichelschmidt[3], H. Yasuoka[3], J. Wosnitza[1,2], Th. Doert[4], M. Baenitz[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany

The Yb-based delafossite $NaYbSe_2$ is a triangular-lattice antiferromagnet with space group (R-3m). In this compound, spin-orbit coupling leads to a pronounced magnetic anisotropy. The absence of magnetic long-range order at zero field is suggestive of a quantum spin-liquid ground state. From specific-heat and magnetization experiments, magnetically ordered states were observed for $H \perp c$ and $H \parallel c$ exceeding 2 and 9 T, respectively. ^{23}Na ($I = 3/2$) NMR probes the microscopic details of the field-induced magnetic structure. Measurements of the $1/T_1$-relaxation rate are consistent with the specific-heat data. At $H \perp c = 5$ T, the magnetization indicates an up-up-down spin arrangement with according asymmetric broadening of the NMR spectra. At $H \parallel c = 16$ T, an umbrella-type configuration of the magnetic moments is revealed, in agreement with a symmetric broadening of the NMR spectra. Low-field measurements reveal a continuous increase of the $1/T_1$-relaxation rate and spectral broadening without signatures of long-range order down to 0.3 K.

TT 24.4 Tue 10:15 HSZ 304

Spin orbit entangled $J = 1/2$ triangular magnets $NaYbCh_2$

(Ch:O,S,Se): pushing a spin liquid into criticality and magnetic order by magnetic fields — •M. Baenitz[1], K.M. Ranjith[1], S. Luther[3], Ph. Schlender[2], T. Reimann[3], S. Khim[1], J. Sichelschmidt[1], B. Schmidt[1], H. Yasuoka[1], H. Kuehne[3], J. Wosnitza[3], and Th. Doert[2] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]TU Dresden, Department of Chemistry and Food Chemistry, D-01062 Dresden, Germany — [3]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, D- 01328 Dresden, Germany

Spin orbit coupling (SOC) brought significant progress to the field of quantum spin liquids (QSLs). Yb-based magnets are prime candidates for the QSL-state and as such the $NaYbCh_2$ series is regarded as a unique platform to study anisotropic planar spin 1/2 triangular lattice magnetism (TLM) with bond frustration. In contrast to $YbMgGaO_4$,which shares the same space group (R-3m), $NaYbCh_2$ lacks inherent lattice distortions and Yb resides on a centrosymmetric position in the $YbCh_6$ octahedron. Our comprehensive study combines bulk- and local- probes and identifies $NaYbCh_2$ as a new class of spin orbit entangled TLMs were the QSL state is realized on a perfect triangular lattice [1,2]. The application of fields in (a,b)-plane transforms the system into a critical regime followed by long range order. We present magnetization, specific heat and Na NMR data down to 300 mK

[1] M. Baenitz et al., Phys. Rev. B 98 (2018)
[2] K.M. Ranjith et al., Phys. Rev. B 99 (2019)

TT 24.5 Tue 10:30 HSZ 304

Spin dynamics in the quantum spin liquid candidate $Na_2BaCo(PO_4)_2$ probed by Electron Spin Resonance — •Christoph Wellm[1,2], Willi Roscher[1], Vladislav Kataev[1], Oleg Janson[1], Bernd Büchner[1,2], Robert J. Cava[3], and Ruidan Zhong[3] — [1]Leibniz Institute for Solid State and Materials Research IFW Dresden, D-01069 — [2]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01062 — [3]Department of Chemistry, Princeton University, Princeton, US-08544

The triangular-lattice magnet $Na_2BaCo(PO_4)_2$ with localized effective spin-1/2 moments of Co^{2+} ions shows strong, exotic magnetic flucuations in absence of long-range order down to 0.3 K with large residual entropy and linear in temperature spinon excitations, making it a very promising candidate for the realization of a quantum spin liquid [1,2]. We report electron spin resonance (ESR) and magnetization results of powder and single crystals of the title compound supporting the scenario of a spin liquid. We relate our results to previous experimental studies [1,2] and theory (talk by W. Roscher et.al. at this conference).

[1] R. Zhong *et al.*, Proc. Natl. Acad. Sci., **116**, pp. 14505-14510 (2019)
[2] N. Li *et al.*, arXiv:1911.11107 (2019)

TT 24.6 Tue 10:45 HSZ 304

DFT calculations of the quantum spin liquid candidate $Na_2BaCo(PO_4)_2$ — •Willi Roscher, Christoph Wellm, Bernd Büchner, Vladislav Kataev, and Oleg Janson — Leibniz Institute for Solid State and Materials Research Dresden, Germany

The recently synthesized triangular lattice magnet $Na_2BaCo(PO_4)_2$ shows effective $S = 1/2$ behavior with strong quantum fluctuations persistent down to 50 mK, rendering it as a candidate for the quantum spin liquid (QSL) ground state [1,2]. Very recent ESR and magnetization measurements hint at a more complex picture with different energy scales. To provide a microscopic insight, we perform band structure DFT calculations using the full-potential code FPLO. We calculate the band structure and Wannier projections for the t_{2g} an e_g states of Co. The evaluated transfer integrals are used to estimate the leading magnetic exchanges, the spin orbit coupling constant and the trigonal crystal field splitting. These two latter parameters are used to assess the electronic ground state and the excitation spectrum of Co^{2+} atoms. Finally, we compare our theoretical findings with new experimental studies.

[1] R. Zhong *et al.*, Proc. Natl. Acad. Sci., **116**, pp. 14505-14510 (2019)
[2] N. Li *et al.*, arXiv:1911.11107 (2019)

TT 24.7 Tue 11:00 HSZ 304

Evidence of one-dimensional magnetic heat transport in the triangular-lattice antiferromagnet Cs_2CuCl_4 — E. Schulze[1,2], S. Arsenijevic[1], L. Opherden[1], A.N. Ponomaryov[1], J. Wosnitza[1,2], T. Ono[3], H. Tanaka[4], and •S.A. Zvyagin[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, 01328 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Osaka Prefecture University, Osaka 599-8531, Japan — [4]Tokyo Institute of Technology, Tokyo 152-8551, Japan

We report on low-temperature heat-transport properties of the spin-1/2 triangular-lattice antiferromagnet Cs_2CuCl_4. Broad maxima in the thermal conductivity along the three principal axes, observed at about 5 K, are interpreted in terms of the Debye model, including the phonon Umklapp scattering. For thermal transport along the *b* axis, we found a pronounced field-dependent anomaly, close to the transition into the three-dimensional long-range-ordered state. No such anomalies were observed for the transport along the *a* and *c* directions. We argue that this anisotropic behavior is related to an additional heat-transport channel through magnetic excitations, that can best propagate along the direction of the largest exchange interaction. Our observations strongly support the quasi-1D spin-liquid scenario with spinons as elementary excitations, proposed for this frustrated antiferromagnet. Besides, peculiarities of the heat transport of Cs_2CuCl_4in magnetic fields up to the saturation field and above are discussed [1].

This work was supported by the DFG.

[1] E. Schulze et al., Phys. Rev. Research 1, 032022(R) (2019).

15 min. break.

TT 24.8 Tue 11:30 HSZ 304

Thermal conductivity of the hyper-hyperkagome spin liquid candidate $PbCuTe_2O_6$ — •Xiaochen Hong[1], Matthias Gillig[1], Shravani Chillal[2], A. T. M. Nazmul Islam[2], Bernd Büchner[1,3,4], Bella Lake[2,5], and Christian Hess[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden (IFW-Dresden), Dresden — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [3]Institute of Solid State Physics, TU Dresden, Dresden — [4]Center for Transport and Device, TU Dresden, Dresden — [5]Technische Universität Berlin, Berlin

Quantum spin liquids (QSLs) are exotic phases of matter formed by interacting quantum spins. QSLs are characterized by the absence of static magnetism and the existence of emergent fractional excitations. Recently, $PbCuTe_2O_6$ was discovered to be a rare QSL candidate with a three-dimensional spin structure. Here we report the thermal conductivity measurements of this compound down to about 50 mK and up to 16 T. Our results show evidence for the gapped spinons in $PbCuTe_2O_6$. Besides, the unusual field dependence of its low temperature thermal conductivity indicates the residual magnetic order is very sensitive to the external field.

TT 24.9 Tue 11:45 HSZ 304

Probing anisotropic static and dynamic magnetic interactions of Fe-kagome $Fe_4Si_2Sn_7O_{16}$ by bulk magnetisation and NMR — •S. Dengre[1], R. Sarkar[1], L. Opherden[2], M. Uhlarz[2], T. Herrmannsdörfer[2], M. Allison.[3], T. Söhnel[3], C.D. Ling[4], J Gardner[5], and H.-H. Klauss[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany — [2]Institute of Resource Ecology and Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, D-01328 Dresden, Germany — [3]School of Chemical Sciences, University of Auckland, Auckland 1142, New Zealand — [4]School of Chemistry, The University of Sydney, Sydney 2006, Australia — [5]Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organization, Menai 2234, Australia

$Fe_4Si_2Sn_7O_{16}$ hosts an undistorted kagome lattice with Fe^{2+} ($3d^6$, $S = 2$) spins. We present results on oriented and unoriented powder samples. The bulk magnetic susceptibility shows the presence of strong planar (XY) rather than *Ising* anisotropy. Both static NMR shift (K) and dynamic spin-lattice relaxation rate ($1/T_1$) NMR reveal a highly anisotropic behaviour in $\parallel$ and $\perp$ orientation of the external field with respect to the Kagome planes. For $\parallel$ orientation, the NMR shift (K) scales linearly with the bulk susceptibility for temperatures ranging from 100 K to 4 K. The NMR shift in $\perp$ orientation shows the onset of AFM correlations at T $\approx$ 30 K by a deviation from the linear scaling. This is also reflected in the $1/T_1$ for $\parallel$ orientation, which starts to decrease at T $\approx$ 30 K.

TT 24.10 Tue 12:00 HSZ 304

Dynamics of an SU(2)-symmetric Kitaev model: spectroscopic signatures of fermionic magnons — •Willian Massashi Hisano Natori[1] and Johannes Knolle[1,2,3] — [1]Imperial College London, London, United Kingdom — [2]Technische Universitat

Munchen, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

In this work, we study the dynamics of an integrable Kugel-Khomskii Hamiltonian defined as an extension of the Kitaev honeycomb model. This model displays a global SU(2) symmetry that leads to S=1 fermionic excitations. We show that these fermions' dynamical response is exactly computed using a few-particle approach and can be experimentally probed with resonant inelastic x-ray scattering. The techniques developed to uncover the dynamics of the Kitaev model are used to compute the expected neutron scattering response. We show that the SU(2) symmetric model exhibits a vison gap three times larger than the spin-1/2 Kitaev model and a broader band of excitations due to the presence of additional Majorana flavors.

TT 24.11 Tue 12:15 HSZ 304

Phonon renormalization in the Kitaev quantum spin liquid — •Alexandros Metavitsiadis and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

We present the self-energy of phonons, magnetoelastically coupled to the two-dimensional Kitaev spin-model on the honeycomb lattice. Fractionalization of magnetic moments into mobile Majorana matter and a static $\mathbb{Z}_2$ gauge field lead to a continuum of relaxation processes comprising two channels. Thermal flux excitations, which act as an emergent disorder, strongly affect the phonon renormalization. Above the flux proliferation temperature, the dispersion of a narrow quasiparticle-hole channel is suppressed in favor of broad and only weakly momentum dependent features, covering large spectral ranges. Our analysis is based on complementary calculations in the low-temperature homogeneous gauge and a mean-field treatment of thermal gauge fluctuations, valid at intermediate and high temperatures.

TT 24.12 Tue 12:30 HSZ 304

Phase Diagram of the Breathing Kagome $S = 1/2$ XY Model with Four-Site Ring Exchange — •Niklas Casper and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

We study the phase diagram of the breathing kagome $S = 1/2$ XY model with four-site ring exchange. This model exhibits trimerization of the nearest neighbor exchange between up-/downward oriented triangles of the kagome lattice. This may be of relevance to compounds like vanadium oxyfluoride $[NH_4]_2[C_7H_{14}N][V_7O_6F_{18}]$.

Though a frustrated quantum spin model, it does not suffer from the sign problem and therefore can be treated by quantum Monte Carlo. In particular, we use the stochastic series expansion method which is extended to treat four-site ring exchange terms residing on the up to next nearest neighbor bow-tie plaquettes by using an update procedure proposed by Roger G. Melko and Anders W. Sandvik [Phys. Rev. E **72**, 026702].

Results for the spin stiffness will be presented in order to study the quantum phase transition belonging to the 3D XY universality class.

TT 24.13 Tue 12:45 HSZ 304

Chromium breathing pyrochlores as a showcase for a variety of pyrochlore Hamiltonians — •Tobias Müller[1], Pratyay Ghosh[2], Yasir Iqbal[3], Ronny Thomale[1], Johannes Reuther[4], Michel J. P. Gingras[5,6], and Harald O. Jeschke[7] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Paul Scherrer Institut, Forschungsstrasse 111, 5232 Villigen PSI, Schweiz Switzerland — [3]Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India — [4]Dahlem Center for Complex Quantum Systems and Fachbereich Physik,Freie Universität Berlin, 14195 Berlin, Germa — [5]epartment of Physics and Astronomy, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada — [6]Quantum Materials Program, Canadian Institute for Advanced Research, MaRS Centre,West Tower 661 University Ave., Suite 505, Toronto, ON, M5G 1M1, Cana — [7]Research Institute for Interdisciplinary Science, Okayama University, Okayama 700-8530, Japa

We investigate all six structurally characterized chromium-based breathing pyrochlores using a combination of density functional theory and pseudofermion functional renormalization group calculations. We show that the variety of chemical compositions leads to distinct magnetic behavior due to the different pyrochlore Hamiltonians realized. We discuss especially the line-like degeneracies in momentum space found in sulfide compounds and an approximate spiral spin liquid in a selenide material. The root cause for these effects are longer-rage exchange couplings up to third nearest neighbor type.

TT 25: Skyrmions I (joint session MA/TT)

Time: Tuesday 9:30–13:00 Location: POT 6

Invited Talk TT 25.1 Tue 9:30 POT 6

Emergent electromagnetic response of nanometer-sized spin textures — •Max Hirschberger — Department of Applied Physics, University of Tokyo, Bunkyo-ku 113-8656, Japan — RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan

A wide array of experimental techniques in condensed matter, including resonant elastic x-ray scattering and real-space imaging using Lorentz transmission electron microscopy, were incorporated to establish the presence of nanometer-sized skyrmion lattices in the new centrosymmetric materials Gd_2PdSi_3 and $Gd_3Ru_4Al_{12}$, with Heisenberg Gd^{3+} magnetic moments and competing interactions. When a conduction electron moves through a topological spin texture, it acquires a quantum mechanical phase (Berry phase) which can strongly modify the dynamical properties of the electron gas. The tiny topological spin textures (skyrmions) in Gd_2PdSi_3 and $Gd_3Ru_4Al_{12}$ are expected to give rise to a giant emergent magnetic field B_{em} of order 500 Tesla. We have recently found quantitative evidence for B_{em} using electrical Hall measurements and thermoelectric properties such as the topological Nernst effect. Ongoing work is focused on the tuning of magnetic interactions in these materials via chemical substitution; moreover, we are employing element-specific resonant x-ray scattering techniques to study the coupling between local moments and conduction electrons in this new class of skyrmion host.

TT 25.2 Tue 10:00 POT 6

Skyrmions in $SrRuO_3$ based heterostructures in tilted magnetic fields? — •Sven Esser[1], Sebastian Esser[1], Anton Jesche[1], Vladimir Roddatis[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Augsburg University, D-86159 Augsburg, Germany — [2]Interface Geochemistry, Helmholtz Centre Potsdam, 14473 Potsdam, Germany

Formation of Néel-type skyrmions at oxide interfaces is supported by Dzyaloshinskii-Moriya (DM) interaction through introducing a breaking of the 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].

Utilizing metal-organic aerosol deposition 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. A contribution of the topological Hall effect to the Hall resistance can be observed for temperatures between 10K and 80K, which may hint at the formation of skyrmions.

Measurements of the angular-dependent Hall resistivity display additional contributions that are not observed in pure SRO thin films and thus most likely related to the SRO/SIO interface.

[1] J. Matsuno *et al.*, Science Adv. **2** (2016) e1600304.

TT 25.3 Tue 10:15 POT 6

Intrinsic stability of magnetic anti-skyrmions in tetragonal inverse Heuslers — •Rana Saha[1], Tianping Ma[1], Abhay K. Srivastava[1], Ankit Sharma[1], Jagannath Jena[1], Vivek Kumar[2], Praveen Vir[2], Claudia Felser[2], and Stuart Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

One of the major topics in spintronics today is the study of chiral non-collinear spin textures of various topologies. Recently, a novel chiral spin texture, magnetic anti-skyrmion that has distinct topological features from that of Bloch and Néel skyrmions, was discovered in tetragonal inverse Heusler, $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Anti-skyrmions have boundaries (the in-plane magnetization region between magnetization pointing up and pointing down) that have a complex structure consisting of successive left hand Bloch, left hand Néel, right hand Bloch, and right hand Néel wall segments. This complex structure is a result of an anisotropic Dzyaloshinskii-Moriya exchange interaction that is set by the symmetry of the underlying lattice. Interestingly, magnetic anti-skyrmions are stable over a wide range of temperature, magnetic field and thickness of the lamella in which they are formed [2]. In this presentation, I will discuss our recent in-situ Lorentz and magnetic force microscopic studies of nucleation, stabilization and size manipulation of anti-skyrmions in tetragonal inverse Heuslers.

[1]Nayak *et al.*, Nature **548**, 561 (2017).
[2]Saha *et al.*, Nat. Commun. **10**, 5305 (2019).

TT 25.4 Tue 10:30 POT 6

Crystal Hall effect in an ultrathin film of $SrRuO_3$(SRO) grown on $SrTiO_3$(STO)[001]: A case of collinear antiferromagnetic insulator — •Kartik Samanta[1], Marjana Ležaić[1], Stefan Blügel[1], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg-University Mainz, 55128 Mainz, Germany

Motivated by the recently observed topological Hall effect in ultra-thin films of SRO grown on STO(001) substrate, we investigate the magnetic ground state and anomalous Hall response of the SRO ultra-thin films by virtue of spin density functional theory(DFT). Our findings reveal that in the monolayer limit of SRO film, large energy level splitting of Ru-t_{2g} states, stabilizes an anti-ferromagnetic insulating magnetic ground state. For the doped insulating state, our calculated electronic transport properties based on Berry curvature analysis show a large Hall response. From the systematic investigation of our results, we find that the large Hall effect is due to a combination of broken time-reversal and crystal symmetries caused by the arrangement of non-magnetic atoms (Sr and O) in the mono-layer of SRO thin film. We identify the emergent Hall effect as a clear manifestation of the so-called crystal Hall effect [1] occurring in compensated antiferromagnets.

We acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 "Skyrmionics" and the Jülich Supercomputing Center(project JIFF40).

[1] L. Šmejkal, *et al.*; arXiv:1901.00445 (2019)

TT 25.5 Tue 10:45 POT 6

Topological Hall effect in thin films of tetragonal inverse Heusler compounds — •Anastasios Markou[1], Peter Swekis[1], Jacob Gayles[1], Dominik Kriegner[1,2], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden

Spin chirality in metallic materials with noncoplanar spin structure gives rise to a Berry phase induced topological Hall effect (THE). Topologically stable nontrivial spin structures, such as skyrmions and antiskyrmions exhibit THE. The THE is a transverse response to an applied current that can be used to distinguish magnetic textures for device applications, such as the racetrack memory. We focus on the Heusler compounds with D_{2d} symmetry [1,2], which recently found to host antiskyrmions [2]. We present the structural, magnetic, and transport properties in thin films of the tetragonal Mn_xPtSn (x=1.4-2.1) and Mn_2RhSn Heusler compounds. We find that the THE appears below spin reorientation temperature, and together with the anomalous Hall effect are strongly dependent on the composition and thickness of the films.

[1]O. Meshcheriakova *et al.*, Phys. Rev. Lett. **113**, 087203 (2014).
[2]A. K. Nayak *et al.*, Nature **548**, 561-566 (2017).

TT 25.6 Tue 11:00 POT 6

Skyrmions in Ta/CoFeB-wedge/MgO — •Christian Denker[1], Hauke Heyen[1], Sören Nielsen[2], Malte Römer-Stumm[2], Nina Meyer[1], Neha Jha[1], Kornel Richter[2], Enno Lage[2], Markus Münzenberg[1], and Jeffrey McCord[2] — [1]Institut für Physik, Universität Greifswald, Germany — [2]Nanoscale Magnetic Materials - Magnetic Domains, Institute for Materials Science, Universität Kiel, Germany

We investigate different generation approaches as well as pinning center distribution and strength for magnetic skyrmions in Ta/CoFeB-wedge/MgO trilayers. Skyrmions appear as a part of the out-of-plane hysteresis or using pulsed in-plane fields and zero-field stable skyrmions result from tilted in-plane remanent magnetic field application. Furthermore, we investigate energy landscapes for skyrmions by current-induced hopping motion in a stripe with regions of different defect types and densities, since skyrmion motion tracking allows us to access the pinning center distribution and strength.

15 min. break.

TT 25.7 Tue 11:30 POT 6

Impact of light and heavy single atomic defects on single magnetic skyrmions — •Imara Lima Fernandes and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Incorporating magnetic skyrmions as future bits of information technology is challenged by the unavoidable defects inherent to any device. Recently, the universality of the skyrmion-defect interaction profiles for the 3*d* and 4*d* elements was established [1], which is mainly dictated by the defect-induced changes in the magnetic exchange interactions. Those defects can be used to enhance the skyrmions detection using all-electrical means via the spin-mixing magnetoresistance (XMR) [2,3]. In the current study based on a full *ab initio* approach, we explore impurities from various parts of the periodic table, which enable different mechanisms determining the skyrmion-defect interactions. We address systematically the case of vacancies, *sp* and 5*d* elements in order to find correlations between their chemical nature and the energetics as well as the electronic properties of skyrmions generated in Pd/Fe/Ir(111) surface.

– Funding provided by the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (ERC-consolidator grant 681405 - DYNASORE).

[1] I. Lima Fernandes *et al.*, Nature Commun. **9**, 4395 (2018).
[2] I. Lima Fernandes *et al.*, arXiv:1906.08838, (2019)
[3] D. M. Crum *et al.*, Nature Commun. **6**, 8541 (2015)

TT 25.8 Tue 11:45 POT 6

Beyond Skyrmions Utilizing alternative magnetic quasiparticles for spintronics devices — •Börge Göbel[1,2], Oleg Tretiakov[3], Stuart S. P. Parkin[2], and Ingrid Mertig[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [3]School of Physics, The University of New South Wales, Sydney, Australia

Skyrmions are considered as the bits in future spintronic devices like the racetrack storage. One issue, which is hindering the realization of this application, is the so-called skyrmion Hall effect: A skyrmion does not move parallel to an applied spin-polarized current. Instead, the skyrmion is pushed towards the edge of the sample where it annihilates. In this talk, I will give an overview about observed or proposed alternative magnetic quasiparticles. The stabilization, as well as the emergent electrodynamic effects will be discussed for the antiskyrmion, the antiferromagnetic skyrmion, the skyrmionium, and the bimeron. These magnetic objects are either attractive from a fundamental point of view, or are advantageous application-wise.

[1] B. Göbel, A. Mook, J. Henk, I. Mertig. PRB 96, 060406(R) (2017) [2] B. Göbel, A. Schäffer, J. Berakdar, I. Mertig, S. Parkin. Sci. Rep. 9, 12119 (2019) [3] B. Göbel, A. Mook, J. Henk, I. Mertig, O. Tretiakov. PRB 99, 060407(R) (2019) [4] B. Göbel, J. Henk, I. Mertig. Sci. Rep. 9, 9521 (2019)

TT 25.9 Tue 12:00 POT 6

Observation of anti-skyrmions in $Mn_2Rh_{0.95}Ir_{0.05}Sn$ Heusler compound — •Jagannath Jena[1], Rolf Stinshoff[2], Rana Saha[1], Abhay K. Srivastava[1], Tianping Ma[1], Hakan Deniz[1], Peter Werner[1], Claudia Felser[2], and Stuart S. P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

Magnetic anti-skyrmions are topologically protected nanoscopic chiral spin textures. They are composed of alternating boundary of Bloch and Néel domain walls. Recently anti-skyrmions have been discovered in a ferromagnetic tetragonal inverse Heusler compound $Mn_{1.4}Pt_{0.9}Pd_{0.1}Sn$ [1]. Here we report the observation of anti-skyrmions in a ferrimagnetic Heusler compound $Mn_2Rh_{0.95}Ir_{0.05}Sn$

using Lorentz transmission electron microscopy. This compound has a lower magnetic moment which orders at 270 K. Our results may pave the way to search for antiskyrmions in a ferrimagnetic material with a very low magnetic moment for future spintronic applications. [1]Nayak *et al.*, Nature **548**, 561 (2017).

TT 25.10 Tue 12:15 POT 6

B20-type MnSi films on Si (111) grown by flash lamp annealing — •Zichao Li[1,2], Yufang Xie[1,2], Viktor Begeza[1,2], Ye Yuan[1,3], Lars Rebohle[1], Manfred Helm[1,2], Kornelius Nielsch[2,4], Slawomir Prucnal[1], 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 — [3]Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, People's Republic of China — [4]Institute for Metallic Materials, IFW-Dresden, Dresden, 01069, Germany

B20-type MnSi is one of the noncentrosymmetric materials hosting magnetic skyrmions, which are promising information carriers in spintronic devices. In this work, we report the preparation of (111)-textured MnSi films on Si substrates. The preparation method only includes the deposition of Mn layers at room temperature and a following process by flash lamp at milli-second. By controlling the thickness of Mn layers and flash energy, we can obtain pure MnSi or mixtures of MnSi and MnSi1.7. Surprisingly, all prepared films show Curie temperatures around 41 K, which is much higher than for bulk MnSi or films reported previously. Magnetic skyrmions are stabilized at the whole temperature range below 41 K and under a much wider magnetic-field range. We speculate that the increased Curie temperature is due to the strain in the MnSi films arising from the MnSi1.7 phase or from the substrate. Our work calls a re-examination of the structural and magnetic properties of B20 MnSi films.

TT 25.11 Tue 12:30 POT 6

Universality of energy barriers of large magnetic skyrmions — •Jan Masell — Center for Emergent Matter Science RIKEN, Wako, Saitama, Japan

Magnetic skyrmions can only decay via singular spin configurations. We analyze the corresponding energy barriers of skyrmions for two distinct stabilization mechanisms, i.e., Dzyaloshinskii-Moriya interaction (DMI) and competing interactions [1]. Based on our numerically calculated collapse paths on an atomic lattice, we derive analytic expressions for the saddle-point textures and energy barriers of large skyrmions. The sign of the spin stiffness and the sign of fourth-order derivative terms in the classical field theory determines the nature of the saddle point and thus the height of the energy barrier. In the most common case for DMI-stabilized skyrmions (positive stiffness and negative fourth-order term) the saddle-point energy approaches a universal upper limit described by an effective continuum theory. For skyrmions stabilized by frustrating interactions, the stiffness is negative and the energy barrier arises mainly from the core of a singular vortex configuration.

[1] B. Heil, A. Rosch, and J. Masell, Phys. Rev. B 100, 134424 (2019)

TT 25.12 Tue 12:45 POT 6

The Chimera skyrmion collapse mechanism in harmonic transition state theory — •Stephan von Malottki[1], Pavel F. Bessarab[2,3], and Stefan Heinze[1] — [1]Institute of Theoretical Physics and Astrophysics, University of Kiel — [2]University of Iceland, Reykjavík, Iceland — [3]ITMO University, St. Petersburg, Russia

Recent studies reveal a new skyrmion annihilation mechanism via the Chimera skyrmion state [1-3]. We study the skyrmion lifetimes for this collapse mechanism in the ultrathin film system Pd/Fe/Ir(111) by a combination of nudged elastic band method calculations and harmonic transition state theory, based on an atomistic spin model parametrised from density functional theory [4]. The skyrmion lifetime has the form of an Arrhenius law and requires the energy barriers and prefactors of all relevant collapse mechanisms [5,6]. We address the crossover from the radial symmetric skyrmion collapse to the Chimera mechanism as well as the challenge of identifying and treating new Goldstone modes correctly.

[1] Meyer *et al.*, Nat. Commun. **10**, 3823 (2019)
[2] Heil *et al.*, Phys. Rev. B **100**, 134424 (2019)
[3] Desplat *et al.*, Phys. Rev. B **99**, 174409 (2019)
[4] von Malottki *et al.*, Sci. Rep. **7**, 12299 (2017)
[5] Bessarab *et al.*, Sci. Rep. **8**, 3433 (2018)
[6] von Malottki *et al.*, Phys. Rev. B **99**, 060409(R) (2019)

TT 26: Complex Oxides: Surfaces and Interfaces (joint session TT/MA/HL)

Time: Tuesday 14:00–15:45 Location: HSZ 02

TT 26.1 Tue 14:00 HSZ 02

Ultradense tailored vortex pinning arrays in $YBa_2Cu_3O_{7-\delta}$ thin films created by He ion beam irradiation — •Max Karrer[1], Bernd Aichner[2], Benedikt Müller[1], Vyacheslav Misko[3], Kristijan L. Mletschnig[2], Meirzhan Dosmailov[4], Johannes D. Pedarnig[4], Franco Nori[3], Reinhold Kleiner[1], Wolfgang Lang[2], and Dieter Koelle[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Germany — [2]Faculty of Physics, University of Vienna, Austria — [3]Theoretical Quantum Physics Group, RIKEN Cluster for Pioneering Research, Wako-shi, Saitama, Japan — [4]Institute of Applied Physics, Johannes Kepler University Linz, Austria

Magnetic fields penetrate a type II superconductor as magnetic vortices. In a clean superconductor they arrange in a hexagonal lattice; by addition of artificial pinning sites many other arrangements are possible. With a focused He ion beam, we fabricate periodic patterns of pinning sites with spacings down to 70 nm in $YBa_2Cu_3O_{7-\delta}$ thin films. In ultradense kagomé-like patterns, magnetic caging of vortices results in unconventional commensurability effects, yielding peaks in the critical current and minima in the resistance versus applied field up to ∼ 0.4 T. The various vortex patterns at different magnetic fields are analyzed by molecular dynamics simulations of vortex motion, and the magnetic field dependence of the critical current is confirmed. These findings open the way for a controlled manipulation of vortices in cuprate superconductors by artificial sub-100 nm pinning landscapes.

[1] B. Aichner *et al.*, ACS Appl. Nano Mater. **2**, 5108–5115 (2019).

TT 26.2 Tue 14:15 HSZ 02

Strain-dependent electronic reconstruction in Sr_2CoIrO_6 double perovskite from DFT+U+SOC calculations — •Jiongyao Wu and Rossitza Pentcheva — Department of Physics and Center for Nanointegration (CENIDE) Universitat Duisburg-Essen, Duisburg, Germany

The double perovskite Sr_2CoIrO_6 (SCIO) can be regarded as a (111)-superlattice of alternating $SrIrO_3$ (SIO) and $SrCoO_3$ (SCO) layers. Here we explore the electronic and magnetic properties in the framework of density functional theory (DFT) including a Hubbard U term and spin-orbit coupling (SOC) with the PBEsol exchange correlation functional. While the end member SIO is metallic with a quenched spin and orbital moment and bulk SCO is a G-type antiferromagnetic (AFM) insulator with spin and orbtial moment of 2.7 and 0.26 μ_B, respectively, the double perovskite SCIO emerges as an AFM Mott insulator with a band gap of ∼ 500 - 600 meV. Additionally, Ir acquires a spin moment of 1.5 μ_B pointing towards a $j = 1/2$ Mott insulating state in SCIO, similar to other iridates. Analysis of the orbital occupation indicates substantial charge transfer from the Ir to the Co ion. Moreover, subtle changes in orbital occupation are observed as the strain is varied from compressive ($a_{\mathrm{NdGaO_3}}$) to tensile ($a_{\mathrm{SrTiO_3}}$).

We acknowledge funding by the German Science Foundation within CRC/TRR80, project G3.

TT 26.3 Tue 14:30 HSZ 02

Sensitivity of non-local fluctuations on surface effects in ultrathin $SrVO_3$ films — •Matthias Pickem, Jan M. Tomczak, and Karsten Held — Institute of Solid State Physics, TU Wien, Austria

Recent experiments show that strong electronic correlations cause the conventional Fermi-liquid state of bulk $SrVO_3$ to be destroyed in films below a critical thickness. However new experimental results challenge the current understanding of the details of this breakdown.

To this end we perform realistic density functional theory (DFT)

+ dynamical mean-field theory (DMFT) calculations of $SrVO_3$ on $SrTiO_3$ substrate. Depending on the simulated interface ($SrVO_3$ termination, surface reconstructions, or additional $SrTiO_3$ capping) we find that different mechanism cause this aforementioned break-down of the Fermi-liquid state.

Furthermore, calculations on the two-particle level (DMFT susceptibilities) reveal that the different interfaces result in vastly different instabilities.

TT 26.4 Tue 14:45 HSZ 02

Planar GHz resonators on $SrTiO_3$: Suppressed losses at temperatures below 1 K — Vincent T. Engl, Nikolaj G. Ebensperger, Lars Wendel, and •Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany

The complex dielectric constant $\hat{\epsilon} = \epsilon_1 + i\epsilon_2$ of $SrTiO_3$ reaches high values $\epsilon_1 \approx 2 * 10^4$ at cryogenic temperatures, while the dielectric losses (ϵ_2) are much stronger than for other crystalline dielectrics. $SrTiO_3$ is a common substrate for oxide thin films, like the superconducting $LaAlO_3/SrTiO_3$ system, but the large ϵ_1 and ϵ_2 restrict high-frequency quantum devices on $SrTiO_3$. Here we present superconducting coplanar Nb resonators on $SrTiO_3$, which we successfully operate in a distant-flip-chip geometry [1] at frequencies that exceed 1 GHz. We find a pronounced and unexpected increase in resonator quality factor Q at temperatures below 1 K, reaching up to $Q \approx 800$. We attribute this to substantial changes of the dielectric losses in $SrTiO_3$ at mK temperatures, and we also detect non-monotonous changes in the temperature-dependent ϵ_1. These findings [2] challenge our present understanding of the dielectric properties of $SrTiO_3$ and at the same time demonstrate that cryogenic high-frequency devices on $SrTiO_3$ are more feasible than previously assumed.

[1] L. Wendel *et al.* arXiv:1911.10518 [cond-mat.supr-con]
[2] V. T. Engl *et al.* arXiv:1911.11456 [cond-mat.supr-con]

TT 26.5 Tue 15:00 HSZ 02

Tuning superconductivity at the $Al_2O_3/SrTiO_3$-interface with light — •Daniel Arnold, Dirk Fuchs, and Roland Schäfer — Institute for Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

The 2-DEG at $SrTiO_3$-based interfaces is sensitive to illumination with visible light [1], which at low temperatures can be used to tune the transition temperature of the superconducting state in a nonvolatile manner [2]. We present studies on an $Al_2O_3/SrTiO_3$ sample with micro bridges running along different crystallographic directions at the interface. We are able to tune the low temperature conductance by illuminating the sample and reverse the altered state by thermal treatment at low temperatures ($T < 15$ K). Transport measurements in dependence of the magnetic field and temperature are conducted in different states, characterized by the tunable but time independent resistance at 1 K. The Berezinskii-Kosterlitz-Thouless transition in this system can be addressed by the current voltage behavior, which simultaneously gives further information on the inhomogeneous nature of the superconducting phase.

[1] M. Yazdi-Rizi et al., PRB 95 (2017)
[2] D. Arnold et al., APL 115 (2019)

TT 26.6 Tue 15:15 HSZ 02

Crystalline anisotropy of magnetoresistance in LAO/STO nanostructures — •Mithun Sheena Prasad[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 $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) provides new opportunities to explore Nano electronic devices. In our group we have developed an industry compatible Nano patterning technique [1] for the LAO/STO interface. Recent studies on this interface have revealed that at low temperature the current is confined to filaments which are linked to structural domain walls in the STO with drastic consequences for example for the temperature dependence of local transport properties. We have investigated magneto-transport in nanostructures having different orientation with respect to the lattice. Our experiments show that not only the resistance but also the magnetoresistance varies with orientation. The magnetoresistance can even change sign for different orientations and again this can change after a warm-up cool-down cycle strongly supporting the model of filamentary charge transport.

[1] M. Z. Minhas, H. H. Blaschek, F. Heyroth, and G. Schmidt, AIP Advances 6, 035002 (2016)

TT 26.7 Tue 15:30 HSZ 02

Study of 2D superconductivity at oxide interfaces by microwave resonators — •Edouard Lesne[1], Yildiz Saglam[1], Daniel Bothner[1], Felix Schmidt[1], Marc Gabay[2], Gary Steele[1], and Andrea Caviglia[1] — [1]Delft University of Technology — [2]Université Paris-Saclay

The emergent two-dimensional electron system (2DES) formed at the interface between LaAlO3 (LAO) and SrTiO3 (STO) insulating oxides has been a subject of great interest in condensed matter physics during the last decade. Recently, (111)-oriented LAO/STO interfaces have been shown to exhibit an electronic correlation driven reconstruction of its band structure and a two-dimensional superconducting (SC) ground state, both tunable by electrostatic field-effect.

Superconducting coplanar waveguide (SCPW) resonators are tools of exquisite sensitivity for probing low energy excitations in quantum materials, due to their intrinsic low ohmic losses and high quality factors, highly relevant to quantum technology platforms. Here, in order to study the superconducting state at the LAO/STO(111) interface, we designed embedded SCPW resonators whose microwave resonance frequency can be tuned by electrostatic gating, manifesting a change of the 2DES superfluid density through a large change of its kinetic inductance. This allows us to map the SC phase diagram in a detection scheme that goes beyond traditional resistive measurements. Our work highlights the potential of such an approach to the fundamental study of superconductivity in complex materials.

TT 27: Topological Semimetals 2

Time: Tuesday 14:00–15:45 Location: HSZ 103

TT 27.1 Tue 14:00 HSZ 103

Deformation of the Fermi surface of NbP under uniaxial strain — •Clemens Schindler, Jonathan Noky, Marcus Schmidt, Claudia Felser, and Johannes Gooth — Max Planck Institut für Chemische Physik fester Stoffe, Dresden, Deutschland

The Weyl semimetal NbP has recently gained a lot of attention due to its peculiar magnetotransport properties. The low cyclotron masses and long relaxation times in the cleanest single-crystalline samples give rise to an extremely large magnetoresistance and pronounced Shubnikov-de Haas (SdH) oscillations at moderate magnetic fields. In this study, we report on the study of the SdH oscillations under uniaxial strain using a three-piezo stack apparatus, combined with ab initio calculations of the band structure. We demonstrate the breaking of fourfold degenerate electron and hole pockets into twofold degenerate ones due to the breaking of the underlying fourfold rotational symmetry of the lattice. The direct, reversible application of uniaxial strain to materials with a sensitive Fermi surface therefore opens a playground for the symmetry manipulation of the electronic waves, in contrast to the application of hydrostatic pressure as well as the indirect determination of the strain dependence of the Fermi surface via magnetostriction oscillations.

TT 27.2 Tue 14:15 HSZ 103

Shubnikov-de Haas oscillations in the Weyl type-II semimetal WTe_2 — •Jasper Linnartz[1], Claudius Müller[1], Martin Bremholm[2], Nigel Hussey[1], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), IMM, Radboud University, Nijmegen, the Netherlands — [2]Department of Chemistry and iNANO, Aarhus University, Aarhus, Denmark

The transition metal dicalcogenide WTe_2 in the Td phase is a Weyl type-II semimetal. By analyzing the Shubnikov-de Haas oscillations superimposed on the quadratic magnetoresistance in WTe_2 up to 30 T and their temperature-dependent amplitude, we determine the Fermi surface and extract the cyclotron masses of the individual pockets.

Following the high resolution quantum oscillation thermopower experiments [1], we determined in total four individual pockets. Above a threshold magnetic field, we discover orbits due to magnetic breakdown due to nested electron and hole pockets which is confirmed by a cyclotron mass analysis.

[1] Z. Zhu et al., Phys. Rev. Lett. 114, 176601 (2015)

TT 27.3 Tue 14:30 HSZ 103

Disorder-induced coupling of Weyl nodes in WTe_2 — •Steffen Sykora[1], Johannes Schoop[1], Bernd Büchner[1,2,3], Christian Hess[1,3], Romain Giraud[1,4], and Joseph Dufouleur[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 — [4]Universite Grenoble Alpes, CNRS, CEA, Grenoble-INP, INAC-Spintec, F-38000 Grenoble, France

We consider theoretically the finite coupling between Weyl nodes due to residual disorder. The results are compared with quantum transport measurements in a WTe_2 nanoflake where the transport time (backscattering) is related to the quantum life time (elastic mean free path) giving evidence for the anisotropic scattering of quasiparticles. Scattering processes within the material specific band structure are evaluated using a renormalization method allowing us to infer a rather short correlation length ($\xi \sim 5$ nm) of the disorder, in agreement with an analytical approach neglecting scattering between different pockets. Our finding indicates that, if intra-node scattering is dominating over inter-node scattering, the coupling between Weyl nodes is significant, a key issue for the observation of many topological properties.

TT 27.4 Tue 14:45 HSZ 103

Anisotropic magnetoresistance and the planar Hall effect in antiperovskite thin films — •Dennis Huang[1], Hiroyuki Nakamura[2], and Hidenori Takagi[1,3,4] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of Arkansas, Fayetteville, Arkansas 72701, USA — [3]University of Stuttgart, 70569 Stuttgart, Germany — [4]University of Tokyo, 113-0033 Tokyo, Japan

Anisotropic magnetoresistance (AMR) and the planar Hall effect (PHE) have garnered increasing attention as probes of the chiral anomaly in Dirac and Weyl semimetals, or helical surface states in topological insulators. However, these techniques are sensitive to additional effects, such as orbital magnetoresistance, and a more detailed understanding of such contributions is needed. Here, we measure AMR and the PHE in thin films of the antiperovskite Sr_3SnO grown by molecular beam epitaxy. Sr_3SnO is predicted to host both massive 3D Dirac fermions and topological surface states protected by mirror symmetry. We investigate the dependence of AMR and the PHE on magnetic field, temperature and film thickness, as well as their relationship to weak (anti)localization.

TT 27.5 Tue 15:00 HSZ 103

Magneto-optical study of the Dirac semimetal Cd_3As_2 in Voigt geometry — •Seulki Roh[1], Ece Uykur[1], Tobias Biesner[1], Lucky Maluna[1], Alex Nateprov[2], Martin Dressel[1], and Artem Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Academiei str. 5, 2028 Chisinau, Moldova

The three-dimensional Dirac semimetals possess Dirac points, which can be considered as a superposition of two Weyl points in reciprocal space. Under a magnetic field, the spin degeneracy can be lifted and a pair of Weyl points with opposite chiralities connected by a zeroth Landau level appears, enabling the charge transfer between the two Weyl points - the so-called chiral pumping effect. In this study, Cd_3As_2 was investigated by optical spectroscopy under external static magnetic field, **B**. The Voigt geometry was employed to parallelize the electric field of incident light, **E**, and the static magnetic field. In the **E** perpendicular to **B** configuration, we observed a pronounced Voigt resonance due to the splitting of the plasma edge. In the $\mathbf{E} \parallel \mathbf{B}$ geometry, we detected an increase of the Drude spectral weight, which could be caused by the chiral pumping effect. In the talk, we will discuss the possible relation between this effect and our observations in more detail.

TT 27.6 Tue 15:15 HSZ 103

Field-induced electron-hole tunneling in nodal-line semimetals revealed by quantum oscillations — •Claudius Müller[1], Thomas Khouri[1], Maarten van Delft[1], Sergio Pezzini[1], Yu-Te Hsu[1], Maxim Breitkreiz[2], Leslie Schoop[3], Antony Carrington[4], Nigel Hussey[1], and Steffen Wiedmann[1] — [1]High Field Magnet Laboratory (HFML-EMFL), IMM, Radboud University, Nijmegen, the Netherlands — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, Germany — [3]Department of Chemistry, Princeton University, New Jersey, USA — [4]H. H. Wills Physics Laboratory, University of Bristol, UK

We report an investigation of de Haas-van Alphen quantum oscillations in the nodal-line semimetal ZrSiS via capacitive magnetometry measurements in high magnetic fields up to 35 T. By carrying out a full angle dependence, we are able to determine the Fermi surface (FS) of ZrSiS which complements but extends the original Shubnikov-de Haas measurements reported in [1]. For H//c, we observe a complex oscillation spectrum originating from individual electron and hole pockets, as well as oscillations caused by magnetic breakdown (MB). The MB orbits can be seen as a manifestation of Klein tunneling in momentum space, first reported in HfSiS [2], although in a regime of partial transmission due to a small spin-orbit gap between adjacent pockets. Comparison of our experimental observations with theoretical predictions provides us with a full picture of the electronic ground state.

[1] S. Pezzini et al., Nature Physics 14, 178 (2018)
[2] M. van Delft et al., Phys. Rev. Lett. 121, 256602 (2018)

TT 27.7 Tue 15:30 HSZ 103

Magneto-optical probe of the fully gapped Dirac band in ZrSiS — •E. Uykur[1], L. Z. Maulana[1], L. M. Schoop[2], B. V. Lotsch[3,4], M. Dressel[1], and A. V. Pronin[1] — [1]1. Physikalishces Institut, Universität Stuttgart, 70569, Stuttgart, Germany — [2]Department of Chemistry, Princeton University, Princeton, NJ, 08544, USA — [3]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [4]Chemistry Department, University of Munich (LMU), 81377 München, Germany

In this study, we present a far-infrared magneto-optical study of gapped nodal-line semimetal ZrSiS in the magnetic fields up to 7 T. Surprisingly, the magneto-optical spectra of ZrSiS can be explained within a simple 2D gapped-Dirac band model. Results demonstrate the inter- and intra-band transitions developing as $\sqrt{B}$ with increasing B-field. The gap and Fermi velocity parameters can be extracted from the magneto-optical study are also consistent with the literature for the mentioned compound. Considering the average response over the Fermi surface is reflected in the optical studies, the narrow distribution of the parameters is expected. Finally, we will present a peculiar field-independent feature appearing in the spectra that might be related to the nodal-line nature of ZrSiS.

TT 28: Twisted Bilayer Graphene (joint session TT/HL)

Time: Tuesday 14:00–15:45 Location: HSZ 201

TT 28.1 Tue 14:00 HSZ 201

Valley splitter and transverse valley focusing in twisted bilayer graphene — •Christophe De Beule[1], Peter Silvestrov[1], Ming-Hao Liu[2], and Patrik Recher[1,3] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [3]Laboratory for Emerging Nanometrology, 38106 Braunschweig, Germany

We study transport through electrostatic barriers in twisted bilayer graphene and show that for certain configurations, electrons from the K (K') valley are transmitted only to the top (bottom) layer, leading to valley-layer locked bulk currents. We show that such a valley splitter is obtained when the potential varies slowly on the Moiré scale and the Fermi energy in the barrier exceeds the kinematic barrier between Dirac electrons from the top and bottom layer. Furthermore, we show that for a given valley the current is transversely deflected, as time-reversal symmetry is broken in each valley separately, resulting in valley-selective transverse focusing at zero magnetic field.

TT 28.2 Tue 14:15 HSZ 201

Quantum capacitive coupling in large-angle twisted graphene layers — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

Magic-angle twisted bilayer graphene (tBLG) has revealed exotic physics of strong correlation in graphene systems and attracted enormous attention on twistronics of 2D materials. In the opposite extreme of large twist angles, relatively less attention has been paid. Due to the required large momentum change, scattering between different graphene layers of large-angle tBLG is forbidden. Through quantum capacitance of individual graphene layers, however, tBLG is electrostatically coupled, though electronically decoupled. Here, I introduce a self-consistent electrostatic model for carrier densities in decoupled tBLG systems and apply the model to perform quantum transport simulations for a recent experiment on a dual-gated large-angle tBLG device [1]. Good agreement between the experiment and theory confirms the electronic decoupling and indicates that the decoupled large-angle tBLG can be the thinnest parallel-plate capacitor in the world. The model can be further generalized to multi-layer systems composed of decoupled graphene sheets.

[1] P. Rickhaus *et al.*, arXiv:1907.00582 (2019).

TT 28.3 Tue 14:30 HSZ 201

Skyrmion lattices in twisted bilayer graphene — •Thomas Bömerich, Lukas Heinen, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

We investigate the groundstate properties of magnetic skyrmions in anomalous Quantum Hall (AQH) systems. In these systems, the topological charge density, which characterizes the winding of a skyrmion, is directly proportional to the electric charge density. Therefore magnetic skyrmions are electrically charged excitations stabilized by Coulomb interactions between each other. At finite densities the skyrmions form regular lattices and can be controlled by external gate voltages. Our theory can be applied to twisted bilayer graphene as there is experimental evidence of ferromagnetic order and an AQH effect at specific fillings.

Starting from a free energy functional, we solve some limiting cases analytically and use micromagnetic simulations to study the lattice structure as a function of skyrmion density and skyrmion radius. From this we obtain a phase diagram with different skyrmion lattices. In particular we analyse the groundstate and its symmetries without external magnetic field. Additionally, we calculate the total magnetization as a function of skyrmion density, which can be used to detect experimental signatures of skyrmions in AQH systems.

TT 28.4 Tue 14:45 HSZ 201

Magnetism of magic-angle twisted bilayer graphene — •Javad Vahedi[1,2], Andreas Honecker[2], Robert Peters[3], and Guy Trambly de Laissardière[2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany — [2]Laboratoire de Physique Théorique et Modélisation, Université de Cergy-Pontoise, France — [3]Department of Physics, Kyoto University, Japan

Recently, correlated insulators and superconductivity have been discovered experimentally in twisted bilayer graphene (TBG) [1]. The Moiré pattern of the bilayers at so-called “magic angles” leads to localization of the low-energy electrons in the AA-stacking regions, reflected by very flat regions in the band structure [2]. This reduction of the kinetic energy enhances the relative importance of interactions and thus renders the bilayer systems much more susceptible to correlation effects than a single layer. We investigate the magnetic instabilities at half filling in TBG using a real-space Hartree-Fock and RPA analysis. We find that at charge neutrality an antiferromagnetic state localized in the AA region emerges for values of the Coulomb interaction U that are an order of magnitude smaller than what would be required to render an antiferromagnetic state in a single graphene sheet. Furthermore, doping of a few electrons per Moiré unit cell pushes the system into a ferromagnetic phase.

[1] Y. Cao *et al.*, Nature **556**, 80 (2018); Nature **556**, 43 (2018)
[2] G. Trambly de Laissardière *et al.*, Nano Letters **10**, 804 (2010)

TT 28.5 Tue 15:00 HSZ 201

Quantum diffusion in twisted bilayer graphene — •Guy Trambly de Laissardière[1], Omid Faizy Namarvar[2,3], Ahmed Missaoui[1], Javad Vahedi[1,4], Andreas Honecker[1], Laurence Magaud[2], and Didier Mayou[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Univ. de Cergy-Pontoise, France — [2]Institut Néel, CNRS, Univ. Grenoble Alpes, France — [3]XLIM, Univ. Limoges, CNRS (UMR 7252), Limoges, France — [4]Department of Physics and Earth Sciences, Jacobs University Bremen, Germany

It has been shown theoretically and experimentally that twisted bilayer graphenes (TBG), forming Moiré patterns, confine electrons in a tunable way as a function of the angle of rotation of one layer with respect to the other. Since 2018 the discovery of correlated insulators and superconductivity at so-called "magic angles" has stimulated an avalanche of experimental and theoretical activities. In the framework of the Kubo-Greenwood formula for the conductivity, we present tight-binding calculations of quantum diffusion properties in TBG at various angles including the first magic angle. We analyze in particular the effect of static defects, the effect of an electric bias and electron-electron interactions. One of the main results is the decisive role of inter-band transitions [1] in the conductivity of TBG at the magic angle.

[1] G. Trambly de Laissardière et al., Phys. Rev. B **93**, 235135 (2016).

TT 28.6 Tue 15:15 HSZ 201

Fractional quantum Hall states for Moiré superstructures in the Hofstadter regime — •Bartholomew Andrews and Alexey Soluyanov — Department of Physics, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

We apply a perpendicular magnetic field to the minimal effective two-orbital Fermi-Hubbard model based on a description of the low-energy physics of twisted bilayer graphene at the first magic angle. Through the use of a Peierl’s substitution, we determine the Landau level splitting and study the structure of the resulting Chern bands for a range of magnetic flux per plaquette. We identify isolated, topological, and flat bands in the spectrum at low energies. We show that, with the inclusion of a nearest-neighbor density-density interaction, fractional quantum Hall states can be realized solely within these flat bands. Specifically, we characterize the $\nu = 1/3$ Laughlin state through the use of change pumping, spectral flow, entanglement scaling, and CFT edge state counting; and we analyze its dependence on orbital mixing. Ultimately, we comment on the applicability of this model for experiment.

TT 28.7 Tue 15:30 HSZ 201

Kernel Polynomial Method applied to Twisted Bilayer Graphene — Van-Nam Do[1], Duy Nguyen Van[1], Anh Le Hoang[1], and •Dario Bercioux[2,3] — [1]Phenikaa Institute for Advanced Study (PIAS), C1 Building, Phenikaa University, Hanoi 10000, Vietnam — [2]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizbal 4, E-20018 San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain

We apply the Kernel Polynomial Method (KPM) [1] for investigating various spectral properties of twisted bilayer graphene. Contrary to standard methods based on Bloch’s theorem, with the use of the KPM we can investigate twisted bilayer graphene with any twist angle, commensurate and incommensurate [2]. We show how within the KPM it is possible to study the evolution of a state, initially localized on one of the layers, to the other one. The resulting oscillating behaviour resembles Fabry-Pérot-like oscillations. We show that the characteristic transfer time between the two layers has a minimal dependence on the twist angle [3]. We further show how the chiral structure of twisted bilayer graphene allows for a finite transverse optical Hall conductivity even in the absence of external magnetic fields [4].

[1] Weiße *et al.*, Rev. Mod. Phys. **78**, 275 (2006).
[2] H. A. Le & V. N. Do, Phys. Rev. B **97**, 125136 (2018).
[3] H. Nam Do, H. Anh Le, & D. Bercioux, Phys. Rev. B **99**, 165127 (2019).
[4] V. Nam Do, H. Anh Le, V. Duy Nguyen, S. Ta Ho & D. Bercioux *in preparation.*

TT 29: Nonequilibrium Quantum Many-Body Systems 2 (joint session TT/DY)

Time: Tuesday 14:00–16:00 Location: HSZ 204

TT 29.1 Tue 14:00 HSZ 204

Robust and ultrafast state preparation by ramping artificial gauge potentials — •Botao Wang, Xiaoyu Dong, F. Nur Ünal, and André Eckardt — Max-Planck-Institut für Physik komplexer Systeme Nöthnitzer Str. 38, D-01387 Dresden, Germany

The implementation of static artificial magnetic fields in ultracold atomic systems has been established as a powerful tool, e.g. for simulating quantum-Hall physics with charge-neutral atoms. Taking an interacting bosonic flux ladder as a minimal model, we investigate protocols for adiabatic state preparation based on ramping up the vector potential (in the form of Peierls phases), which is engineered to give rise to the desired magnetic flux. We find that the time required for adiabatic state preparation dramatically depends on the spatial pattern of Peierls phases used to create the flux. This is explained by the fact that, while different patterns (i.e. vector potentials) just correspond to different gauges for static fluxes, they induce different electric fields during the ramp. Remarkably, we find that for an optimal choice, it allows for preparing the ground state almost instantaneously. This provides a novel concept for shortcuts to adiabaticity and may open up a new way for robust state preparation.

TT 29.2 Tue 14:15 HSZ 204

Non-equilibrium steady state solutions of time-periodic driven Luttinger liquids — •Serena Fazzini[1], Piotr Chudinski[2], Chirstoph Dauer[1], Imke Schneider[1], and Sebastian Eggert[1] — [1]Physik und OPTIMAS, Technische Universität Kaiserslautern — [2]School of Mathematics and Physics, Queens Univ. Belfast

The recent development of Floquet engineering has made periodic driving a versatile tool for achieving new phases not accessible in static equilibrium systems. We now study the exact Floquet steady states of the periodically driven Tomonaga-Luttinger liquid without resorting to any high frequency approximations. We show that the time-dependent Schrödinger equation can be solved analytically for a large class of driven interacting 1D systems, which give the resulting non-equilibrium steady states. Remarkably, we observe regions of instabilities as a function of total momentum where the solution is not of Floquet form, which implies a loss of time translational invariance and therefore heating of excitations. For small driving amplitudes the instabilities are close to the naively expected resonance condition $n\omega = 2vq$, but for stronger driving the heating regions separate a rich structure of bands of steady state solutions. Physical consequences are discussed.

TT 29.3 Tue 14:30 HSZ 204

Periodically Driven Manybody System: a Density Matrix Renormalization Group Study — •Imke Schneider[1], Shaon Sahoo[2], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517506, India

Driving a quantum system periodically in time can profoundly alter its long-time dynamics and trigger exotic quantum states of matter. We propose a new DMRG method which directly deals with the Fourier components of the eigenstates of a periodically driven system using Floquet theory. With this new method we can go beyond effective Hamiltonians and take into account higher Floquet modes. Numerical results are presented for the isotropic Heisenberg antiferromagnetic spin-1/2 chain under both local (edge) and global driving for energies, spin-spin correlation and temporal fluctuations. As the frequency is lowered, the spin system enters into a Floquet regime with coherent excitations of a large number of Floquet modes, which shows characteristic quantum correlations that cannot be described by any effective static model.

TT 29.4 Tue 14:45 HSZ 204

Suppression of the horizon effect in pairing correlation functions of *t*-*J* chains after a quantum quench — Ansgar Kühn, Lorenzo Cevolani, and •Salvatore R. Manmana — Institut für Theoretische Physik, U. Göttingen

We investigate the time evolution of density, spin, and pairing correlation functions in one-dimensional t-J models following a quantum quench using the time-dependent density matrix renormalization group. While density and spin correlation functions show the typical light-cone behavior over a wide range of parameters, in pairing correlation functions it is strongly suppressed. This is supported by time-dependent BCS theory, where the light cone in the pairing correlation functions is found to be at least two orders of magnitude weaker than in the density correlator. These findings indicate that in global quantum quenches not all observables are affected equally by the excitations induced by the quench.

We acknowledge financial support by SFB/CRC 1073 (project B03) of the DFG.

[1] Phys. Rev. A **98**, 013616 (2018).

TT 29.5 Tue 15:00 HSZ 204

Iterative path integral summations for nonequilibrium quantum transport — •Stephan Weiss, Simon Mundinar, and Jürgen König — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

We have developed a numerically exact scheme, the **I**terative **S**ummation of **P**ath-**I**ntegrals (ISPI), to calculate observable of interest in quantum transport setups out of equilibrium [1,2]. Our main focus aims at small interacting quantum dot systems which are coupled to ferromagnetic [2] as well as superconducting leads in a nonequilibrium environment. We take into account small to intermediate Coulomb interactions, finite lead polarizations as well as finite superconducting gap parameters and finite temperature for the respective setups. Our method treats spin-dependent resonant-tunnelling processes in a natural manner. Examples of the tunnelling current are presented for different setups.

[1] S. Weiss, R. Hützen, D. Becker, J. Eckel, R. Egger, and M. Thorwart, Phys. Stat. Sol. B 250, 2298 (2013).
[2] S. Mundinar, Ph. Stegmann, J. König, and S. Weiss, Phys. Rev. B 99, 195457 (2019).

TT 29.6 Tue 15:15 HSZ 204

Mobility of the Fermi polaron for strong couplings — •Stefan Wittlinger[1], Lode Pollet[1], and Andrey Mishchenko[2] — [1]LMU Munich, Munich, Germany — [2]RIKEN, Wako, Japan

We present an algorithmic scheme to calculate the mobility of the Fermi polaron, an impurity immersed into a Fermi bath, for strong couplings. In general, Monte Carlo simulations of the Fermi polaron problem suffer from the fermionic sign problem. For our scheme, we find a wide parameter range with a tractable sign problem. The perturbative expansion of the interaction is sampled using the diagrammatic determinantal quantum Monte Carlo algorithm. The sampling is done in imaginary time, which requires analytical continuation. Most theoretical treatments of the Fermi polaron problem only consider s-wave interactions or rely on the heavy particle approximation. Our scheme allows for the study of more realistic potentials by also considering higher order scattering terms. It also allows for the study of the problem without the heavy particle approximation. I will present results for a repulsive potential well for a wide range of masses and varying interaction ranges. Possible connections to the Anderson orthogonality catastrophe of the infinite mass case will also be discussed.

TT 29.7 Tue 15:30 HSZ 204

Chiral kinetic theory avoiding anomalies — •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

The anomalous term $\sim \vec{E}\vec{B}$ in the balance of the chiral density can be rewritten as quantum current in the classical balance of density. This term is derived from the quantum kinetic equations for systems with SU(2) structure within a completely conserving approach and it is suggested that the term is of kinetic origin instead of anomaly. 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. 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. [Eur. Phys. J. B 92 (2019) 176, Phys. Lett. A 383 (2019) 1362, Phys. Rev. B 94 (2016) 165415, Phys. Rev. B 92 (2015) 245425 errata:

Phys. Rev. B93 (2016) 239904(E), Phys. Rev. B 92 (2015) 245426

TT 29.8 Tue 15:45 HSZ 204

Optical excitation of magnons in an easy-plane antiferromagnet: Application to Sr_2IrO_4 — •Urban F. P. Seifert[1,2] and Leon Balents[2,3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA — [3]Canadian Institute for Advanced Research, Toronto, Ontario, Canada M5G 1M1

Recent experiments show that ultrafast radiation at energies below the optical gap can create coherent magnetic excitations in Mott insulating antiferromagnets. In this talk, we introduce a quantum theory for the interaction of a (classical) light field with the magnetic degrees of freedom in the paradigmatic two-dimensional antiferromagnet Sr_2IrO_4. The reduced space group symmetry of the crystal allows for several channels for spin-operator bilinears to couple to the electric field. Integrating out high-energy degrees of freedom in a Keldysh framework, we derive induced effective fields which enter the equations of motion of the low-energy mode of in-plane rotations which couple to the out-of-plane magnetization. Considering a pump-probe protocol, these induced fields excite magnetization oscillations which can subsequently probed, e.g. using Kerr rotation. We discuss how the induced fields depend on polarization and frequency of the driving light, and our study applies to both resonant and non-resonant regimes. Crucially, the induced fields depend on the two-magnon density of states, thus allowing for further insight into properties of the magnetic excitation spectrum.

TT 30: Frustrated Magnets - Spin Liquids 2 (joint session TT/MA)

Time: Tuesday 14:00–15:15 Location: HSZ 304

TT 30.1 Tue 14:00 HSZ 304

Theory of partial quantum disorder in the stuffed honeycomb Heisenberg antiferromagnet — •Urban F. P. Seifert and Matthias Vojta — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Recent numerical results [Gonzalez *et al.*, Phys. Rev. Lett. **122**, 017201 (2019); Shimada *et al.*, J. Phys. Conf. Ser. **969**, 012126 (2018)] point to the existence of a partial-disorder ground state for a spin-1/2 antiferromagnet on the stuffed honeycomb lattice, with 2/3 of the local moments ordering in an antiferromagnetic Néel pattern, while the remaining 1/3 of the sites display short-range correlations only, akin to a quantum spin liquid.

In this talk, we derive an effective model for this disordered subsystem, by integrating out fluctuations of the ordered local moments, which yield couplings in a formal $1/S$ expansion, with S being the spin amplitude. The result is an effective triangular-lattice XXZ model, with planar ferromagnetic order for large S and a stripe-ordered Ising ground state for small S, resulting from frustrated Ising interactions. Within semiclassical analysis, the transition point between the two orders is located at $S_c = 0.646$, being very close to the relevant case $S = 1/2$. Near $S = S_c$ quantum fluctuations tend to destabilize magnetic order. We conjecture that this applies to $S = 1/2$, thus explaining the observed partial-disorder state.

TT 30.2 Tue 14:15 HSZ 304

Dirac Spin Liquid on the Spin-1/2 Triangular Heisenberg Antiferromagnet — •Shijie Hu[1], Wei Zhu[2], Sebastian Eggert[1], and Yin-Chen He[3] — [1]Physik und OPTIMAS, Technische Universität Kaiserslautern — [2]Natural Sciences, Westlake Institute of Advanced Study, Hangzhou — [3]Perimeter Institute, Waterloo

We study the spin liquid candidate of the spin-1/2 J_1-J_2 Heisenberg antiferromagnet on the triangular lattice by means of density matrix renormalization group (DMRG) simulations. By applying an external Aharonov-Bohm flux insertion in an infinitely long cylinder, we find unambiguous evidence for gapless U(1) Dirac spin liquid behavior. The flux insertion overcomes the finite size restriction for energy gaps and clearly shows gapless behavior at the expected wave-vectors. Using the DMRG transfer matrix, the low-lying excitation spectrum can be extracted, which shows characteristic Dirac cone structures of both spinon-bilinear and monopole excitations. Finally, we confirm that the entanglement entropy follows the predicted universal response under the flux insertion [1].

[1] Phys. Rev. Lett. **123**, 207203 (2019).

TT 30.3 Tue 14:30 HSZ 304

Phonon attenuation in $\mathbb{Z}_2$ quantum spin liquids — •Johannes Lang[1], Francesco Piazza[1], Roderich Moessner[1], and Matthias Punk[2] — [1]Max-Planck Institut für Physik komplexer Systeme, Dresden, Deutschland — [2]Ludwig-Maximilians-Universität München, München, Deutschland

In $\mathbb{Z}_2$ quantum spin liquids low lying excitations in the form of visons can couple to lattice vibrations. The high degree of frustration in the spin lattice results in an enlarged unit cell for the visons, which in turn has characteristic signatures in phonon attenuation.

TT 30.4 Tue 14:45 HSZ 304

Rank-2 Coulomb Spin Liquids from Classical Spins — •Owen Benton[1], Han Yan[2], Ludovic Jaubert[3], and Nic Shannon[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Okinawa Institute of Science and Technology Graduate University — [3]CNRS Bordeaux

Coulomb spin liquids are well studied spin liquid states exhibiting emergent electromagnetism, having a coarse-grained description corresponding to Maxwell's laws. It has recently been appreciated that even more exotic scenarios are possible, realizing generalizations of electromagnetism with rank-2 electric and magnetic fields. These are of particular interest since the emergent charges of the rank-2 electromagnetism can be fractons, with fundamentally constrained mobility.

In this talk I will describe an approach to finding simple, bilinear models, for classical spins which realize rank-2 Coulomb phases at low temperature. Such models provide access to rank-2 Coulomb phase physics in a setting amenable to efficient numerical study and also suggest directions to look for rank-2 Coulomb phases in experiment.

Remarkably, we find that a traceless, vector-charged, rank-2 Coulomb phase can be generated by perturbing a simple Heisenberg model on the pyrochlore lattice with breathing anisotropy and weak Dzyaloshinskii-Moriya interactions. This enables us to identify Yb-based breathing pyrochlores as potential candidate systems and to make explicit predictions for how the rank-2 Coulomb phase would manifest itself in experiment.

TT 30.5 Tue 15:00 HSZ 304

Single-site magnetic anisotropy governed by interlayer cation charge imbalance in triangular-lattice $AYbX_2$ — •Ziba Zangenehpourzadeh, Stanislav Avdoshenko, Jeroen van den Brink, and Liviu Hozoi — IFW Dresden, 01069 Dresden, Germany

The behavior in magnetic field of a paramagnetic center is characterized by its g tensor. Here we shed light on the anisotropy of the g tensor of Yb^{3+} $4f^{13}$ ions in $NaYbX_2$ and $NaYbO_2$, layered triangular-lattice materials suggested to host spin-liquid ground states. Using quantum chemical calculations we show that, even if the ligand-cage trigonal distortions are significant in these systems, the decisive role in realizing strongly anisotropic, g factors is played by interlayer cation charge imbalance effects. The latter refer to the asymmetry experienced by a given Yb center due to having higher ionic charges at adjacent metal sites within the magnetic ab layer. This should be a rather general feature of $4f^{13}$ layered delafossites: less interlayer positive charge is associated with stronger in-plane magnetic response [1].

[1] Z. Zangeneh, et al, Phys. Rev. B **100**, 174436 (2019).

TT 31: Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 1

Time: Wednesday 9:30–13:00 Location: HSZ 03

TT 31.1 Wed 9:30 HSZ 03

Shining new light on long standing questions: Recent insights into the understanding of low frequency excess flux noise — •Anna Ferring-Siebert, Fabian Kaap, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Low frequency excess flux noise (LFEFN), which scales as $1/f^{\alpha}$, strongly impairs the performance of superconducting quantum devices (SQDs) such as SQUIDs and Qubits. Although it was believed for quite a long time that its magnitude $\sqrt{S_\Phi}$ and exponent α are fairly independent of the device material and inductance, there meanwhile exist hints for the contrary. It is also known that LFEFN somehow depends on the equipment used for device fabrication, but the reason for that remained unknown up to now.
In this contribution, we first discuss the origin of fabrication induced LFEFN as well as means to minimize it. In particular, we show that commercial deposition equipment often yield material layers containing magnetic impurities causing LFEFN. Whithin this context, we further present how we modified commercial sputter sources to reduce LFEFN as well as indications for a correlation between the LFEFN amplitude and the dc-magnetization of deposited material layers. Finally, we discuss recent measurements investigating the dependence of LFEFN on device inductance suggesting that energy sensitivity rather than magnetic flux noise is the more appropriate figure of merit for describing LFEFN.

TT 31.2 Wed 9:45 HSZ 03

Post-production Tile-and-Trim Process for Superconducting Lumped Element Resonators and Transmission Line Resonators in Microwave SQUID Multiplexers — •Felix Ahrens, Patrick Paluch, Daniel Richter, Constantin Schuster, Mathias Wegner, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Heidelberg University, Germany

Microwave SQUID multiplexing (μMUXing) is likely the most promising technique to read out large metallic magnetic calorimeter (MMC) detector arrays. Here, high-quality superconducting GHz resonators based either on transmission lines or lumped-element inductors and capacitors are used for frequency encoding. These resonators are typically designed to have a bandwidth of $\sim$1 MHz to maintain the very fast signal rise time of MMCs and the frequency spacing between two neighbouring channels is set to $\sim$10 MHz to yield a cross-talk level below 10^{-4}. However, due to fabrication inaccuracies, the resonance frequency of micro-fabricated resonators differs very often from the design value and the frequency spacings between neighbouring resonators severely scatter. In order to overcome the resulting μMUX performance degradation e.g. due to an enhanced cross-talk level a post-production fine-tuning of the resonance frequencies is essential. In this contribution we present our post-production tile-and-trim processes allowing to adjust the resonance frequency of both lumped element and transmission line resonators within a microwave SQUID multiplexer.

TT 31.3 Wed 10:00 HSZ 03

Superconducting qubit devices: fabrication suite — •Wei Liu, Kok Wai Chan, Tianyi Li, Johannes Heinsoo, Vasilii Sevriuk, Caspar Ockeloen-Korppi, Jani Tuorila, Juha Hassel, Juha Vartiainen, Kuan Yen Tan, Jan Goetz, and Mikko Mottonen — IQM Finland Oy, Vaisalantie 6, 02130 Espoo, Finland

Scalable quantum computing architecture and fabrication processes have been a hot research topic in the past decade. We focus on the realization of a quantum computer based on superconducting qubits with a fast qubit reset and initialization techniques, utilizing a quantum-circuit refrigerator. We present the fabricated devices and results achieved to date, which includes resonators with high quality factors, $> 10^6$, long qubit lifetime > 0.02 ms and 3D integration techniques such as airbridges.

TT 31.4 Wed 10:15 HSZ 03

Reaching the ultimate energy resolution of a quantum detector — •Bayan Karimi[1], Fredrik Brange[1,2], Danilo Nikolic[3], Joonas T. Peltonen[1], Peter Samuelsson[2], Wolfgang Belzig[3], and Jukka P. Pekola[1] — [1]QuESTech and QTF Centre of Excellence, Department of Applied Physics, Aalto University, 00076 Aalto, Finland — [2]Department of Physics and NanoLund, Lund University, Box 188, SE-221 00 Lund, Sweden — [3]QuESTech and Fachbereich Physik, Universität Konstanz, D-78467, Germany

We present a radio-frequency thermometer based on a zero-bias anomaly of a tunnel junction between a superconductor and proximitized normal metal [1,2]. It features noninvasive detection and essentially uncompromised sensitivity down to the lowest temperatures of below 20 mK in contrast to commonly used finite bias thermometers that dissipate orders of magnitude more power and lose their sensitivity at low temperatures. Using this thermometer we demonstrate detection of equilibrium fluctuations of temperature in a system of about 10^8 electrons exchanging energy with phonon bath at a fixed temperature [3].

[1] B. Karimi, J. P. Pekola, Phys. Rev. Appl. **10**, 054048 (2018).
[2] B. Karimi, D.anilo Nikolić, T. Tuukkanen, J. T. Peltonen, W. Belzig, J. P. Pekola, arXiv:1911.02844 (2019).
[3] B. Karimi, F. Brange, P. Samuelsson, J. P. Pekola, arXiv:1904.05041 (2019).

TT 31.5 Wed 10:30 HSZ 03

Development of RF-Power Dividers for the Josephson Arbitrary Waveform Synthesizer — •Hao Tian, Oliver Kieler, Ralf Behr, Rüdiger Wendisch, Rolf-Werner Gerdau, Karsten Kuhlmann, and Johannes Kohlmann — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany

The JAWS, based on pulse-driven series arrays of SNS Josephson Junctions (JJs) at 4 K, enables spectrally pure AC voltages to be synthesized from DC up to MHz. To simplify the experimental set-up and to increase the JJs operated by a single PPG channel, we designed two types of on-chip power dividers. One type is a two-stage serial-parallel power divider, the second type is a one-stage Wilkinson power divider. The outputs of the power dividers are equipped with DC-block capacitors and LCR filters. Different designs were simulated, integrated to JJs arrays and fabricated. The results showed that the test chips containing a 2-stage serial-parallel power divider and 2000 JJs are operational up to a maximum clock frequency of 13 GHz. Spectrally pure sinusoidal waveforms of 19 mV (RMS) could be synthesized with sigma-delta code amplitudes of 50%. The 1-stage Wilkinson power divider integrated with 1000 JJs and 3000 JJs can operate up to a clock frequency of 15 GHz. We successfully synthesized spectrally pure output voltages of 17.6 mV (RMS) and 33 mV (RMS). This work was partly supported by the EMPIR programme co-financed by the Participating States and from the EU H2020 programme (JRP 15SIB04 QuADC) and by the German BMWi (project ZF4104104AB7).

TT 31.6 Wed 10:45 HSZ 03

Fluxoid dynamics in high impedance long Josephson junctions — •Micha Wildermuth[1], Lukas Powalla[1], Konrad Dapper[1], Yannick Schön[1], Jan Nicolas Voss[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,3,4] — [1]Institute of Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute for Solid-State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]National University of Science and Technology MISIS, Moscow, Russia — [4]Russian Quantum Center, Skolkovo, Moscow, Russia

The dynamics of Josephson vortices in long Josephson junctions is a well-known example of soliton physics and allows to study highly nonlinear effects on a mesoscopic scale. We experimentally study the characteristics of a Josephson junction with electrodes having a large kinetic inductance fraction which provides an additional degree of freedom. The London penetration depth exceeds the stack thickness which results in an incomplete screening of magnetic fields and in fluxoids with an altered shape. We present transport measurements of long Josephson junctions with electrodes made from disordered oxidized aluminum showing current steps with and without external magnetic fields and the IV-characteristics resemble the Fiske and zero-field steps. Magnetic field dependent measurements also show a very similar behavior to conventional long Josephson junctions.

TT 31.7 Wed 11:00 HSZ 03

Study of the relaxation and decoherence in 2D fluxoniums — •Farshad Foroughi, Karthik Bharadwaj, Luca Planat, Arpit Ranadive, Cecile Naud, Olivier Buisson, Nicolas Roch, and Wiebke Hasch-Guichard — univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38000 Grenoble, France

High anharmonicity and wide frequency tunability of the Fluxonium qubit make it an indispensable candidate for emerging quantum computers. Moreover fluxonium qubit in a 3D cavity or environment, when biased at sweet spot, shows very high relaxation time at the order of 10 ms[1]. However 2D and on-chip qubits are more favorable to scale up. The transition from 3D to 2D is not trivial as the coupling to the unwanted degrees of freedom increases a lot. In this work we coupled the fluxonium qubit to on-chip lumped element and distributed resonators. We have studied effect of different qubit parameters on the coherence times T1 and T2.

[1] I. M. Pop et al., Nature 508, 369-372 (2014)

15 min. break.

TT 31.8 Wed 11:30 HSZ 03

Kinetic Inductance of thin Al Films using a Resonant Circuit — •Lorenz Fuchs, Christian Baumgartner, Dieter Schuh, Nicola Paradiso, Dominique Bougeard, and Christoph Strunk — Institute for Experimental and Applied Physics, University of Regensburg

Direct measurement of the magnetic penetration depth λ on thin films with a thickness $d \ll \lambda$ has been challenging ever since. We use a resonant circuit to determine the complex impedance of a superconducting thin film meander in the few MHz regime [1]. The meander is patterned into a 15nm thick aluminum film that is grown on a GaAs substrate. From the imaginary part of the impedance we determine the kinetic inductance of the superconducting condensate and from vortex motion in the pinning potential and from the real part a dissipative contribution caused by quasi-particle excitations and/or vortex motion. A small change of the total inductance of the system due to the kinetic inductance $L_{kin} = \mu_0\lambda^2/d$ of the superconductor below its critical temperature T_c leads to a significant decrease of the resonance frequency f_0. The system is sensitive to changes of inductance smaller than 50 pH, which can compete with the accuracy of more standard two-coil mutual inductance techniques [2]. Examination of the basic features of this technique will provide the basis for further investigation of proximity induced superconductivity in InAs 2DEGs with large spin-orbit coupling.

[1] R. Meservey and P.M. Tedrow, J. Appl. Phys. 40, 2028 (1969)
[2] T. Lemberger et al., Phys. Rev. B, 76, 094515 (2007)

TT 31.9 Wed 11:45 HSZ 03

Superconducting granular aluminum resonators resilient to magnetic fields up to 1 Tesla — •Alexandru Ionita, Kiril Borisov, Dennis Rieger, Patrick Winkel, Markus Wessbecher, Fabio Henriques, Francesco Valenti, Martin Spiecker, Daria Gusenkova, Wolfgang Wernsdorfer, and Ioan Pop — Physikalisches Institut, KIT, Karlsruhe, Germany

Superconducting granular aluminum (grAl) is an attractive high-kinetic inductance material with proven applicability in superconducting qubits [1, 2] and microwave detectors [3]. As the magnetic field is a double-edged sword, which provides an important control knob to superconducting circuits but could also lead to higher quasiparticle population and induced vortices, we investigate the field resilience of grAl superconducting resonators. We carried out reflection measurements in both in-plane and perpendicular external magnetic fields, which tune the resonance frequency by up to 70 MHz. The internal quality factor remains on the order of 10^5 in the single photon regime under in-plane magnetic field up to 1 T [4]. Moderate perpendicular field has a beneficial effect on the resonator properties and leads to a small increase of the internal quality factor by 15 %. We further discuss the field-dependence of self-Kerr coefficient [5], rate of quasi-particle relaxation [3] and coupling to spin-1/2 magnetic impurities.

[1] L. Grünhaupt, M. Spiecker, Nat. Mat. 18(8), 816 (2019).
[2] P. Winkel, arXiv: 1911.02333
[3] F. Valenti, Phys. Rev. Appl. 11, 054087 (2019
[4] K. Borisov (in preparation)
[5] N. Maleeva, Nat. Comm. 9(1), 3889 (2018)

TT 31.10 Wed 12:00 HSZ 03

Resistance tuning of disordered nanowires by current pulses and their electrical response at low temperatures — •Jan Nicolas Voss[1], Yannick Schön[1], Micha Wildermuth[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,3,4] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Russian Quantum Center, Skolkovo, Moscow, Russia — [4]National University of Science and Technology MISIS, Moscow, Russia

Superconducting nanowires made from granular aluminium have unique electrical properties at low temperatures. They originate from the intrinsic network of Josephson junctions in the material and the spatial restrictions to dimensions that are of the order of the superconducting coherence length. We present a novel method, which allows changing the nanowire resistance by modifying the intrinsic junction network by electrical pulses. With this method, we test the quantum phase slip model for the wires at millikelvin temperatures.

We have observed a transition from an insulating over a metallic to a superconducting response in about a two hundred individual resistance steps. The measurement results are compared with theoretical predictions.

TT 31.11 Wed 12:15 HSZ 03

Rabi Oscillations in a Superconducting Nanowire Circuit — •Yannick Schön[1], Jan Nicolas Voss[1], Micha Wildermuth[1], Andre Schneider[1], Sebastian T. Skacel[1], Martin P. Weides[1,3], Jared H. Cole[4], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,5,6] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]University of Glasgow, Glasgow, United Kingdom — [4]RMIT University, Melbourne, Australia — [5]National University of Science and Technology MISIS, Moscow, Russia — [6]Russian Quantum Center, Skolkovo, Moscow, Russia

Disordered oxidized (granular) aluminum is a new material for superconducting quantum circuits, featuring not only a very high kinetic inductance but also microwave resonators with high quality factors. Applied to wires of nanometer scale it allows for a pronounced nonlinear microwave response.

We investigate the circuit quantum electrodynamics of superconducting nanowire oscillators. The sample circuit consists of a capacitively shunted nanowire with a width of about 20 nm and a varying length up to 350 nm, capacitively coupled to an on-chip resonator. By applying microwave pulses we observe Rabi oscillations, measure coherence times and the anharmonicity of the circuit. Despite the very compact design, simple top-down fabrication and high degree of disorder in the granular aluminum material, we observe lifetimes in the microsecond range.

TT 31.12 Wed 12:30 HSZ 03

Implementation of a transmon qubit using superconducting granular aluminum — •Patrick Winkel[1], Kiril Borisov[2], Lukas Grünhaupt[1], Dennis Rieger[1], Martin Spiecker[1], Francesco Valenti[1,3], Alexey V. Ustinov[1,4], Wolfgang Wernsdorfer[1,2,5], and Ioan M. Pop[1,2] — [1]Physikalisches Institut, KIT, Karlsruhe, Germany — [2]Institute of Nanotechnology, KIT, Karlsruhe, Germany — [3]Institut für Prozessdatenverarbeitung und Elektronik, KIT, Karlsruhe, Germany — [4]Russian Quantum Center, MISIS, Moscow, Russia — [5]Institut Néel, CNRS, Grenoble, France

The high kinetic inductance offered by granular aluminum (grAl) has recently been employed for linear inductors in superconducting high-impedance qubits and kinetic inductance detectors. Due to its large critical current density compared to typical Josephson junctions, its resilience to external magnetic fields, and its low dissipation, grAl may also provide a robust source of non-linearity for strongly driven quantum circuits, topological superconductivity, and hybrid systems. Having said that, can the grAl non-linearity be sufficient to build a qubit? Here we show that a small grAl volume shunted by a thin film aluminum capacitor results in a microwave oscillator with an anharmonicity of 4.48 MHz, two orders of magnitude larger than its spectral linewidth, effectively forming a transmon qubit. Resonance fluorescence measurements of the fundamental transition yield an intrinsic qubit linewidth corresponding to a lifetime of 16 μs. This linewidth remains below 150 kHz for in-plane magnetic fields up to 70 mT.

TT 31.13 Wed 12:45 HSZ 03

Amplitude and frequency sensing of microwave fields with

a superconducting transmon qubit — •Maximilian Kristen[1], Andre Schneider[1], Alexander Stehli[1], Tim Wolz[1], Sergey Danilin[2], Hannes Rotzinger[1], Alexey V. Ustinov[1,3,4], and Martin Weides[1,2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]University of Glasgow, Glasgow, UK — [3]National University of Science and Technology MISIS, Moscow, Russia — [4]Russian Quantum Center, Moscow, Russia

Experiments with quantum circuits require careful calibration of the applied pulses and fields over a large frequency range. Here, we demonstrate how frequency and local amplitude of a microwave signal can be inferred from the ac Stark shifts of higher transmon levels. In time-resolved measurements we employ Ramsey fringes, allowing us to detect the amplitude of the system's transfer function over a range of several hundreds of MHz with an energy sensitivity on the order of 1e-4. The presented sensing method can facilitate pulse correction for high fidelity quantum gates in superconducting circuits and allows for the characterization of arbitrary microwave fields for experiments with hybrid microwave systems.

TT 32: Superconductivity: Theory 2

Time: Wednesday 9:30–10:45 Location: HSZ 103

TT 32.1 Wed 9:30 HSZ 103

Josephson lattice model for phase fluctuations of local pairs in copper oxide superconductors — •Sergey Brener[1,2], Malte Harland[1], Alexander Lichtenstein[1], and Mikhail Katsnelson[3] — [1]Universität Hamburg — [2]The Hamburg Centre for Ultrafast Imaging — [3]Radboud Universiteit, Nijmegen, Niederlande

We derive an expression for the effective Josephson coupling from the microscopic Hubbard model. It serves as a starting point for the description of phase fluctuations of local Cooper pairs in $d_{x^2-y^2}$-wave superconductors in the framework of an effective XY model of plaquettes, the Josephson lattice. The expression for the effective interaction is derived by means of the local-force theorem, and it depends on local symmetry-broken correlation functions that we obtain using the cluster dynamical mean-field theory. Moreover, we apply the continuum limit to the Josephson lattice to obtain an expression for the gradient term in the Ginzburg-Landau theory and compare predicted London penetration depths and Kosterlitz-Thouless transition temperatures with experimental data for $YBa_2Cu_3O_{7-x}$.

TT 32.2 Wed 9:45 HSZ 103

Phase sensitive determination of nodal d-wave order parameter in single band superconductors — •Jakob Böker[1], Miguel Sulangi[2], 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

Determining the exact pairing symmetry of a superconducting order parameter remains to be a challenge of great experimental effort. Recently a new method utilizing quasiparticle interference (QPI) measurements based on scanning tunneling spectroscopy was proposed. It states that the momentum-integrated QPI data, antisymmetrized with respect to bias voltage, provides a robust phase sensitive tool to distinguish sign-changing $s_\pm$ from sign-preserving s_{++} superconductivity in the iron based superconductors. Here we discuss that the same quantity can be used to visualize the sign-changing character of a single band nodal d-wave order parameter, relevant for the cuprate and likely for the infinite-layer nickelate superconductors. Further, using a realistic approach accounting for Cu-Wannier functions, we model STM data of zinc-doped $Bi_2Sr_2CaCu_2O_{8+\delta}$ to directly compare our theory with experimental results.

TT 32.3 Wed 10:00 HSZ 103

Communal pairing in spin-imbalanced Fermi gases — •Darryl Foo — University of Cambridge

A spin-imbalanced Fermi gas with an attractive contact interaction forms a superconducting state whose underlying components are superpositions of Cooper pairs that share minority-spin fermions. This superconducting state includes correlations between all available fermions, making it energetically favorable to the Fulde-Ferrell-Larkin-Ovchinnikov superconducting state. The ratio of the number of up- and down-spin fermions in the instability is set by the ratio of the up- and down-spin density of states in momentum at the Fermi surfaces, to fully utilize the accessible fermions. We present analytical [EPL 126 67003 (2019)] and complementary Diffusion Monte Carlo results [arXiv:1910.13582] for the state.

TT 32.4 Wed 10:15 HSZ 103

Weak localization corrections to the thermal conductivity in s-wave superconductors — •Lucia Gonzalez Rosado[1,2], Fabian Hassler[2], and Gianluigi Catelani[1] — [1]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

We study thermal conductivity in disordered conventional superconductors, focusing on the weak localization (WL) effect and using a Green's function diagrammatic technique in Nambu space. We obtain the WL correction to the thermal conductivity from the diffusive behavior of the low-energy modes, and calculate it explicitly in two dimensions, both for fixed phase-coherence length and for fixed phase-coherence time. We show that the correction depends in some temperature regimes on an emergent energy scale ε_*. We show that this scale is experimentally measurable for dirty superconductors at high temperatures.

TT 32.5 Wed 10:30 HSZ 103

Experimental consequences of Bogoliubov Fermi surfaces — Clara Johanna Lapp and •Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden

Superconductors involving electrons with orbital degrees of freedom can have internally anisotropic pairing states that are impossible in single-band superconductors. For example, in even-parity multiband superconductors that break time-reversal symmetry, nodes of the superconducting gap are generically inflated into two-dimensional Bogoliubov Fermi surfaces. The detection and characterization of these quasiparticle Fermi surfaces requires the understanding of their experimental consequences. We derive the low-energy density of states for various nodal structures. Based on this, we calculate the low-temperature forms of the electronic specific heat, the thermal conductivity, the magnetic penetration depth, and the NMR spin-lattice relaxation rate, in the clean limit.

TT 33: Correlated Electrons: Method Development 1

Time: Wednesday 9:30–12:45 Location: HSZ 201

TT 33.1 Wed 9:30 HSZ 201

Density functional perturbation theory with DFT+U in the mixed-basis framework — •Rolf Heid — Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology

DFT+U is a viable tool to improve description of materials, where the standard DFT exchange-correlation potentials fail to catch essential properties of electronic correlation. While phenomenological in nature, it is numerically efficient and also gives access to energy derivatives, e.g. forces and force constants. Most applications to lattice dynamics properties have been based on the direct method (supercells and forces), while the linear response approach has been rarely used.

Here I describe a combination of DFT+U and density functional perturbation theory (DFPT) in the framework of the mixed-basis approach, an efficient method based on norm-conserving pseudopotentials employing a combination of plane waves and tailored local functions for the expansion of the valence states. The DFPT extension of the mixed-basis method [1,2] has been extensively applied in the past. The present DFT+U implementation employs the fully rotationally invariant form [3] in its relativistic extension [4]. Its usefulness is demonstrated for compounds containing 3d or 4f/5f elements.

[1] R. Heid et al., Phys. Rev. B **60**, R3709 (1999).
[2] R. Heid et al., Phys. Rev. B **81**, 174527 (2010).
[3] A.I. Liechtenstein et al., Phys. Rev. B **52**, R5467 (1995).
[4] A. B. Shick et al., Europhys. Lett. **69**, 588 (2005).

TT 33.2 Wed 9:45 HSZ 201

TRILEX² approach: towards the calculation of realistic systems — •Evgeny A. Stepanov[1], Silke Biermann[2], and Alexander I. Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, Germany — [2]Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France

A theoretical description of strongly correlated realistic systems is a challenging issue. A state-of-art method that allows to obtain single-particle properties of a corresponding multi-band electronic problem is the dynamical mean field theory (DMFT). Starting from DMFT, it is known that a consistent calculation of two-particle susceptibilities can be done via a ladder diagram that necessarily contains local vertex corrections. However, a calculation of these vertices is the most complicated and time consuming part of numerical approaches that describe nonlocal collective effects diagrammatically beyond DMFT. In some cases, a description of collective electronic fluctuations can be performed in a much simpler way using the GW+DMFT theory. However, the GW+DMFT in its original form accounts for the screening of the local Coulomb interaction only in the charge channel. Thus, the effect of the magnetic fluctuations in the nonlocal self-energy is missing. Recently, some of us introduced a computationally inexpensive TRILEX² approach [PRB 100, 205115 (2019)] that describes nonlocal many-body effects in the GW+DMFT style, but allows for a simultaneous account for collective excitations in different (charge, spin, etc.) bosonic channels. Here, we apply this method to a multi-band Hubbard model to explore orbital and spin fluctuations.

TT 33.3 Wed 10:00 HSZ 201

Strong-coupling formula for momentum-dependent susceptibilities in dynamical mean-field theory — •Junya Otsuki[1], Kazuyoshi Yoshimi[2], Hiroshi Shinaoka[3], and Yusuke Nomura[4] — [1]Research Institute for Interdisciplinary Science, Okayama University, Okayama Japan — [2]Institute for Solid State Physics, University of Tokyo, Chiba, Japan — [3]Saitama University, Saitama, Japan — [4]University of Tokyo, Tokyo, Japan

Computing momentum-dependent susceptibilities in the dynamical mean-field theory (DMFT) requires solving the Bethe-Salpeter equation, which demands large computational cost. Exploiting the strong-coupling feature of local fluctuations, we derive a simplified formula that can be solved at a considerably lower cost [1]. This formula allows us to estimate an effective intersite interaction, which is reduced to a well-known formula in the strong-coupling limit, such as the kinetic exchange and RKKY interactions. We present some applications of this formula to demonstrate its validity and applicability.

[1] J. Otsuki, K. Yoshimi, H. Shinaoka, Y. Nomura, Phys. Rev. B **99**, 165134 (2019)

TT 33.4 Wed 10:15 HSZ 201

Fixed point and thermodynamic stability of DMFT — •Erik van Loon[1] and Friedrich Krien[2] — [1]University of Bremen, Bremen, Germany — [2]Jožef Stefan Institute, Ljubljana, Slovenia

We consider the hysteresis region and critical end point of the DMFT metal-insulator transition by analyzing the fixed point equation and the Landau free energy.

TT 33.5 Wed 10:30 HSZ 201

Bandwidth renormalization due to the intersite Coulomb interaction — Yann in 't Veld[1], •Malte Schüler[2,3], Tim Wehling[2,3], Mikhail Katsnelson[1], and Erik van Loon[2,3] — [1]Institute for Molecules and Materials, Radboud University — [2]Bremen Center for Computational Materials Science, University Bremen — [3]Institute for Theoretical Physics, University Bremen

The theory of correlated electrons is currently moving beyond the paradigmatic Hubbard U, towards the investigation of intersite Coulomb interactions. Recent investigations have revealed that these interactions are relevant for the quantitative description of realistic materials. Physically, intersite interactions are responsible for two rather different effects: screening and bandwidth renormalization. We use a variational principle to disentangle the roles of these two processes and study how appropriate the recently proposed Fock treatment of intersite interactions is in correlated systems. The magnitude of this effect in graphene is calculated based on cRPA values of the intersite interaction. We also apply the variational principle to benzene and find effective parameters comparable to those obtained by ab-initio density matrix downfolding.

TT 33.6 Wed 10:45 HSZ 201

Single-boson exchange decomposition of the vertex function — •Friedrich Krien[1,3], Angelo Valli[2,3], and Massimo Capone[3] — [1]Institut Jozef Stefan, Ljubljana, Slovenia — [2]TU Wien, Austria — [3]SISSA, Trieste, Italy

We present a decomposition of the four-point vertex function which imparts a physical interpretation of the vertex in terms of the exchange of bosons of three flavors. The proposed decomposition does not require the matrix inversion of the Bethe-Salpeter equation and avoids the vertex divergences intrinsic to the traditional parquet decomposition. We discuss parametrizations of the vertex function in terms of the Hedin three-leg vertex.

15 min. break.

TT 33.7 Wed 11:15 HSZ 201

Symmetric improved estimators for continuous-time quantum Monte Carlo — •Josef Kaufmann[1], Patrik Gunacker[1], Alexander Kowalski[2], Markus Wallerberger[1], Giorgio Sangiovanni[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Continuous-time quantum Monte Carlo in the hybridization expansion is the current method of choice for solving the multiorbital Anderson impurity model. However, the results suffer from notoriously high noise at large Matsubara frequencies. Previously, this problem has been addressed e.g. by improved estimators [1]

We now go beyond this by deriving equations of motion for Green's functions symmetrically with respect to all time arguments. The resulting equations relate the one- and two-particle Green's function to correlators of up to six particles at four times [2], which can be computed by worm sampling [3, 4]. Finally, we arrive at self-energies and vertex functions that are practically noiseless at all frequencies.

This increase in precision leads to improved convergence behavior in dynamical mean-field theory calculations, as well as more reliable analytical continuation to real frequencies.

[1] H. Hafermann et al., PRB 85, 205106 (2012)
[2] J. Kaufmann, P. Gunacker et al., PRB 100, 075119 (2019)
[3] P. Gunacker et al., PRB 92, 155102 (2015)
[4] M. Wallerberger et al., CPC 235, 388 (2019)

TT 33.8 Wed 11:30 HSZ 201

Novel approach to non-local correlations: dual boson diagrammatic monte carlo — •Matteo Vandelli[1,2], Evgeny Stepanov[1], Angel Rubio[2], and Alexander Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

A long list of interesting physical phenomena arises due to strong interactions among electrons, but the mechanisms behind them are not fully understood yet. One of the most successful methods to deal with correlations is Dynamical Mean Field Theory (DMFT). However diagrammatic extensions are needed to capture non-local correlations. In particular dual theories are very promising, since they are based on an exact transformation. Recently Gukelberger et al. [PhysRevB.96.035152] have proven that the combination of Dual Fermion approach with diagrammatic Monte Carlo (DiagMC@DF) reproduces very accurately the results based on numerically exact Monte Carlo benchmarks. We expanded this scheme so that we could include non-local interactions appearing in the Extended Hubbard model. In order to achieve this goal, we combined diagrammatic Monte Carlo with Dual Boson approach (DiagMC@DB). The main advantage of this technique is that it can capture the interplay between competing instabilities. Furthermore the algorithm samples all the possible Feynman diagrams, as opposed to other diagrammatic approaches that arbitrarily select only some topologies.

TT 33.9 Wed 11:45 HSZ 201

Quantum Dynamics Made Fast: Achieving Linear Time-Scaling for Nonequilibrium Green Functions — •Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

The accurate description of nonequilibrium dynamics in correlated quantum-many-body systems remains to be a driving force for current research in condensed-matter physics and beyond. Among others, the nonequilibrium Green functions (NEGF) method has proven to be a powerful tool to predict quantum dynamics[1]. However, NEGF simulations are computationally expensive due to their T^3 scaling with the simulation duration T . With the introduction of the generalized Kadanoff–Baym ansatz[2] (GKBA), T^2 scaling could be achieved for second order Born (SOA) selfenergies[3], which has substantially extended the scope of NEGF simulations. Recently[4], we could show that GKBA-NEGF simulations can be performed with order T^1 scaling for SOA and even GW selfenergies. Here, we show numerical results for various many-body approximations and demonstrate that tremendous computational speed-up can be achieved.

[1] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[2] P. Lipavský *et al.*, Phys. Rev. B **34**, 6933 (1986)
[3] S. Hermanns *et al.*, Phys. Scr. **2012** 014036 (2012)
[4] N. Schlünzen *et al.*, submitted, arXiv:1909.11489

TT 33.10 Wed 12:00 HSZ 201

Functional renormalization group for a large Moiré unit cell — •Lennart Klebl, Dante Kennes, and Carsten Honerkamp — RWTH Aachen University, Aachen, Germany

Layers of two-dimensional materials arranged at a twist angle with respect to each other lead to enlarged unit cells with potentially strongly altered band structures, offering a new arena for novel and engineered many-body ground states. For the exploration of these, renormalization group methods are an appropriate, flexible tool that takes into account the mutual influence of competing tendencies. We show how the functional renormalization group known from simpler two-dimensional systems can be employed for large unit cells of Moiré superlattices, providing a description on the atomic scale and absorbing available ab-initio information on the model parameters. For the case of twisted bilayer graphene models, we explore the leading ordering tendencies depending on the band filling and the range of interactions. The results indicate a delicate balance between distinct magnetically ordered ground states.

TT 33.11 Wed 12:15 HSZ 201

Efficient simulation of the Dynamics in Two-Dimensional Quantum Spin Systems with Isometric Tensor Networks — •Sheng-Hsuan Lin and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

We introduce a numerical method to efficiently simulate the dynamical spin structure factor of two-dimensional quantum spin systems. The time evolution of truly two-dimensional systems is made possible using recently introduced isometric tensor network states [1]. We benchmark the algorithm by considering two paradigmatic models: First, we compare our results for the transverse field Ising model on square lattice with the prediction of spin wave theory. Second, we consider the Kitaev model on the honeycomb lattice and compare to the exact solution.

[1] arXiv preprint arXiv:1902.05100 (2019)

TT 33.12 Wed 12:30 HSZ 201

Orientational order parameters for arbitrary quantum systems* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The concept of quantum-mechanical nematic order, which is important in systems such as superconductors, is based on an analogy to classical liquid crystals, where order parameters are obtained through orientational expansions. We generalize this method to quantum mechanics based on an expansion of Wigner functions. This provides a systematic framework for the derivation of quantum order parameters, which unifies all known types of quantum orientational order into one framework and has a natural connection to the classical case. Moreover, new order parameters allow to find new orientational quantum phases. The method is demonstrated for Fermi liquids and spin systems. In addition, we construct new order parameters for molecular systems that cannot be properly described with the usual nematic tensors.

**Funded by the Deutsche Forschungsgemeinschaft (DFG) – WI 4170/3-1*

TT 34: Correlated Electrons: f-Electron Systems and Heavy Fermions 1

Time: Wednesday 9:30–13:00 Location: HSZ 204

TT 34.1 Wed 9:30 HSZ 204

Crystal-field wave function of $CeCu_2Si_2$ across T_c and T_K studied with linear polarized x-ray absorption — •andrea marino[1,2], andrea amorese[1], martin sundermann[2,3], kai chen[4], gertrud zwicknagl[5], maurits haverkort[6], frank steglich[1], liu hao tjeng[1], and andrea severing[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Dipartimento di Fisica, Politecnico di Milano, Milano, Italy — [3]Institute of Physics II, University of Cologne, Cologne, Germany — [4]Helmholz Zentrum Berlin (HZB) BESSY, Berlin, Germany — [5]Institute for Mathematical Physics, Technical University Braunschweig, Braunschweig, Germany — [6]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

We have investigated the crystal-field wave functions of $CeCu_2Si_2$ in the temperature range between 250 mK and 300 K, i.e. from well below to well above the superconducting transition temperature $T_c = 0.6$ K and the Kondo temperature $T_K \approx 10$ K using Ce $M_{4,5}$ x-ray absorption spectroscopy (XAS). The experiments in the mK regime were performed with the new mK insert at the DEIMOS beamline at synchrotron SOLEIL in France. The overall temperature dependence of the linear dichroism in the XAS is well explained with the thermal occupation of excited crystal-field states. Small deviations are discussed in terms of hybridization of f-electrons and conduction bands, supported by the temperature dependence of the f^0 satellite in the isotropic XAS spectra.

TT 34.2 Wed 9:45 HSZ 204

Temperature and Momentum Dependences of the Kondo Peak in the Heavy-Fermion System $CeRh_2Si_2$ — •Georg Poelchen[1], Susanne Schulz[1], Monika Güttler[1], Max Mende[1], Alexander Generalov[2], Christoph Geibel[3], Cornelius Krellner[4], Steffen Danzenbächer[1], James W Allen[5], Clemens Laubschat[1], Yuri Kucherenko[6], and Denis V Vyalikh[7,8] — [1]IFMP, TU Dresden, Germany — [2]Max IV Laboratory, Lund, Sweden — [3]MPI for Chemical Physics of Solids, Dresden, Germany — [4]Kristall- und Materiallabor, Goethe-Universität Frankfurt, Germany — [5]Randall Laboratory, University of Michigan, USA — [6]Institute for Metal Physics, National Academy of Science, Ukraine — [7]DIPC, San Sebastian, Spain — [8]IKERBASQUE, Bilbao, Spain

Ultra-violet angle-resolved photoemission spectroscopy (UV-ARPES) was used to explore the temperature dependences of different surface terminations of the antiferromagnetic Kondo lattice $CeRh_2Si_2$. Spectra were taken from Ce- and Si-terminated surfaces in a wide temperature range, and reveal characteristic $4f$ patterns for weakly (surface) and strongly (bulk) hybridized Ce, respectively. Surprisingly, the temperature dependence of the Fermi level peak points to a considerably larger effective Kondo temperature at the surface, likely due to a higher local-moment effective degeneracy.

Further, we derived the k-resolved dispersion of the Kondo peak which is also found to be distinct due to different sets of itinerant bands to which the $4f$ states couple, highlighting that the Kondo physics vary remarkably between surface and bulk of the Kondo lattice material.

TT 34.3 Wed 10:00 HSZ 204

$TbRh_2Si_2$ and $TbIr_2Si_2$: Single crystal growth and characterization — •Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

In the last decades, many studies on RT_2Si_2 (R = rare earth, T = transition metal) ternary silicides have been made. The compounds which crystallize in the bodycentered tetragonal $ThCr_2Si_2$ structure exhibit exceptional magnetic properties such as superconductivity, valence fluctuations or the Kondo effect. In recent years, we have started to systematically investigate the magnetic properties of RRh_2Si_2 compounds, which present exciting surface properties, strongly influenced by the 4f-magetism [1,2]. So far, the magnetism of $TbRh_2Si_2$ and $TbIr_2Si_2$ has been studied on polycrystalline samples [3,4]. These compounds show antiferromagnetic order below $T_N = 92$ K and $T_N = 84$ K respectively with a magnetic ordering vector k = (001). In this contribution, we present the details of the crystal growth of single crystals of these two compounds grown by Bridgman method from indium flux. We show the results of specific heat, specific resistivity and magnetization measurements, with the focus on the magnetic transition [5].

[1] M. Güttler et al., Sci. Rep. 6, 24254 (2016)
[2] A. Generalov et al., Nano Lett. 17, 811 (2017).
[3] S. Quezel et al., Solid State Commun. 49, 7 (1984)
[4] T. Shigeoka et al., Physics Procedia, 75, 837-844 (2015)
[5] K. Kliemt et al., Cryst Res. Technol. 1900116 (2019)

TT 34.4 Wed 10:15 HSZ 204

Superconductivity and heavy-fermion behavior in locally non-centrosymmetric LnIr$_2$As$_2$ (Ln = La and Ce) — •Seunghyun Khim, Markus König, and Christoph Geibel — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

Compounds containing atoms with a large atomic number are considered a candidate for the realization of unconventional phenomena induced by spin-orbit splitting of degenerated bands and orbitals. In combination with a non-centrosymmetric crystal structure, the resulting asymmetric spin-orbit coupling (ASOC) gives rise to spin-momentum coupled electronic structures. Appearance of superconductivity or strong electronic correlations within these electronic structures could lead to nontrivial phases. Accordingly, LnIr$_2$As$_2$ (Ln = La and Ce) in the $CaBe_2Ge_2$-type structure are promising systems because of the presence of the 5d-orbital element as well as of the lack of local inversion symmetry on each sublayer in the unit cell. Here, we present studies on single crystals of $LaIr_2As_2$ and $CeIr_2As_2$. We discover superconductivity in $LaIr_2As_2$ with a transition temperature T_c = 1.5 K. The Sommerfeld coefficient is $\gamma_0 \sim 9$ mJ/mol-K^2, implying weak electronic correlations. $CeIr_2As_2$, on the other hand, shows enhanced effective mass due to the Kondo interactions between the Ce^{3+} magnetic moments and itinerant electrons. Below 5 K, the specific-heat C/T increases with decreasing T to reach ~ 350 mJ/mol-K^2 at 0.5 K, revealing non-Fermi liquid character. We discuss the physical properties of these compounds in detail, in view of the possible ASOC.

TT 34.5 Wed 10:30 HSZ 204

Quasiparticle bands in the locally non-centrosymmetric heavy-fermion $CeRh_2As_2$ — •Évrard-Ouicem Eljaouhari[1,2], Sébastien Burdin[2], and Gertrud Zwicknagl[1] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany — [2]LOMA, Université de Bordeaux, France

In the study of heavy-fermion materials, non-centrosymmetric ones have gained much interest in the past decade. Indeed, their lack of inversion symmetry in combination with strong spin-orbit coupling (SOC) and magnetic interactions can lead to the emergence of novel phenomena such as unvoncentional superconductivity and quantum phase transitions.

Of particular significance is the new non-centrosymmetric heavy-fermion $CeRh_2As_2$ for which some interesting properties have been reported. For example, measurements have shown the existence of a quasi-quartet crystal electric field (CEF) ground state which would normally not be expected in a tetragonal system. Also and as for other non-centrosymmetric superconductors, a Rashba-type SOC which leads to the splitting of the Fermi surface into two and to the possibility of mixing singlet-triplet superconducting states is expected.

In order to get deeper understanding of this compound and its properties, a realistic modeling of its electronic structure is needed. In this talk we present our results on the quasiparticle bands of $CeRh_2As_2$ which have been calculated thanks to the Renormalised Band method which proceeds from a relativistic description of the electronic structure and accounts for CEF effects and for the mass renormalisation.

TT 34.6 Wed 10:45 HSZ 204

$CeRu_2P_2$ and $CeCo_2P_2$: Single Crystal Growth Method and Magnetic Properties — •Fabian Feldmann, Marius Peters, Johannes Hellwig, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut Goethe Universität Frankfurt/Main

CeT_2P_2 (T = Co, Ru) are rare-earth ternary phosphides with tetragonal $ThCr_2Si_2$ -type crystal structure. $CeRu_2P_2$ is an intermediate valent system [1],[2] and $CeCo_2P_2$ is an antiferromagnet with a rather high Néel temperature $T_N = 440$ K [3], most likely due to an interplay of 3d and 4f magnetism, although Ce is close to a non-magnetic Ce^{4+} state.

Here, we present the high-temperature metal-flux technique that was used to obtain millimeter-sized single crystals. Furthermore, we show magnetic measurements for both systems. $CeCo_2P_2$ shows anisotropic behavior above the ordering temperature, which is unexpected for itinerant 3d magnetism. $CeRu_2P_2$ as a reference system without the d magnetism of Co also shows anisotropic behavior and may indicate that $CeCo_2P_2$ also exhibits some remaining Ce 4f magnetism [4].

[1] A. Amorese et al., Phys. Rev. B **93**, 165134 (2016)
[2] T. Fujiwara et al., J. Phys.: Conf. Ser. **273**, 012112 (2011)
[3] Y. Tian et al., Physica B **512**, 75 (2017)
[4] K. Kliemt et al., Cryst. Res. Technol., 1900116 (2019)

TT 34.7 Wed 11:00 HSZ 204

Orientation of ground-state orbital in $CeCoIn_5$ and $CeRhIn_5$ — •Martin Sundermann[1,2], Andrea Amorese[1,2], Fabio Strigari[1], Brett Leedahl[2], Liu Hao Tjeng[2], Maurits W. Haverkort[3], Hlynur Gretarsson[4,2], Hasan Yavaş[4], Marco Moretti Sala[5], Eric D. Bauer[6], Priscila F. S. Rosa[6], Joe D. Thompson[6], and Andrea Severing[1,2] — [1]2. Physikalisches Institut, Universität zu Köln — [2]Max Planck Institut für Chemische Physik fester Stoffe, Dresden — [3]Institut für Theoretische Physik, Universität Heidelberg — [4]PETRA III, Deutsches Elektronen-Synchrotron (DESY), Hamburg — [5]European Synchrotron Radiation Facility (ESRF), Grenoble, Frankreich — [6]Los Alamos National Laboratory, New Mexico, USA

We present core-level non-resonant inelastic x-ray scattering (NIXS) data of the heavy fermion compounds $CeCoIn_5$ and $CeRhIn_5$ measured at the Ce $N_{4,5}$-edges. The higher than dipole transitions in NIXS allow determining the orientation of the Γ_7 crystal-field ground-state orbital within the unit cell. The crystal-field parameters of the $CeMIn_5$ compounds and related substitution phase diagrams have been investigated in great detail in the past; however, whether the ground-state wave function is the Γ_7^+ (x^2-y^2) or Γ_7^- (xy orientation) remained undetermined. We show that the Γ_7^- doublet with lobes along the (110) direction forms the ground state in $CeCoIn_5$ and $CeRhIn_5$. A comparison is made to the results of existing DFT+DMFT calculations.

15 min. break.

TT 34.8 Wed 11:30 HSZ 204

Investigation of Ce-based Materials with Multiple Inequivalent Kondo-sites. — Jardoslav Valenta[1], Petr Opletal[1], Jan Fikáček[1], Elen Duverger Nedellec[1], Jiří Pospíšil[1], Shinsaku Kambe[2], Hironori Sakai[2], Yo Tokunaga[2], Russel E Walstedt[3], Robert Küchler[4], Jacintha Banda[4], Manuel Brando[4], and •Jeroen Custers[1] — [1]Dept. of Condensed Matter Physics, Charles University, Ke Karlovu, 5, 121 16 Praha, Czech Republic — [2]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai-mura, Ibaraki 319-1195, Japan — [3]Physics Department, The University of Michigan, Ann Arbor, MI 48109, USA — [4]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, D-01187 Dresden, Germany

The vast majority of heavy fermion compounds investigated in close proximity to a magnetic quantum phase transition exhibit only one crystallographic site for the Rare Earth or Actinide ion. Here we present results on ongoing research on several Ce–based compounds with multiple Ce-sites. Recent ^{115}In NQR/NMR results on Ce_3PtIn_{11} which has two inequivalent Ce-sites, show evidence for two quantum critical points. Each can be associated with a particular Ce-site. Our investigation on a series of $(Ce_{1-x}La_x)_3Al_{11}$ reveals that, up to $x = 0.25$, we substitute La for Ce on the Ce2 site only. As the parent compound Ce_3Al_{11} has 2 sites (Ce1: 2 atoms/f.u.; Ce2: 1 atom/f.u.) we thus can follow the evolution of removing one Kondo-site step by step. Finally we will present our first results on $Ce_3Rh_5Ge_7$. This novel compound harbors 3 inequivalent Ce-sites.

TT 34.9 Wed 11:45 HSZ 204

Valence effect in the thermopower of Eu systems — •Ulrike Stockert[1], Silvia Seiro[2,1], Nubia Caroca-Canales[1], Elena Hassinger[1], and Christoph Geibel[1] — [1]MPI for Chemical Physics of Solids, Dresden — [2]Institute for Solid State Research, IFW, Dresden

$EuIr_2Si_2$ and $EuNi_2P_2$ have been classified as valence-fluctuating (VF) materials with a strongly temperature-dependent Eu valence. At low temperature T the effective charge carrier masses are significantly enhanced due to hybridization between the Eu 4f and the conduction electron states. The relative importance of hybridization and valence fluctuations in Eu-based VF systems is not yet clear and a topic of current interest.

We present thermal conductivity and thermopower data for $EuIr_2Si_2$ and $EuNi_2P_2$ in the temperature range beween 2 K and 300 K. The thermal conductivities of both materials are conventional with differences arising due to different crystal quality. By contrast, the thermopowers of $EuIr_2Si_2$ and $EuNi_2P_2$ exhibit large values and a characteristic T dependence that cannot be explained satisfactorily by simple hybridization models. Instead, we may describe the thermopower by taking into account the temperature-dependence of the Eu valence, which leads to additional thermopower contributions due to variations in the chemical potential. These findings corroborate the relevance of the valence fluctuations for understanding the properties of $EuIr_2Si_2$ and $EuNi_2P_2$ at intermediate temperatures.

TT 34.10 Wed 12:00 HSZ 204

Crystal growth of the valence fluctuating system $EuPd_2Si_2$ — •Marius Peters, Kristin Kliemt, Eunhyung Cho, Doan-My Tran, Franz Ritter, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt

The study of collective phenomena raising from enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice-degrees of freedom. One system providing such a strongly coupled phase transition is $EuPd_2Si_2$ of the $ThCr_2Si_2$ structural type, showing a temperature induced valence transition of europium between the energetically vicinal valence states Eu^{2+} and Eu^{3+} at about 170K [1]. First reports on the synthesis of single crystals came up only recently [2], but a deep investigation of the valence transition in this compound is still missing.

We approached the ternary Eu-Pd-Si system using differential thermal analysis to map the local composition phase diagram. We used the Bridgman and the Czochralski method fort he successful growth of mm-sized single crystals of $EuPd_2Si_2$. In this contribution we will present chemical and structural characterization of these crystals and some preliminary physical measurements around the valence transition.

[1] E. V. Sampathkumaran et al., Journal of Physics C14, L237 (1981).
[2] Y. Onuki et al., Philosophical Magazine 97, 3399 (2017).

TT 34.11 Wed 12:15 HSZ 204

Crystal growth and characterization of isotope-pure $YbRh_2Si_2$ (^{171}Yb, ^{173}Yb, ^{174}Yb) — •Sebastian Witt[1], Susanna Rongstock[1], Thanh Duc Nguyen[1], Manuel Brando[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe University, Frankfurt, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

A central question in condensed matter research concerns the interplay between quantum criticality and unconventional superconductivity in strongly correlated electron systems such as heavy-electron systems. Recently, superconductivity was also discovered in the quantum-critical material $YbRh_2Si_2$ at 2mK [1]. So far the interplay between electronic and nuclear moments of Yb and its impact on the superconductivity is not settled. For that reason, it is essential to investigate $YbRh_2Si_2$ samples with a well-defined Yb nuclear spin.

In this talk, we report the crystal growth with the entire range of nuclear spin number in the single crystals (^{171}Yb: I = 1/2, ^{173}Yb: I = 5/2, ^{174}Yb: I = 0). For the crystal growth we developed a new setup for small masses, especially for the metallothermic reduction of metallic Yb from Yb_2O_3. Besides the single crystal characterization (Laue, PXRD) we will present measurements of the resistivity and isotopic composition. To investigate the influence of nuclear spin on the electronic degrees of freedom, we will show the heat capacity around the antiferromagnetic transition at 70mK.

[1] E. Schuberth et al., Science, 351, 485-488 (2016).

TT 34.12 Wed 12:30 HSZ 204

Extremely weak magnetic exchange in metallic 4f-electron system leads to enormous magnetocaloric effect — •Thomas Gruner[1], Jiasheng Chen[1], Dongjin Jang[2], Jacintha Banda[3], Christoph Geibel[3], Manuel Brando[3], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]KRISS, Daejeon, Republic of Korea — [3]MPI CPfS, Dresden, Germany

Traditional cryogenic demagnetisation refrigerators for the temperature range $40\,\mathrm{mK} < T < 2\,\mathrm{K}$ use hydrated paramagnetic salts as cooling agents. This often imposes significant restrictions on equipment designs due to the weak thermal conductivity and the need for hermetic sealing of these insulating materials. Recently, we showed that certain Yb-based metallic materials provide attractive alternatives [1]. In a search for even more appropriate materials we investigated a number of Heusler- and half-Heusler compounds and studied their structural, magnetic, transport and magnetocaloric properties, enabling us to select a particularly promising Yb system.

Our measured data evidence metallic behaviour, the absence of superconductivity and a stable trivalent Yb^{3+} state, without any sign of a significant Kondo interaction. This new compound can be easily brought into shape, making the production of powerful cooling pills much simpler compared to commonly used paramagnetic salt or garnet refrigerants. By performing different demagnetisation tests, we demonstrated the feasibility of a simple, economical and durable alternative for traditional cooling devices for temperatures down to 120 mK.

[1] Jang, Gruner et al.; Nature Commun.; **6**, 8680 (2015)

TT 34.13 Wed 12:45 HSZ 204

Visualizing the Kondo lattice crossover in an Yb-based heavy fermion system with Compton scattering — •Monika Güttler[1], Kurt Kummer[2], Akihisa Koizumi[3], Kristin Kliemt[4], Cornelius Krellner[4], Clemens Laubschat[1], and Denis Vyalikh[5,6] — [1]IFMP, TU Dresden, Germany — [2]ESRF, Grenoble, France — [3]Graduate School of Material Science, University of Hyogo, Japan — [4]Kristall- und Materiallabor, Physikalisches Institut, Goethe-Universität Frankfurt, Germany — [5]DIPC, San Sebastian, Spain — [6]IKERBASQUE, Bilbao, Spain

With the breakdown of coherent Kondo scattering with rising temperature, the Fermi surface (FS) in rare earth Kondo lattices is expected to transition from the *large* FS counting the $4f$ moments, which form entangled quasiparticles with huge masses with the conduction states, to the *small* FS with decoupled and localized $4f$ moments. A direct observation of this transition with temperature has however remained elusive because conventional probes of the FS in Kondo lattices require high magnetic fields which might reconstruct the FS or cannot work reliably at elevated temperatures. Using high-resolution Compton scattering we overcome these limitations and show that the FS topology in the prototypical Kondo lattice $YbRh_2Si_2$ undergoes pronounced changes between 14 K and 300 K in zero magnetic field. We present clear evidence for a largely restored small FS at room temperature which could not be observed before. Our results set an upper bound for the relevant energy scale of the complex Kondo crossover phenomenon in $YbRh_2Si_2$.

TT 35: Frustrated Magnets - Strong Spin-Orbit Coupling 1 (joint session TT/MA)

Time: Wednesday 9:30–13:00 Location: HSZ 304

Invited Talk TT 35.1 Wed 9:30 HSZ 304

Field-induced magnetic order in the Kitaev material α-$RuCl_3$ — •Lukas Janssen — Technische Universität Dresden, Dresden, Germany

α-$RuCl_3$ has recently been intensely debated in the context of a potential field-induced spin-liquid phase. However, interesting physics can be observed in this material also at field strengths below and above the putative spin-liquid regime. In this combined experimental and theoretical work, we demonstrate the existence of a novel ordered phase at intermediate field strengths, characterize its nature, and discuss implications for the dominant exchange interactions present in this material.

Talk includes results obtained with Christian Balz, Stephen E. Nagler, and Matthias Vojta.

TT 35.2 Wed 10:00 HSZ 304

Field-induced quantum phase transitions in α-RuCl$_3$ — •Sebastian Bachus[1], Yoshifumi Tokiwa[1], Vladimir Tsurkan[2], Alois Loidl[2], Anton Jesche[1], Alexander A. Tsirlin[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Recently the observation of a half-integer quantized thermal Hall effect in the Kitaev material α-RuCl$_3$, possibly indicating chiral Majorana edge modes, attracted considerable attention [1]. It arises in a finite field range exceeding the critical field for long-range antiferromagnetic order. We utilize a high-resolution alternating field method for the precise determination of the truly adiabatic magnetocaloric effect or magnetic Grüneisen parameter down to ~ 1 K and in magnetic fields up to 15 T. Together with accompanying heat capacity measurements, it allows us to determine the entropy evolution when tuning the system into and out of the presumed topological Kitaev quantum spin liquid regime as a function of the applied field. We present a comprehensive analysis of the thermodynamic data and comparison to [2].

Work supported by the German Science Foundation via Project No. 107745057 (TRR80).

[1] Y. Kashara *et al.*, Nature 559, 227-231 (2018).
[2] C. Balz *et al.*, Phys. Rev. B 100, 060405(R) (2019).

TT 35.3 Wed 10:15 HSZ 304

High-Field Quantum Disordered State in α-RuCl$_3$ — •Anuja Sahasrabudhe[1], David Kaib[2], Stephan Reschke[3], Raphael German[1], Thomas Koethe[1], Jonathan Buhot[4], Dmytro Kamenskyi[4], Ciarán Hickey[5], Petra Becker[6], Vladimir Tsurkan[3,7], Alois Loidl[7], Seung-Hwan Do[8], Kwang-Yong Choi[8], Markus Grüninger[1], Stephen Winter[2], Zhe Wang[1,9], Roser Valentí[2], and Paul van Loosdrecht[1] — [1]Institute of Physics II, University of Cologne — [2]Institut für Theoretische Physik, Goethe-Universität Frankfurt — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [4]High Field Magnet Laboratory (HFML - EMFL), Radbound University, Nijmegen — [5]Institute for Theoretical Physics, University of Cologne — [6]Institute for Geology and Mineralogy, University of Cologne — [7]Institute of Applied Physics, MD2028 Chisinau — [8]Department of Physics, Chung-Ang University, Seoul — [9]Institute of Radiation Physics, Helmholtz Zentrum Dresden-Rossendorf

Layered α-RuCl$_3$ does not show a true Kitaev quantum spin liquid state due to the presence of additional interactions leading to magnetic ordering at low temperature. This ordering can be suppressed by applying a moderate in-plane magnetic field, leading to a novel high field phase. Using Raman and THz spectroscopy, combined with an exact diagonalization study, we show that the induced high field state can be identified as a partially-polarized quantum disordered magnetic state characterised by a gapped multi-particle continuum out of which a bound-state emerges as well as a sharp single-particle response.

TT 35.4 Wed 10:30 HSZ 304

Pressure-dependent investigation of the elastic constants in α-RuCl$_3$ — •A. Hauspurg[1,2], S. Zherlitsyn[1], T. Yanagisawa[3], V. Felea[1], V. Tsurkan[4], K.-Y. Choi[5], S.-H. Do[5], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Hokkaido University, Sapporo, Japan — [4]Institute of Physics, University of Augsburg, Germany — [5]Department of Physics, Chung-Ang University, Seoul, South Korea

As a paradigmatic example of the realization of Kitaev physics on a honeycomb lattice, α-RuCl$_3$ serves for numerous experimental investigations of fundamental physics of this model. Yet it shows a striped AF groundstate with evidence for a field-induced quantum spin liquid state. We performed investigations of the elastic constants by means of propagating ultrasound waves in this intriguing compound. Under variable magnetic fields, temperatures, and pressures we obtain further insight into its phase diagram. We will show evidence of pressure-dependent contributions of competing Kitaev and Heisenberg terms, which results in a suppression of the antiferromagnetically ordered phase at low temperatures.

TT 35.5 Wed 10:45 HSZ 304

Pressure-induced dimerization and Kitaev spin liquid regime of α-RuCl$_3$ — •Quirin Stahl[1], Gaston Garbarino[2], Tobias Ritschel[1], Francisco J. Martinez-Casado[3], Gilberto Fabbris[4], Joerg Strempfer[4], Maximilian Kusch[1], Anna Isaeva[1,5], Thomas Doert[5], Randirley Beltrán Rodríguez[6], Rajyavardhan Ray[6], Silvina P. Limandri[7], Maria Roslova[5], Liviu Hozoi[6], Ravi Yadav[6], Jeroen van den Brink[6,8], Gaël Bastien[6], Anja U.B. Wolter[6], Bernd Büchner[1,6], and Jochen Geck[1] — [1]IFMP, TU Dresden, Germany — [2]ESRF, Grenoble, France — [3]ILL, Grenoble, France — [4]APS, Argonne National Laboratory, USA — [5]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [6]IFW Dresden, Germany — [7]IFEG, National University of Córdoba, Argentina — [8]Institute of Theoretical Physics, TU Dresden, Germany

Recently, the honeycomb material α-RuCl$_3$ has been identified as a possible realization of the Kitaev model, rendering this material an ideal platform for exploring Kitaev magnetism experimentally. However, the onset of long-range magnetic order at $T_N = 7$ K and ambient pressure, i.e. the absence of a spin liquid ground state, implies that α-RuCl$_3$ deviates from the ideal Kitaev model under these conditions. We therefore set out to elucidate whether α-RuCl$_3$ can be driven into the true Kitaev regime by means of hydrostatic pressure. Our x-ray diffraction and extended x-ray absorption fine structure studies reveal a rich structural phase diagram, including pressure induced Ru-Ru dimerization as well as a high-symmetry rhombohedral phase. The latter is indeed found to be very close to the ideal Kitaev model.

TT 35.6 Wed 11:00 HSZ 304

Giant coupling between phonons and Majorana fermions in a Kitaev spin liquid — •Dirk Wulferding[1,2], Youngsu Choi[3], Yann Gallais[4], Clément Faugeras[5], Peter Lemmens[1,2], Seung-Hwan Do[6], and Kwang-Yong Choi[3] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]LENA, TU-BS, Braunschweig, Germany — [3]Chung-Ang Univ., Seoul, Korea — [4]Univ. Paris-Diderot, Paris, France — [5]LNCMI Grenoble, France — [6]Oak Ridge National Lab, USA

In the Kitaev honeycomb candidate material α-RuCl$_3$ a continuum of fractionalized Majorana fermions exists which can be directly probed by Raman spectroscopy [1-5]. In-plane magnetic fields gap the continuum, thereby confining it energetically to the regime of optical phonons. Using high-field Raman spectroscopy [6], we shine a light onto the interplay of Majorana fermions and phonons, which results in a drastic reduction of the phonon lifetimes together with a renormalization of phonon energies.

Work supported by QUANOMET NL-4 and DFG LE967/16-1.

[1] Sandilands, et al., Phys. Rev. Lett. 114, 147201 (2014)
[2] Knolle, et al., Phys. Rev. Lett. 113, 187201 (2014)
[3] Glamazda, et al., Phys. Rev. B 95, 174429 (2017)
[4] Glamazda, et al., Nat. Commun. 7, 12286 (2016)
[5] Sahasrabudhe, et al., arXiv:1908.11617 (2019)
[6] Wulferding, et al., arXiv:1910.00800 (2019)

15 min. break.

TT 35.7 Wed 11:30 HSZ 304

Thermal Transport of the Kitaev spin-liquid candidate α-RuCl$_3$ — Richard Hentrich[1], •Matthias Gillig[1], Xiaochen Hong[1], Federico Caglieris[1], Maria Roslova[2], Anna Isaeva[1,2], Thomas Doert[2], Uli Zeitler[3], Matija Culo[3], Maryam Shahrokhvand[3], Bernd Büchner[1,4], and Christian Hess[1,4] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, TU Dresden, Germany — [3]High Field Magnet Laboratory (HFML-EFML), Radboud University Nijmegen, 6525 ED Nijmegen, The Netherlands — [4]Center for Transport and Devices, TU Dresden, Germany

α-RuCl$_3$ currently is the best known candidate material for realizing Kitaev physics. Previous experiments on the longitudinal thermal conductivity revealed a strong coupling of he magnetic and phononic subsystems which results in a strongly magnetic field dependent thermal conductivity due to the field-induced opening of a gap [1]. Furthermore, a sizeable thermal Hall effect has been observed which triggered the search for signatures of fractionalized thermal transport due to topological edge modes near an in-plane field value of 8 T where long-range magnetic order is suppressed but the spin gap is still small [2].

Here we focus on low-temperature and high-field (up to 30 T) studies of the thermal transport which suggest the persistence of low-energy field-dependent modes up to the highest field studied at 30 T.

[1] R. Hentrich et al., Phys. Rev. Lett. **120**, 117240 (2018)
[2] Y. Kasahara et al., Nature **559**, 227 (2018)

TT 35.8 Wed 11:45 HSZ 304

Magnetic properties of two sodium ruthenates Na_2RuO_3 and Na_3RuO_4 — •Vera P. Bader[1], Alexander A. Tsirlin[1], Anton Jesche[1], Clemens Ritter[2], and Philipp Gegenwart[1] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Institut Laue-Langevin, Grenoble, France

Ruthenates show a diversity of magnetic phenomena, e.g. due to transitions between the non-magnetic $J = 0$ state and excited $J = 1$ levels in Ru^{4+} [1] or due to strong Ru-O covalency in the case of Ru^{5+} [2]. Powder samples of Na_2RuO_3 and Na_3RuO_4 were prepared via solid state reactions in a controlled atmosphere. The Ru^{4+} ions in Na_2RuO_3 form honeycomb layers which are stacked along the crystallographic c-axis. The measured diffraction pattern could be simulated under the assumption of stacking faults. The inverse susceptibility deviates from the Curie-Weiss behaviour and shows a downward bending in the high temperature region indicating a paramagnetic Van Vleck contribution which would be expected for a $J = 0$ ground state. In Na_3RuO_4 the Ru^{5+} ions form isolated tetramers which are composed of two equilateral triangles. The magnetic susceptibility reveals an antiferromagnetic transition at 30 K while the heat capacity data show two successive phase transitions at 25 K and 28 K. Up to now, the origin of the two phase transitions is not known. Neutron diffraction reveals the absence of symmetry lowering upon both transitions and the development of incommensurate magnetic order.

[1] J. Chaloupka et al., arXiv:1910.00074 (2019)
[2] A. Hariki et al., PRB 96 155135 (2017)

TT 35.9 Wed 12:00 HSZ 304

On the charge transfer energy in iridates: a HAXPES study — •Daisuke Takegami[1], Deepa Kasinathan[1], Klaus Wolff[1], Simone Altendorf[1], Chun-Fu Chang[1], Katharina Hoefer[1], Anna Meléndez-Sans[1], Yuki Utsumi[1], Federico Meneghin[1], Thai Duy Ha[1], Chien-Han Yen[1], Kai Chen[2], Chang-Yang Kuo[1,3], Yen-Fa Liao[3], Ku-Ding Tsuei[3], Ryan Morrow[4], Sabine Wurmehl[4], Beluvalli E. Prasad[1], Martin Jansen[5], Alexander Komarek[1], Philipp Hansmann[1], and Liu Hao Tjeng[1] — [1]MPI for Chemical Physics of Solids, Dresden, Germany — [2]Institute of Physics II, University of Cologne, Cologne, Germany — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]Leibniz Institute for Solid State and Materials Research IFW Dresden, Dresden, Germany — [5]MPI for Solid State Research, Stuttgart, Germany

We have investigated the electronic structure of iridates in the double perovskite crystal structure containing either Ir^{4+} or Ir^{5+} using HAXPES. The experimental valence band spectra can be well reproduced using tight binding calculations including only the Ir 5*d*, O 2*p* and O 2*s* orbitals with parameters based on the down-folding of the DFT band structure results. We found that regardless the A and B cations, the A_2BIrO_6 iridates have essentially zero O 2*p* to Ir 5*d* charge transfer energies. They are extremely covalent systems with the consequence is that the magnetic exchange interactions become very long-ranged, thereby hampering the materialization of the Kitaev model. Nevertheless, it still would be possible to realize a spin-liquid system using the iridates with a proper tuning of the competing exchange interactions.

TT 35.10 Wed 12:15 HSZ 304

Magnetization density distribution of Sr_2IrO_4: Deviation from a *local* $j_{\text{eff}} = 1/2$ picture — Jaehong Jeong[1], •Benjamin Lenz[2,3], Arsen Gukasov[1], Xavier Fabreges[1], Andrew Sazonov[4], Vladimir Hutanu[4], Alex Louat[5], Cyril Martins[6], Silke Biermann[3,7], Veronique Brouet[5], Yvan Sidis[1], and Philippe Bourges[1] — [1]Laboratoire Léon Brillouin, CEA Saclay, Gif-sur-Yvette, France — [2]IMPMC, Sorbonne Université, Paris, France — [3]CPHT, Ecole Polytechnique, Palaiseau, France — [4]Institute of Crystallography, RWTH Aachen, Germany — [5]LPS, Université Paris-Saclay, Orsay, France — [6]LCPQ, Université Paul Sabatier, Toulouse, France — [7]Collège de France, Paris, France

5*d* iridium oxides are of huge interest due to the potential for new quantum states driven by strong spin-orbit coupling. The $j_{\text{eff}} = 1/2$ state of Sr_2IrO_4 is such a state and consists of a quantum superposition of the three t_{2g} orbitals with nearly equal population, which stabilizes an unconventional Mott insulating state.
Here, we report an anisotropic and aspherical magnetization density distribution measured by polarized neutron diffraction in a magnetic field up to 5T at 4K, which strongly deviates from a *local* $j_{\text{eff}} = 1/2$ picture. Theoretical considerations based on a momentum-dependent composition of the $j_{\text{eff}} = 1/2$ orbital and an estimation of the different contributions to the magnetization density casts the applicability of an effective one-orbital $j_{\text{eff}} = 1/2$ Hubbard model into doubt.
The analogy to the superconducting copper oxide systems might thus be weaker than commonly thought.

TT 35.11 Wed 12:30 HSZ 304

Magnetodielectric and magnetoelastic coupling in the frustrated fcc antiferromagnet $(NH_4)_2IrCl_6$ — •Nazir Khan and Alexander A. Tsirlin — Experimental Physics VI, University of Augsburg, 86135 Augsburg, Germany

Magnetodielectric and magnetoelastic phenomena in the fcc antifluorite $(NH_4)_2IrCl_6$ single crystal have been investigated using thermodynamic, dielectric and magnetostriction measurements. The compound is an antiferromagnetic Mott insulator with the charge gap Δ=0.9 eV and Néel temperature T_N=2.2 K. The antiferromagnetic ordering leads to a decrease in temperature-dependent dielectric constant at zero applied field. Further, in the magnetically ordered state the dielectric constant and macroscopic sample length show a strong magnetic field dependence. The dielectric constant increases monotonically with increasing field without any saturation up to a field 14 T where it exhibits a magnetocapacitance of about 0.6%. The magentodielectric phenomenon in the present system is believed to be due to the magnetostrictive effects and spin-phonon coupling. The magnetostrictive effects are evident from the temperature and field dependence of the macroscopic length change. Spin-phonon coupling results when the energy scale of a soft phonon mode associated with the rotation of $IrCl_6$ octahedra becomes comparable with that of a magnetic interaction or magnetic field.

[1] T. Katsufuji *et al.*, Phys. Rev. B **64**, 054415 (2001)
[2] Jaye K. Harada *et al.*, Phys. Rev. B **93**, 104404 (2016)

TT 35.12 Wed 12:45 HSZ 304

$MgIrO_3$ and $ZnIrO_3$: new hyperhoneycomb iridates — •Alexander O. Zubtsovskii and Alexander A. Tsirlin — EP VI, EKM, University of Augsburg, Germany

Iridates with edge-sharing IrO_6 octahedra host Kitaev interactions and show unusual magnetic behavior triggered by the exchange anisotropy and frustration. Here, we report two new compounds, $MgIrO_3$ and $ZnIrO_3$, obtained by the ionic substitution into the hyperhoneycomb beta-Li_2IrO_3. Crystal structures studied by synchrotron x-ray diffraction and high-resolution electron microscopy show lower symmetry than the parent compound, because Mg^{2+} and Zn^{2+} as divalent cations occupy different positions than Li^+. Magnetic behavior is characterized using magnetization and heat capacity measurements as well as muon spin relaxation.

TT 36: Many-body Systems: Equilibration, Chaos and Localization II (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: HÜL 186

TT 36.1 Wed 9:30 HÜL 186

Many-body dynamical localization in the kicked Bose-Hubbard chain — Michele Fava[1], Rosario Fazio[2,3], and •Angelo Russomanno[4] — [1]Rudolf Peierls Centre for Theoretical Physics, Clarendon Laboratory, University of Oxford, Oxford OX1 3PU, UK — [2]Abdus Salam ICTP, Strada Costiera 11, I-34151 Trieste, Italy — [3]Dipartimento di Fisica, Universit\'a di Napoli "Federico II", Monte S. Angelo, I-80126 Napoli, Italy — [4]Max-Planck-Institut f\"ur Physik Komplexer Systeme, N\"othnitzer Strasse 38, D-01187, Dresden, Germany

We show that a clean kicked Bose-Hubbard model exhibits a many-body dynamically localized phase. This phase shows ergodicity breaking and we can argue that this property persists in the large-size limit: the Floquet states violate eigenstate thermalization and then the asymptotic value of local observables depends on the initial state and is not thermal. This implies that the system does not generically heat up to infinite temperature, for almost all the initial states. Differently from many-body localization here the entanglement entropy linearly increases in time. This increase corresponds to space-delocalized Floquet states which are nevertheless localized across specific subsectors of the Hilbert space: In this way the system is prevented from randomly exploring all the Hilbert space and does not thermalize.

TT 36.2 Wed 9:45 HÜL 186

Entanglement clusters in many-body localized systems — •Kevin Hemery, Adam Smith, and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Strasse 1, D-85748 Garching, Germany

A complete understanding of the many body localized (MBL)-ergodic transition is still missing. We investigate this phenomenon by analysing the entanglement structure of the eigenstates of the Heisenberg chain in presence of a disordered field. Our method is based on a combination of the two-site mutual information and a graph theory clustering algorithm.

First we test our approach by recovering the scaling behaviour of the number of entangled clusters across the phase transition, which has previously been extracted using the full density matrix. On the MBL side, we access large systems by using the so-called "DMRG-X" algorithm, a variational matrix-product-states based method. We compare our results to predictions drawn from renormalisation group based theories of the thermalisation avalanche.

TT 36.3 Wed 10:00 HÜL 186

Emergent localization in euclidean random matrices without small parameter — •Anton Kutlin and Ivan Khaymovich — Max Planck Institute for the Physics of Complex Systems, D-01187 Dresden, Germany

We study the wave functions localization properties for the isotropic euclidean random matrix (ERM) model in arbitrary dimension. Due to its generality, this model arises naturally in various physical contexts such as studies of vibrational modes [1,2], artificial atomic systems [3,4], liquids and glasses [5-7], ultracold gases and photon localization phenomena [8,9]. We generalize the known[10,11] renormalization group (RG) approach, formulate universal sufficient conditions for localization in ERM models and inspect a striking duality of the wave function spatial structure between ERMs and translation-invariant (TI) models with a diagonal disorder[12]. Finally, we discuss possible extensions of the approach to anisotropic models.

[1] B. Ash et al., PRE 98, 042134 (2018) [2] A. Amir et al., PRX 3, 021017 (2013) [3] A. de Paz et al., PRL 111, 185305 (2013) [4] P. I. Karpov et al., PRE 97, 062157 (2018) [6] J .Rehn et al., Phil. Trans. R. Soc. A 374: 20160093 (2016) [7] J. Rehn et al., PRB 92, 085144 (2015) [8] T. Scholak et al., PRA 90, 063415 (2014) [9] A. Gero et al., PRA 88, 023839 (2013) [10] A. L. Burin et al., Pis'ma Zh. Eksp. Teor. Piz. 50, No. 6, 304-306 (1989). [11] L. S. Levitov, PRL 64, 547 (1990). [12] X. Deng et al., PRL 120, 110602 (2018).

TT 36.4 Wed 10:15 HÜL 186

Ergodization times and dynamical glass in classical Josephson junction chains — •Carlo Danieli[1], Mithun Thudiyangal[2], Yagmur Kati[3], and Sergej Flach[4] — [1]Max Planck Institute for the Physics of Complex Physics, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Mathematics and Statistics, University of Massachusetts, Amherst MA 01003-4515, USA — [3]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, Korea — [4]Center for Theoretical Physics of Complex Systems, Institute for Basic Science, Daejeon, Korea

Models of classical Josephson junction chains turn integrable in the limit of large energy densities or small Joseph- son coupling strength. Close to these limits, the Josephson coupling between superconducting grains induces a short range network. We compute distributions of finite-time averages of grain charges and extract the ergodization time TE which controls their convergence to ergodic delta distributions. We relate TE to the statistics of the fluctuations in time of the grain charges, which are dominated by fat tails. The ergodization time TE grows anomalously fast upon approaching the integrable limit as compared to the Lyapunov time TΛ - the inverse largest Lyapunov expo- nent. The microscopic reason for the observed behavior - which we labeled dynamical glass - is rooted in a growing number of grains evolving over long time in a regular fashion due to low probability of resonant interactions with the neighboring ones. We conjecture that the observed dynamical glass is Josephson junction networks irrespective of their dimensionality. Ref: Phys.Rev.Lett. 122 054102 (2019).

TT 36.5 Wed 10:30 HÜL 186

Real-time dynamics of string breaking in quantum spin chains — •Roberto Verdel[1], Fangli Liu[2], Seth Whitsitt[2], Alexey V. Gorshkov[2,3], and Markus Heyl[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187-Dresden, Germany — [2]Joint Quantum Institute, NIST/University of Maryland, College Park, MD 20742, USA — [3]Joint Center for Quantum Information and Computer Science, NIST/University of Maryland, College Park, MD 20742, USA

String breaking is a central dynamical process in theories featuring confinement, where a string connecting two charges decays at the expense of the creation of new particle-antiparticle pairs. In this talk, we show that this process can also be observed in quantum Ising chains [1], where domain walls get confined either by a symmetry-breaking field or by long-range interactions. Our main finding is that string breaking occurs, in general, as a two-stage process: First, the initial charges remain static and stable; yet, the connecting string can undergo complex dynamics. In the second stage, which can be severely delayed due to dynamical constraints happening in the previous phase, the string finally breaks. We analyse the constrained many-body dynamics of the first stage and its consequences for the final string breaking or the suppression of it.

References: [1] R. Verdel, F. Liu, S. Whitsitt, A. V. Gorshkov, and M. Heyl, (2019), arXiv:1911.11382 [cond-mat.stat-mech].

TT 36.6 Wed 10:45 HÜL 186

Dynamics of strongly interacting systems: From Fock-space fragmentation to Many-Body Localization — •Giuseppe De Tomasi[1], Daniel Hetterich[2], Pablo Sala[3], and Frank Pollmann[4] — [1]TUM Munich/Cambridge University — [2]TUM Munich — [3]TUM Munich — [4]TUM Munich

We study the t-V disordered spinless fermionic chain in the strong coupling regime, t/V –> 0. Strong interactions highly hinder the dynamics of the model, fragmenting its Hilbert space into exponentially many blocks in system size. Macroscopically, these blocks can be characterized by the number of new degrees of freedom, which we refer to as movers. We focus on two limiting cases: Blocks with only one mover and the ones with a finite density of movers. The former many-particle block can be exactly mapped to a single-particle Anderson model with correlated disorder in one dimension. As a result, these eigenstates are always localized for any finite amount of disorder. The blocks with a finite density of movers, on the other side, show an MBL transition that is tuned by the disorder strength. Moreover, we provide numerical evidence that its ergodic phase is diffusive at weak disorder. Approaching the MBL transition, we observe sub-diffusive dynamics at finite time scales and find indications that this might be only a transient behavior before crossing over to diffusion.

15 min. break

TT 36.7 Wed 11:15 HÜL 186

Impact of pertubations on expectation value dynamics — •Robin Heveling, Lars Knipschild, and Jochen Gemmer — University of Osnabrueck, Osnabrueck, Germany

Recently it was advocated by several groups that a variety of pertubations in condensed matter type systems may have "generic" effects on the dynamics of expectation values [1,2,3]. We investigate this approach numerically and to some extend analytically, scrutinizing various ways of modelling said generic effects.

[1] L. Dabelow, P. Reimann, Perturbed relaxation of quantum many-body systems, arXiv:1903.11881
[2] J. Richter et al., Exponential damping induced by random and realistic pertubations, arXiv:1906.09268
[3] L. Knipschild, J. Gemmer, Stability of quantum dynamics under constant Hamiltonian pertubations, arXiv:1811.00381

TT 36.8 Wed 11:30 HÜL 186

Influence of drive smoothness on the Floquet MBL transition — •Tobias Gulden[1,2], Asaf Diringer[2], and Netanel Lindner[2] — [1]IST Austria — [2]Technion - Israel Institute of Technology

We investigate how the critical driving amplitude at the Floquet MBL-to-ergodic phase transition changes between smooth and non-smooth driving over a large range of frequencies. To this end we study numerically a disordered spin-1/2 chain which is periodically driven by a sine or a square-wave drive, respectively. In both cases the critical driving amplitude increases monotonically with the frequency, and at large frequencies it is identical for the two drives. However, at low and intermediate frequencies the critical amplitude of the square-wave drive depends strongly on frequency, while the one of the cosine drive is almost constant in a wide frequency range. By analyzing the density of drive-induced resonances we conclude that this difference is due to resonances induced by higher harmonics in the Fourier spectrum which are present (absent) in the spectrum of the square-wave (sine) drive.

TT 36.9 Wed 11:45 HÜL 186

Periodic projections in quantum spin chains — •S. Harshini Tekur[1], Arnd Bäcker[2,1], and David J. Luitz[1] — [1]MPI für Physik komplexer Systeme, Dresden — [2]TU Dresden, Institut für Theoretische Physik

We investigate a new class of systems where a driven, disordered spin chain is opened by the addition of a periodic projection at one end of the chain, in analogy with classical or quantum maps with escape. The evolution operator over one period then becomes sub-unitary with a complex spectrum inside the unit circle. This class of systems exhibits several interesting properties, which we demonstrate by studying its level statistics, entanglement dynamics and spectral features like exceptional points which are unique to non-normal matrices. These may also be experimentally realized in a set-up where certain configurations of the spin chain are post-selected after a measurement.

TT 36.10 Wed 12:00 HÜL 186

Long-lived coherence in driven spin systems: from two- to infinite spatial dimensions — •Walter Hahn and V. V. Dobrovitski — QuTech, Delft University of Technology, Lorentzweg 1, 2628 CJ Delft, The Netherlands

We study dipolar-coupled quantum many-spin systems with local disorder, subject to periodic pulse driving, in different spatial dimensions: from two-dimensional to (effectively) infinite-dimensional systems. Using direct numerical simulations, we show that these systems exhibit long-lived magnetization response for all dimensions, despite strong fluctuations in the spin-spin couplings, and corresponding strong singularities in the spin dynamics. We observe the long-lived magnetization response for the initial polarization being either along the driving pulses, or along the axis conserved by the internal Hamiltonian. For longer time delays, the magnetization echoes exhibit an even-odd asymmetry, i.e. the system's response is modulated at the period which is twice the period of the driving. The above results are corroborated by a Floquet-operator analysis.

This work was supported by Dutch Research Council (NWO) and by DARPA DRINQS program.

TT 36.11 Wed 12:15 HÜL 186

Disorder-free localization in an interacting two-dimensional lattice gauge theory — •Petr Karpov[1,2], Roberto Verdel[1], Yi-Ping Huang[1,3], Markus Schmitt[1,4], and Markus Heyl[1] — [1]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, Dresden 01187, Germany — [2]National University of Science and Technology "MISiS", Moscow, Russia — [3]The Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland — [4]University of California, Berkeley, California 94720, USA

Recently, disorder-free localization has been introduced as a new mechanism for ergodicity breaking in homogeneous systems caused by local constraints imposed by gauge invariance [1,2]. Here, we show that disorder-free localization can occur in genuinely interacting systems in two spatial dimensions. Specifically, we show that the quantum link model can become nonergodic by providing a strict bound on the localization-delocalization transition through an unconventional classical percolation problem. We investigate the quantum dynamics in this system by means of an improved classical network description [3] endowed with a time-dependent variational principle.

[1] A. Smith, J. Knolle, D.L. Kovrizhin, and R. Moessner, Phys. Rev. Lett. **118**, 266601 (2017).

[2] M. Brenes, M. Dalmonte, M. Heyl, and A. Scardicchio, Phys. Rev. Lett. **120**, 030601 (2018).

[3] M. Schmitt and M. Heyl, SciPost Phys. **4**, 013 (2018).

TT 36.12 Wed 12:30 HÜL 186

Learning many-body localization indicators directly from the Hamiltonian — •Alexander Gresch, Lennart Bittel, and Martin Kliesch — Heinrich-Heine University, Düsseldorf, Germany

Many-body localization (MBL) captures the phenomenon that the propagation of correlations in disordered quantum systems can be strongly suppressed due to interference effects. Quantum systems undergoing MBL do practically not equilibrate but instead preserve local signatures of their initial conditions for arbitrarily long times. This property makes such systems potential candidates for storage devices in quantum computation. However, a full analytical understanding has not been achieved and numerical approaches have to deal with the exponential growth of the Hilbert space dimension. Hence, approximate methods have been proposed. A recent approach uses artificial neural networks for distinguishing MBL states from non-localized ones, which allows to calculate the phase diagram of the transition. The already proposed deep learning schemes require an expensive preprocessing, e.g. the eigenstates of the Hamiltonian or their entanglement spectrum, as inputs.

In this work, we investigate the Heisenberg spin chain with random local magnetic field. We demonstrate that an MBL-prediction is possible from the given disorder parameters alone without any preprocessing. We guide the learning process via several different indicators for MBL that have previously served as a basis for numerical studies. Here, we provide new insights in their predictive capabilities from a machine learning perspective.

TT 36.13 Wed 12:45 HÜL 186

Anderson Localization in a Rydberg Composite — •Matthew Eiles, Alexander Eisfeld, and Jan-Michael Rost — Max Planck Institute for the Physics of Complex Systems, 38 Noethnitzer Str. Dresden 01187

We demonstrate the localization of a Rydberg electron in a Rydberg composite, a system containing a Rydberg atom coupled to a structured environment of neutral ground state atoms. This localization is caused by weak disorder in the arrangement of the atoms and increases with the number of atoms M and principal quantum number ν. We develop a mapping between the electronic Hamiltonian in the basis of degenerate Rydberg states and a tight-binding Hamiltonian in the so-called "trilobite" basis, and then use this concept to pursue a rigorous limiting procedure to reach the thermodynamic limit in this system, taken as both M and ν become infinite, in order to show that Anderson localization takes place. This system provides avenues to study aspects of Anderson localization under a variety of conditions, e.g. for a wide range of interactions or with correlated/uncorrelated disorder.

TT 37: Skyrmions II (joint session MA/TT)

Time: Wednesday 9:30–13:00 Location: POT 6

Invited Talk TT 37.1 Wed 9:30 POT 6

Anatomy of skyrmion-defect interactions and their impact on detection protocols — •Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic skyrmions are topological swirling spin-textures with enormous potential for new technologies that store, transport and read information. However, imperfections are intrinsic to any real device, affecting the detection, nucleation, type of motion and velocity of a skyrmion. I will discuss our first-principles investigations of the electronic, magnetic and transport properties of single skyrmions interacting with 3d and 4d impurities embedded in PdFe/Ir(111). We found that the obtained energy landscape has a universal shape as function of the defect's electron filling, enabling predictions of the repulsive or attractive nature of the impurity [1]. This finding can be used to design complex energy profiles with targeted properties via atom-by-atom manufacturing of multi-atomic defects. Finally, I address how the latter affect the electronic structure and the chiral orbital magnetism, with consequences for the efficiency of skyrmion detection protocols, either all-electrical [2,3] or optical [4]. — Work done with I. L. Fernandes, J. Bouaziz, D. M. Crum, M. dos Santos Dias, M. Bouhassoune, I. Gede Arjana, J. Chico and S. Blügel and supported by the EU Horizon 2020 via ERC-consolidator Grant No. 681405–DYNASORE.

[1] Fernandes *et al.*, Nat. Commun. **9**, 4395 (2018); [2] Fernandes *et al.*, ArXiv:1906.08838; [3] Crum *et al.*, Nat. Commun. **6**, 8541 (2015); [4] dos Santos Dias *et al.*, Nat. Commun. **7**, 13613 (2016)

TT 37.2 Wed 10:00 POT 6

Electrical and optical manipulation of magnetic skyrmions — •Felix Büttner[1], Bastian Pfau[2], Lucas Caretta[1], Kai Litzius[1], Michael Schneider[2], Guiseppe Mercurio[3], Marie Böttcher[4], Bertrand Dupé[4], Johan Mentink[5], Stefan Eisebitt[2], and Geoffrey Beach[1] — [1]MIT, Cambridge, MA, USA — [2]MBI, Berlin, Germany — [3]XFEL, Hamburg, Germany — [4]University of Mainz, Germany — [5]RU Nijmegen, The Netherlands

Magnetic skyrmions are nanoscale twisted spin textures with a topology equivalent to the unit sphere. Skyrmions exhibit fascinating quasi-particle physics, including skyrmion gyration [1], inertia [1], the skyrmion Hall effect [2], topological damping [3], sub-ns switching [4], and ultra-fast motion [5]. They are also promising candidates for several data storage and data processing technologies. In this context, fast and energy efficient operation is key. In this talk I will give a brief overview of our latest results of on skyrmion displacement by nanosecond spin-orbit torque current pulses and ultrafast light pulses. The main part of the talk will focus on the physics and speed of optically induced topological switching (skyrmion nucleation) and how this is different from classical bubble behavior. These results will be discussed from a theoretical and experimental perspective.

[1] Büttner et al., Nat Phys 11, 225 (2015). [2] Litzius et al., Nat Phys 13, 170 (2017). [3] Büttner et al., Sci Rep 8, 4464 (2018). [4] Büttner et al., Nat Nano 12, 1040 (2017). [5] Caretta et al., Nat Nano 13, 1154 (2018).

TT 37.3 Wed 10:15 POT 6

Manipulation of magnetization and spin textures via femtosecond laser — •Nina Novakovic[1,2], Mohamad-Assaad Mawass[1], Oleksii Volkov[3], Wolfgang-Dietrich Engel[4], Denys Makarov[3], and Florian Kronast[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, 12489, Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24/25, 14476, Potsdam, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf e. V., Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [4]Max Born Institute Berlin, Max-Born-Str. 2A, 12489 Berlin, Germany

Ultrafast optical control of magnetization recently became a rising field of study in magnetic thin film research, as micrometer sized domains manipulated at a small timescale may lead to faster and denser memory devices. We investigate different magnetic textures, such as bubbles and skyrmions under the influence of femtosecond laser pulses by means of photoelectron emission microscopy.

We present helicity dependent transition between stripe and bubble domains in CoPt multilayers. Moreover, manipulation of individual bubbles by tuning down laser fluence and external field is demonstrated. With the introduction of Ta layer at the interface in the CoPt system, we increase the influence of DMI. This allows us to study the formation and annihilation of skyrmions via fs laser and discuss important parameters which are required to attain reliable and efficient helicity dependent switching process, such as magnetic field and laser fluence and polarization.

TT 37.4 Wed 10:30 POT 6

Quantum Damping of Characteristic Skyrmion Eigenmodes due to Spontaneous Magnon Decay — •Alexander Mook, Jelena Klinovaja, and Daniel Loss — Department of Physics, University of Basel, CH-4056 Basel

The three characteristic and magnetically active modes of skyrmion crystals, i.e., the anticlockwise, breathing, and clockwise mode [1], are experimental probes that reveal information on the stability and behavior of the topologically nontrivial magnetic texture.

Herein, we show that the combination of a noncollinear texture and lowly dispersive Landau-level-like nature of magnon bands in skyrmion crystals installs strong three-particle interactions. These lead to spontaneously decaying magnons, i.e., to an intrinsic zero-temperature quantum damping, which manifests as lifetime broadening of the quasiparticle peak in the spectral function.

By varying the external magnetic field the characteristic modes can be brought “in resonance” with a flat mode, strongly enhancing their damping. This finding establishes skyrmion crystals as a platform to study the quantum mechanical phenomenon of spontaneous quasiparticle decay.

[1] M. Mochizuki, Phys. Rev. Lett. **108**, 017601 (2012)

TT 37.5 Wed 10:45 POT 6

Current-driven magnetic Skyrmions in constrained geometries — •Martin Stier[1], Richard Strobel[1], Wolfgang Häusler[2], and Michael Thorwart[1] — [1]Universität Hamburg, Jungiusstraße 9, 20355 Hamburg — [2]Universität Augsburg, Universitätsstr. 1, 86135 Augsburg

From a principle point of view, magnetic Skyrmions are ultimately stable and thus do basically not interact with their environment. This is in stark contrast to experimental findings, where Skyrmions are strongly influenced by the shape, roughness and the quality of the sample. We show how the current-driven dynamics and the number of Skyrmions are influenced by geometric constrictions in the wire, its edge roughness and magnetic impurities within the material. We discuss several scenarios in detail, e.g., Skyrmion trapping or acceleration, and Skyrmion destruction or creation. These findings may help to develop tailored microscopic memory devices involving Skyrmions.

TT 37.6 Wed 11:00 POT 6

Evolution of topological charge during transitions between magnetic states — •Igor Lobanov — ITMO University, Saint Petersburg, Russia — Saint Petersburg State University, Russia

Stability of magnetic skyrmions and other topological structures is an important prerequisite for the development of magnetic storage and computing devices. Evaluation of lifetime of magnetic states and the most probable transition scenario can be performed using harmonic transition state theory [1,2] and minimum energy path (MEP) calculation. Results on annihilation of skyrmionium to the ferromagnetic state are presented. There, the initial state and the final state are both of zero topological charge, but the charge is not necessarily conserved during the transition between the states. Several MEPs for the skyrmionium annihilation are identified, corresponding activation energies and transition rates are systematically compared, while variation of the topological charge along each MEP is analyzed. The dependence of lifetime on the lattice constant is studied, the resulting switching of the preferable path is demonstrated. The calculated MEPs give us a hint for optimal control of nucleation and annihilation of topologically protected structures.

This work was funded by the Russian Science Foundation (Grant No. 19-72-10138).

1. G. Fiedler, J. Fidler, J. Lee, T. Schrefl, R. L. Stamps, H. B. Braun, and D. Suess, J. Appl. Phys. 111, 093917 (2012)

2. P.F. Bessarab, V.M. Uzdin, H. Jonsson, Phys. Rev. B 85, 184409 (2012)

15 min. break.

TT 37.7 Wed 11:30 POT 6

Topological Phase Transition Controls Magnon Spin Currents — •Sebastián A. Díaz[1], Tomoki Hirosawa[2], Jelena Klinovaja[1], and Daniel Loss[1] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Physics, University of Tokyo, Tokyo, Japan

Using magnons in insulating magnets as information carriers is a highly promising approach for low-power consumption devices free of Joule heating. Here we show that a ferromagnetic skyrmion crystal provides a novel platform for switchable magnon currents. Taking advantage of a topological phase transition in the magnon spectrum, we show that an external magnetic field allows one to turn on and off chiral magnon currents carried by topological edge states. We identify concrete systems for experimental implementations. Our proposal establishes a profound connection between the fields of magnetic skyrmions and topological magnonics controlled by magnetic fields.

[1] S. A. Díaz, T. Hirosawa, J. Klinovaja, and D. Loss, arXiv:1910.05214.

TT 37.8 Wed 11:45 POT 6

Mixed Topology Ring States in skyrmions of mixed Weyl semimetals — •Matthias Redies[1,2], Fabian Lux[1,2], Patrick

Buhl[3], Jan-Philipp Hanke[1], Stefan Blügel[1], and Yuriy Mokrousov[1,3] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Physics, RWTH Aachen University, 52056 Aachen, Germany — [3]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany

Various properties of Weyl semimetals are currently attracting significant attention. Recently, the concept of a magnetic mixed Weyl semimetal (MWS) has been put forward e.g. in 2D ferromagnets [1], and various prospects of these materials have been suggested. In such 2D materials the Weyl points are exhibited in the mixed space of **k**-vectors and the magnetization direction. We investigate the effect that skyrmionic order has on electronic transport properties of MWSs. Our analysis reveals the emergence of robust ring-like edge states, carrying local orbital moment, which mediate the transition between two different Chern insulator phases appearing in the skyrmion lattice of MWSs. We discuss the properties of such mixed topology ring states and their possible applications.

We acknowledge funding from Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 “Skyrmionics".

[1] Hanke *et al.*, Nature Comm. **8**, 1479 (2017), ibid. **10**, 3179 (2019)

TT 37.9 Wed 12:00 POT 6

Skyrmion Breathing Modes in Synthetic Ferri- and Antiferromagnets — •Martin Lonsky and Axel Hoffmann — Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL 61801, United States of America

Magnetic multilayers that combine strong spin-orbit interaction with lacking inversion symmetry can give rise to the presence of topologically nontrivial spin textures, so-called magnetic skyrmions, at room temperature. Recent studies have indicated strongly enhanced propagation velocities of skyrmions in antiferromagnets and compensated ferrimagnets [1]. At the same time, it is unclear how magnetic compensation may affect dynamic excitations of magnetic skyrmions, such as breathing modes which entail an oscillation of the skyrmion size at GHz frequencies [2]. Here, we present micromagnetic simulations of these excitations in synthetic ferri- and antiferromagnets. The observed features in the calculated power spectra show a systematic dependence on the coupling strength between the individual magnetic layers and are related to pure breathing modes as well as to hybridizations of breathing and spin wave modes that are characteristic for the considered geometry. Based on these simulations, we then discuss the impact of these results for potential skyrmion sensing and other applications.

This work is supported by the Deutsche Forschungsgemeinschaft (DFG) through the research fellowship LO 2584/1-1.

[1] L. Caretta et al., Nat. Nanotechnol. 13, 1154-1160 (2018)
[2] M. Garst et al., J. Phys. D: Appl. Phys. 50, 293002 (2017)

TT 37.10 Wed 12:15 POT 6

Spin waves in skyrmions with various topological charges — •Levente Rózsa and Ulrich Nowak — Universität Konstanz, Konstanz, Deutschland

Magnetic skyrmions offer promising prospects for the development of magnonic devices. The most widely studied mechanism to date for the stabilization of skyrmions is the Dzyaloshinsky-Moriya interaction (DMI). Although a wide variety of localized spin wave modes has been predicted theoretically in DMI-stabilized skyrmions [1], their experimental observation via excitation by a homogeneous external field has been restricted to breathing and gyrational modes. This can be attributed to the angular momentum selection rules enforced by the cylindrically symmetric spin structure. In contrast to the DMI, frustrated Heisenberg exchange interactions (FHEI) may stabilize different types of skyrmions with various topological charges [2]. Here we theoretically investigate how the types of localized magnons and the selection rules are modified in FHEI-stabilized skyrmions. The competition between FHEI and DMI is also considered, which was demonstrated to distort the shape of the different types of skyrmions [3].

[1] M. Garst et al., J. Phys. D: Appl. Phys. **50**, 293002 (2017).
[2] A. O. Leonov et al., Nat. Commun. **6**, 8275 (2015).
[3] L. Rózsa et al., Phys. Rev. B **95**, 094423 (2017).

TT 37.11 Wed 12:30 POT 6

Transverse susceptibility of skyrmion lattice order in Cu_2OSeO_3 and MnSi — •Denis Mettus[1], Felix Rucker[1], Andreas Bauer[1], Helmuth Berger[2], Markus Garst[3], Achim Rosch[4], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]École Polytechnique Federale de Lausanne, Lausanne, Switzerland, Switzerland — [3]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [4]Institute for Theoretical Physics, Universität zu Köln, D-50937 Köln, Germany

The observation of skyrmion lattice flow in chiral magnets under spin-transfer torques at exceptionally small spin current densities has generated great interest concerning the underlying pinning and coupling mechanisms. While the spin currents in MnSi represent spin-polarized charge currents, similar spin torque effects due to tiny magnon currents are observed in the electrical insulator Cu_2OSeO_3. We report systematic measurements of the transverse ac susceptibility of MnSi and Cu_2OSeO_3 as a function of the amplitude and frequency of the excitation field. In our study we cover the response of the magnetization in the limits of local scales up to large scales of the entire texture. We discuss our results in the context of unpinning effects due to spin transfer torques as well as different stabiliziation mechanisms of skyrmion lattice order.

TT 37.12 Wed 12:45 POT 6

Skyrmion-Skyrmion and Skyrmion-Edge Interactions studied with SP-STM — •Jonas Spethmann, André Kubetzka, Roland Wiesendanger, and Kirsten von Bergmann — University of Hamburg

For the design of potential skyrmion-based devices, a deep understanding of the interactions between individual skyrmions and between skyrmions and magnetic nanostructure boundaries is fundamental. In order to study these interactions, we investigate the magnetic field dependent size and shape of multiple skyrmions confined in islands of PdFe bilayer on Ir(111) using spin-polarized STM. When the external magnetic field is reduced, the skyrmion size increases [1]. This forces adjacent skyrmions to interact with each other or with the edge of the PdFe island. Such interactions may manifest in form of skyrmion deformation, displacement or annihilation. Due to our operation temperature of 4 K or lower, the skyrmions do not spontaneously revert back to the spin spiral phase at small or even zero magnetic fields. Instead, we obtain metastable topological states, which provide an interesting starting point for further investigations. Additionally, by modification of the PdFe island-edge, we are able to study the influence of different types of edges on the spin spiral state and on the skyrmion-edge interactions.

[1] N. Romming et al., PRL 114: 177203, 2015.

TT 38: Topological Superconductors

Time: Wednesday 11:00–12:45 Location: HSZ 103

Invited Talk TT 38.1 Wed 11:00 HSZ 103

Nematic superconductivity in the superconducting doped topological insulators $Nb_xBi_2Se_3$ and $Sr_xBi_2Se_3$ — •Kristin Willa[1,2], Matthew Smylie[1,3], Roland Willa[1,2], Ulrich Welp[1], Genda Gu[4], and Wai-Kwong Kwok[1] — [1]Argonne National Laboratory, Lemont, USA — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Hofstra University, Hempstead, USA — [4]Brookhaven National Laboratory, Upton, USA

Spontaneous rotational-symmetry breaking in the superconducting state of the doped topological insulator Bi_2Se_3 has attracted significant attention as a candidate for topological superconductivity. We have studied the normal and the superconducting state of $Nb_xBi_2Se_3$ and $Sr_xBi_2Se_3$ using magnetoresistance, magnetization, penetration depth and specific heat. While no sign of a symmetry breaking of the three-fold in plane crystal symmetry is observed in the normal state, we find a clear two-fold in plane symmetry of the upper critical field in the superconducting state. This large basal-plane anisotropy of H_{c2} (Γ=3.5) is attributed to a two-component gap structure $\eta = (\eta_1, \eta_2)$. A quantitative analysis of our data excludes more conventional sources of this twofold anisotropy and gives clear evidence for nematic superconductivity and some indications for topological superconductivity in both $Nb_xBi_2Se_3$ and $Sr_xBi_2Se_3$.

TT 38.2 Wed 11:30 HSZ 103

Structurally-driven nematicity of odd-parity superconductivity in $Sr_xBi_2Se_3$ — •Aleksandr Kuntsevich, Yuri Selivanov, Victor Martovitskii, and Aleksandr Rakhmanov — P.N. Lebedev Physical Institute, 119991, Moscow, Russia

Superconductivity(SC) in doped (by Cu, Sr or Nb) topological insulator Bi_2Se_3 attracts a great deal of attention as odd-parity topological one, with an exotic nematic vector order parameter.On a structural level it is unknown where exactly the dopant atoms are located in the lattice and how this placement controls SC properties.

$Sr_xBi_2Se_3$ is the most structurally perfect member of this family, it demonstrates stability of SC, and ∼100% SC fraction. We improved the crystalline quality, showed that that SC in $Sr_xBi_2Se_3$ is induced by very low doping level, and strongly depends on the specific arrangement of Sr atoms in the host matrix [1].

We also managed to obtain purely single-block crystals. The x-ray diffraction shows that these single crystals are either weakly stretched or compressed uniaxially in the basal plane. In the SC state, the upper critical field H_{c2} has a twofold rotational symmetry and depends on the sign of the strain: in the stretched samples the maximum of H_{c2} is achieved when H is transverse to the strain axis, while in the compressed samples this maximum is observed when the field is along the strain direction. This result is naturally explained within the nematic SC coupled to the strain. This observation is a novel experimental evidence for the odd-parity SC in $Sr_xBi_2Se_3$[2].

[1] AYK *et al* Materials**12**, 3899,2019
[2] AYK *et al* PRB**100**, in press,2019

TT 38.3 Wed 11:45 HSZ 103

Transport study on bulk $PtBi_2$ and $Pt_{1-x}Rh_xBi_2$ at very low temperature — •Valentin Labracherie, Arthur Veyrat, and Joseph Dufouleur — Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany

Weyl Semimetals are a new class of material with chiral spin texture discovered in the last decade. They host quasiparticles with linear excitations, the Weyl fermions, which have definite spin chirality. These bulk states come as pairs of Dirac cones connected to each other at their interface with some trivial materials. Weyl fermions are expected to exhibit new effects like Fermi arcs and chiral anomaly for which electrons are pumped from one cone to the other, breaking the conservation of the chiral charge. Due to that, we have the appearance of a planar hall effect and anisotropic negative magnetoresistance when the electrical and magnetic field are aligned.

Several candidates to Weyl semimetal have also shown superconducting states at very low temperature and a lot of efforts has been made to see if these superconducting states is link to topology or not. I will present here transport measurement on $PtBi_2$, a Weyl semimetal which show a superconducting state at 0.6K and we investigate the effect of Rh doping on its superconducting properties.

TT 38.4 Wed 12:00 HSZ 103

^{125}Te NMR studies of 1T-$MoTe_2$ under pressure -Towards superconductivity mediated by Weyl Fermions — •H. Yasuoka[1], T. Fujii[1,2], K.M. Ranjith[1], M.O. Ajeesh[1], M. Schmidt[1], T. Mito[2], M. Nicklas[1], C. Felser[1], A. Mackenzie[1], and M. Baenitz[1] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]School of Science, University of Hyogo Hyogo, Japan

1T-$MoTe_2$ is claimed to be one of the type-II Weyl semimetals, and has attracted much attention due to its exotic physical properties stemming from the topological (line nodal) band structure where the electron and hole pockets are touching at the Fermi energy. One of the most preeminent features is the occurrence of superconductivity which is stabilized under pressure up to around T_c=7K. In order to understand the superconductivity, we have employed the ^{125}Te NMR technique under pressure (up to 2.17 GPa) and measured the NMR line profile and nuclear magnetic relaxation, determining the Knight shift and low lying magnetic excitations. Using the same NMR tuning circuit, we have also measured the pressure and temperature (T) dependences of the resonant frequency, and extracted the T-dependence of the upper critical field H_{c2}. The results are not in accord with simple WHH model, but are well fit to an empilical formula, $H_{c2}(T) = H_{c2}(0)[1-\frac{T}{T_c}]^{\alpha}$. By doing this, we obtained $H_{c2}(0)$=1.50T, T_c= 3.81K, and α=1.1 at 2.17 GPa. A superconducting signature has been observed in $K(T)$ and $1/T_1T(T)$ at around 2.5 K (2.17GPa, 0.46T). We present detailed NMR results and try to explore the superconductivity from the microscopic point of view.

TT 38.5 Wed 12:15 HSZ 103

Strongly correlated superconductor with polytypic 3D Dirac points — Sergei Borisenko[1], •Volodymyr Bezguba[1,2], Alexander Fedorov[1,3], Yevhen Kushnirenko[1], Vladimir Voroshnin[3], Mihai Sturza[1], Saicharan Aswartham[1], and Alexander Yaresko[4] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Kyiv Academic University, 03142 Kyiv, Ukraine — [3]Helmholtz-Zentrum Berlin fur Materialien und Energie — [4]Max-Planck-institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Topological superconductors should be able to provide essential ingredients for quantum computing, but are very challenging to realize. Spin-orbit interaction in iron-based superconductors opens the energy gap between the p-states of pnictogen and d-states of iron very close to the Fermi level, and such p-states have been recently experimentally detected. Density functional theory predicts existence of topological surface states within this gap in $FeTe_{1-x}Se_x$ making it an attractive candidate material. Here we use synchrotron-based angle-resolved photoemission spectroscopy and band structure calculations to demonstrate that $FeTe_{1-x}Se_x$ (x=0.45) is a superconducting 3D Dirac semimetal hosting type-I and type-II Dirac points and that its electronic structure remains topologically trivial.

TT 38.6 Wed 12:30 HSZ 103

Phase-tunable second-order topological superconductor — •Selma Franca, Dmitri Efremov, and Ion Cosma Fulga — IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstr. 20, 01069 Dresden, Germany

Two-dimensional second-order topological superconductors (SOTSCs) have gapped bulk and edge states, with zero-energy Majorana bound states localized at corners. Motivated by recent advances in Majorana nanowire experiments, we propose to realize a tunable SOTSC as a two-dimensional nanowire array. We show that the coupling between the Majorana modes of adjacent wires can be controlled by phase-biasing the device, allowing one to access a variety of topological phases. We characterize the system using scattering theory, which provides access to its transport properties and its topological invariants. The setup is robust against disorder, both in the nanowires themselves and in the Josephson junctions formed between adjacent wires. Further, we identify a parameter regime in which an initially trivial system is rendered topological upon adding disorder, providing an example of a second-order topological Anderson phase.

TT 39: Focus Session: Frontiers in Cryogenic Particle Detection

Time: Wednesday 15:00–18:30 Location: HSZ 03

Invited Talk TT 39.1 Wed 15:00 HSZ 03

Magnetic Micro-Calorimeters: Present success stories, concepts and visions — •Andreas Fleischmann — Heidelberg University, Heidelberg, Germany

Micro-calorimeters are energy dispersive detectors, which can be optimized for the detection of various kinds of particles, ranging from single visible photons over x-ray to hard gamma-rays, including alpha- and beta-particles as well as neutral molecules with some keV of kinetic energy. Operated in a purely thermal mode, micro-calorimeters can achieve arbitrarily good energy resolution, provided a low enough detector temperature. And indeed, in the last decade single channels as well as arrays of micro-calorimeters have become indispensable instruments in numerous fields of science ranging from quantum information, molecular and atomic physics over astro-particle physics to nuclear forensics and homeland security. In this review talk we will present some of the fascinating detector systems, discuss the physics and design considerations of magnetic micro-calorimeters and try to identify promising paths for future developments.

Invited Talk TT 39.2 Wed 15:30 HSZ 03

Ultra-Sensitive Microwave Kinetic Inductance Detectors from the Optical to the Far Infrared — •Jochem Baselmans[1,2], Pieter de Visser[1], Stephen Yates[1], Lorenza Ferrari[1], Vignesh Murugesan[1], David Thoen[2], and Akira Endo[2] — [1]SRON Netherlands Institute for Space Research — [2]Delft University of Technology

Near future space-based observatories for the far-infrared and for the optical will need large arrays of cryogenic detectors with unprecedented sensitivity. Aluminium based Microwave Kinetic Inductance Detectors (MKIDs) are the most promising for these applications. MKIDs are superconducting resonators whose resonant frequency and Q factor are modified due to photon absorption. They are read-out using a microwave readout signal at the unperturbed resonant frequency. These devices can be well described using the standard Mattis-Bardeen theory, with the added complexity that the quasiparticle energy distribution is modified by the absorption of readout photons with E = $hf_{readout} << \Delta$. At T<$T_c/8$ this process creates excess quasiparticles proportional to $\sqrt{P_{readout}}$, which limits the sensitivity. Since decreasing $P_{readout}$ is impossible due to excess noise sources we reduce the device volume. This results in a Noise Equivalent Power $NEP = 6 \cdot 10^{-20}\ W/\sqrt{Hz}$, 4-5 times better than previously reported For optical MKIDs, capable of single photon spectroscopy, an additional issue is the escape of high energy phonons from the aluminium film into the substrate. I will discuss recent experiments that use thin membranes to significantly reduce the phonon loss. This drastically increases the resolving power to 50 for 402 nm photons.

Invited Talk TT 39.3 Wed 16:00 HSZ 03

LTS dc-SQUID sensors for TES and MMC readout — •Jörn Beyer — Physikalisch-Technische Bundesanstalt, Berlin, Germany

The superconducting quantum interference device (SQUID) is a highly sensitive detector for magnetic flux or any physical quantity that can be efficiently converted into flux. Current sensors based on LTS SQUIDs are practically unrivalled to operate two categories of superconducting cryogenic detectors, namely transition edge sensors (TESs) and metallic magnetic calorimeters (MMCs). Applications of TES detectors range from the bolometric detection of sub-millimeter waves to calorimetric detection of X- and gamma-rays. MMCs so far address primarily high-energy applications, for instance spectrometry of soft and hard X-rays or radionuclide spectrometry. In this contribution, basic technology and design concepts of LTS dc-SQUID current sensors are presented. Efficient signal coupling as well as circuit configurations such as SQUID cascades, SQUID arrays, SQUID sensors with differential output and SQUID-based multiplexers will be discussed. LTS dc-SQUIDs already provide adequate performance for a range of readout applications of single TESs and MMCs as well as of arrays of these detectors. Still, further improvement of sensor functionality and noise is possible. Refined lithographic technology can be employed to realize SQUID sensors with sub-micrometer-sized Josephson junctions as well as fine-pitch superconducting pick-up coils. Recent progress on these developments will be presented.

15 min. break.

Invited Talk TT 39.4 Wed 16:45 HSZ 03

CRESST and NUCLEUS: The low-energy frontier of Dark Matter and neutrino physics — •Raimund Strauss — Technische Universität München

The CRESST and NUCLEUS experiments are moving the low-energy frontier in astroparticle physics with cryogenic calorimeters. Their common detector technology is based on single crystals equipped with tungsten transition-edge-sensors that are operated at temperatures of about 10mK. CRESST has achieved the world-best energy thresholds for nuclear recoils in the 10eV regime and is currently the leading experiment for sub-GeV Dark Matter searches. In this talk, I will present recent results on low-mass Dark Matter acquired during the latest measurement campaign at the Gran Sasso underground laboratory (LNGS) in Italy, and discuss the future Dark Matter program of CRESST. The NUCLEUS experiment aims for the exploration of coherent-elastic neutrino nucleus scattering (CEvNS) at a nuclear power reactor. It opens a new window to study the fundamental properties of neutrinos and to probe physics beyond the Standard Model of Particle Physics. Accessing energies down to the 10 eV regime enables to fully exploit the strongly enhanced cross section of CEvNS which leads to a miniaturization of neutrino detectors. A new detector concept based on gram-scale cryogenic calorimeters establishes a fiducial-volume cryogenic detector. NUCLEUS is fully funded and will be installed at the CHOOZ nuclear power plant in France. I will present first results from a prototype cryogenic detector and discuss the extensive physics program of NUCLEUS.

Invited Talk TT 39.5 Wed 17:15 HSZ 03

Large Array of Superconducting Transition-Edge Sensors for High Sensitive Photon and Particle Detectors — •Luciano Gottardi — SRON - Netherlands Institute for Space Research, Utrecht , The Netherlands

Superconducting Transition-Edge Sensors (TES) have proven to achieve very high sensitivity in detecting small temperature changes. TES-based detectors are employed in many low temperature imaging instruments in the field of gamma-ray spectroscopy, X-ray and infrared astrophysics, CMB-polarization experiments and optical instrumentation. We will present the cutting-edge technology of the X-ray Integral Field Unit on board of the future ESA Advanced Telescope for High-Energy Astrophysics (Athena). The detector baseline consists of 3200 micro-calorimeters based on superconducting MoAu transition-edge sensors (TES's) from NASA-Goddard read out in the MHz bandwidth using Frequency Division Multiplexing (FDM), based on Superconducting QUantum Interference Devices (SQUIDs) from SRON/VTT. The proposed design calls for devices with high quantum efficiency and a breakthrough energy resolution of 2.5 eV at 5.9 keV. The focus of this paper will be on our recent efforts in the optimization of the NASA/Goddard MoAu and the SRON TiAu TES pixel design to improve on the superconducting transition uniformity, the noise, and to minimize non-linearity effects. This technology is potentially interesting as well for the development of high resolution X-ray cameras for monitoring the quality of the plasma in nuclear fusion reactors or for the search of axions-like particles.

TT 39.6 Wed 17:45 HSZ 03

Beta Spectrometry Measurements with Metallic Magnetic Calorimeters — •Michael Paulsen[1,2], Jörn Beyer[1], Lina Bockhorn[3,4], Christian Enss[2], Sebastian Kempf[2], Karsten Kossert[4], Martin Loidl[5], Riham Mariam[5], Ole Nähle[4], and Matias Rodrigues[5] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [3]Institut für Festkörperphysik, Leibniz University, Hannover, Germany — [4]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany — [5]CEA, LIST, Laboratoire National Henri Becquerel, Saclay, France

Precise measurements of beta spectra shapes are relevant in radionuclide metrology, e.g. when determining the activity of samples containing beta emitting isotopes and in fundamental research. Metallic Magnetic Calorimeters (MMCs) are energy-dispersive low-temperature detectors that are particularly suitable for beta spectrometry as they can be employed for wide energy ranges while having high energy resolution. We present beta spectra of ^{99}Tc ($E_{max} = 293.8\,\mathrm{keV}$) and ^{36}Cl ($E_{max} = 709.5\,\mathrm{keV}$) measured with MMC-based beta spectrometers along with a discussion of how systematic bremsstrahlung effects can be reduced for high energy spectra ($E_{max} > 500\,\mathrm{keV}$) using a dedicated absorber preparation or an unfolding algorithm.

TT 39.7 Wed 18:00 HSZ 03

Development and optimisation of metallic magnetic calorimeter arrays towards ECHo-100k — •Federica Mantegazzini, Arnulf Barth, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, Robert Hammann, Sebastian Kempf, Clemens Velte, and Tom Wickenhäuser — Kirchhoff-Institute of Physics, Heidelberg University, Germany

The Electron Capture in ^{163}Ho (ECHo) experiment has been designed for the determination of the effective electron neutrino mass exploiting the electron capture spectrum of ^{163}Ho. The detector technology is based on metallic magnetic calorimeters (MMCs) loaded with ^{163}Ho and operated at millikelvin temperature. For the first phase of the experiment, ECHo-1k, MMC arrays consisting of 72 pixels have been microfabricated and implanted with high purity ^{163}Ho source reaching an activity of about 1 Bq per pixel. The implanted detectors have been successfully operated and characterised, reaching an energy resolution below 5 eV. For the next phase of the experiment, ECHo-100k, the planned activity per pixel is 10 Bq and the required number of pixels simultaneously operated will be 12000. Therefore, a new dedicated MMC array chip which allows for highly efficient ^{163}Ho implantation and multiplexed read-out as well as optimised detector performances has been designed and produced. We present preliminary results obtained in the characterisation of the ECHo-100k chip and we discuss the future plans towards the next phase of the ECHo experiment.

TT 39.8 Wed 18:15 HSZ 03

MOCCA: operating a full 4k-pixel molecule camera for the position and energy resolved detection of neutral molecular fragments — •Dennis Schulz[1], Steffen Allgeier[1], Christian Enss[1], Andreas Fleischmann[1], Lisa Gamer[1], Loredana Gastaldo[1], Julia Hauer[1], Sebastian Kempf[1], Oldřich Novotný[2], Sebastian Spaniol[2], and Andreas Wolf[2] — [1]Kirchhoff-Institute for Physics, Heidelberg University — [2]Max-Planck-Institute for Nuclear Physics, Heidelberg

The MOCCA detector is a high-resolution, large-area molecule camera based on metallic magnetic calorimeters and read out with SQUIDs that has the ability to detect neutral molecule fragments with keV kinetic energies. MOCCA is an array of 64 × 64 quadratic pixels with a side length of 700 μm and covers a total detection area of 4.5 cm × 4.5 cm with a filling factor of 99.5 %. It will be deployed at the Cryogenic Storage Ring CSR at the Max Planck Institute for Nuclear Physics in Heidelberg, a storage ring built to prepare and store molecular ions in their rotational and vibrational ground states, enabling studies on electron-ion interactions. To reconstruct the reaction kinematics, MOCCA is able to measure the energy and position of multiple incident particles hitting the detector simultaneously.

We present the fabrication of Through-Wafer Vias together with new measurements of a full-scale MOCCA detector, demonstrating the readout principle, multi-hit capability, and energy resolution of less than 200 eV, combined with a very low cross-talk between pixels.

TT 40: Topological Josephson Junctions

Time: Wednesday 15:00–17:00 Location: HSZ 103

TT 40.1 Wed 15:00 HSZ 103

Second Chern number and non-Abelian Berry phase in topological Josephson matter — •Hannes Weisbrich, Raffael L. Klees, Gianluca Rastelli, and Wolfgang Belzig — Universität Konstanz

Topology and related quantized numbers play an important role in condensed matter physics in various topics. For instance, it has been theoretically proposed that the first Chern number is related to a quantized transconductance in topological Josephson matter [1]. Higher dimensional topological phases characterized by the second Chern number can describe even more complex quantum states, e.g. the four dimensional quantum Hall effect [2]. Hereby we present a first theoretical proposal for topological Josephson matter with a non-trivial second Chern number. We show that a double quantum dot in contact with several superconducting leads can implement such exotic topological state. Moreover the lowest pair of Andreev states shows a non-Abelian Berry phase which can be used to perform arbitrary rotations within the twofold degenerate subspace by adiabatic changes of the superconducting phases. Finally, we discuss a measurement protocol for the second Chern number by means of a combination of non-Abelian Berry rotations and polarized microwave spectroscopy [3].

[1] R.-P. Riwar et al., Nat. Commun. 7, 11167 (2016).
[2] S. C. Zhang and J. Hu, Science, 294(5543), 823-828 (2001).
[3] R. L. Klees et al., arXiv:1810.11277 (2018).

TT 40.2 Wed 15:15 HSZ 103

Detection of Majorana modes via supercurrents through quantum dots — •Jens Schulenborg and Karsten Flensberg — Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

Experimental techniques to verify Majorana fermions are of current interest. A prominent test is the effect of Majoranas on the Josephson current between two wires linked via a normal junction.

This talk presents the case of a quantum dot connecting the two superconductors and the sign of the supercurrent in the trivial and topological regimes under grand-canonical equilibrium conditions, explicitly allowing for parity changes due to, e.g., quasi-particle poisoning. We find that the well-known supercurrent reversal for odd quantum dot occupancy (π-junction) in the trivial case[1] does not occur in the presence of Majoranas in the wires. However, we also find this to be a mere consequence of Majoranas being zero energy states, and therefore one cannot conclude that the lack of supercurrent sign reversal is a discriminating signature of Majoranas.

[1] B. I. Spivak et al., Phys. Rev. B **43**, 4 (1991)

TT 40.3 Wed 15:30 HSZ 103

Transverse Josephson current in magnetic TI junction — •Oleksii Maistrenko[1], Benedikt Scharf[2], Dirk Manske[1], and Ewelina Hankiewicz[2] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]Institut für theoretische Physik (TP4), Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Josephson junctions based on 3D topological insulators offer intriguing possibilities to realize unconventional p-wave pairing and Majorana modes. In particular, such junctions exhibit non-chiral, counterpropagating Majorana modes for a superconducting phase bias $\phi = \pi$ [1]. We show how by applying an appropriately oriented in-plane magnetic field in the junction, we can switch these Majorana modes to a regime in which they become unidirectional. One can understand this switching behavior from the interplay between the magnetic field and the spin-momentum locking of the topological insulator. Interestingly, the application of the in-plane magnetic field is also accompanied by a net transverse supercurrent that can be a sizable fraction of the longitudinal supercurrent. This current might be spin polarized. Magnetic Josephson junctions based on 3D topological insulators thus present a versatile platform for manipulating Majorana modes and controlling transverse supercurrents.

[1] L. Fu and C. L. Kane, Phys. Rev. Lett. **100**, 96407 (2008)

TT 40.4 Wed 15:45 HSZ 103

Topologically nontrivial Andreev bound states — •Pasquale Marra[1,2] and Muneto Nitta[2] — [1]Graduate School of Mathematical Sciences, The University of Tokyo — [2]Department of Physics, Keio University

Andreev bound states are low energy excitations appearing below the particle-hole gap of superconductors, and are expected to be topologically trivial. Here, we report the theoretical prediction of topologically *nontrivial* Andreev bound states in one-dimensional superconductors. These states correspond to another topological invariant defined in a synthetic two-dimensional space, the particle-hole Chern number, which we construct in analogy to the spin Chern number in quantum spin Hall systems. Nontrivial Andreev bound states have distinct features and are topologically nonequivalent to Majorana bound states. Yet, they can coexist in the same system, have similar spectral signatures, and materialize with the concomitant opening of the particle-hole gap. The coexistence of Majorana and nontrivial Andreev bound state is the direct consequence of "double dimensionality", i.e., the dimensional embedding of the one-dimensional system in a synthetic two-dimensional space, which allows the definition of two distinct topological invariants ($\mathbb{Z}_2$ and $\mathbb{Z}$) in different dimensionalities.

TT 40.5 Wed 16:00 HSZ 103

Current–phase relation in a long topological Josephson junction — •Stefan Backens[1] and Alexander Shnirman[1,2] — [1]Institute for Theoretical Condensed Matter Physics (TKM), KIT, Karlsruhe, Germany — [2]Institute of Nanotechnology, KIT, Karlsruhe, Germany

The surface of a 3D topological insulator (TI) can be gapped out, e. g., by a proximity-induced superconducting order parameter. We consider a Josephson junction formed by two s-wave superconductors on a TI surface. In this geometry, the surface spectrum comprises electronic modes localised around the junction in addition to scattering modes. Taking into account the contributions of both scattering states and bound states, we analyse the phase dependence of the Josephson current mediated by the TI surface modes. The impact of their spectrum combining spin–orbit coupling and (induced) s-wave superconductivity is of particular interest.

TT 40.6 Wed 16:15 HSZ 103

Improving topological superconductivity in two-dimensional Josephson junctions — •Aidan Wastiaux and Falko Pientka — Max-Planck Institut für Physik komplexer Systeme, Noethnitzer Straße 38 01187 Dresden

Two-dimensional Josephson junctions in a magnetic field are a new platform to host localized Majorana bound states (MBS) [1]. While recent experiments [2,3] have confirmed the possibility of engineering such a topological phase, improvements are needed to stabilize it. It is therefore important to predict suitable values of the microscopic parameters in order to realize a robust topological phase in Josephson junctions (see [4,5]).

In this talk, we extend previous work to the case of large Zeeman energies and identify optimal regimes (i.e., with a large spectral gap protecting the MBS), based on a combination of analytical and numerical results. Moreover, we compare the planar Josephson junction to a nanowire proximitized by two superconductors with a phase difference.

[1] Pientka et al., PRX 7, 021032 (2017)
[2] Fornieri et al., Nature 569, 89-92 (2019)
[3] Ren et al., Nature 569, 93-98 (2019)
[4] Setiawan et al., PRB 99, 220506 (2019); Setiawan et al., PRB 99, 174511 (2019)
[5] Scharf et al., PRB 99, 214503 (2019)

TT 40.7 Wed 16:30 HSZ 103

Manipulation of Majorana qubits in the Josephson junction on helical edges — •Sang-Jun Choi, Calzona Alessio, and Trauzettel Bjoern — Institute of Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Topological Josephson junctions constitute a promising platform to observe the exotic properties of Majorana fermions (MFs). Hosting MFs – especially in a Josephson junction setup – enables us (i) to manipulate the coupling between MFs via the phase difference of the superconductors and (ii) measure the fermion parity of two MFs by the sign of the supercurrent. First experimental hints for the existence of MFs in Josephson junctions have recently been established by a measurement of the fractional Josephson effect.

We theoretically study the Josephson effect on a U-shaped quantum spin Hall edge channel which hosts four MFs and hence describes a single Majorana qubit. Two distinct knobs – chemical potential and superconducting phase difference – are used to tune the various couplings among the MFs. As a result, we find two kinds of finite rotations of the Majorana qubit around x- and z-axis. We identify signatures of Lamor precession and Rabi oscillations in this setup. Additionally, we show that the rotated (Majorana qubit) state can be read-out by measuring the supercurrent. Finally, we propose an experimental protocol that is able to detect the non-Abelian nature of the MFs.

TT 40.8 Wed 16:45 HSZ 103

Quantized phase-coherent heat transport of helical Majorana modes — •Alexander G. Bauer[1], Benedikt Scharf[2], Ewelina M. Hankiewicz[2], Laurens W. Molenkamp[3], and Björn Sothmann[1] — [1]Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany — [2]Institute of Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat,University of Würzburg, Am Hubland,97074 Würzburg, Germany — [3]Physikalisches Institut, EP3, Universität Würzburg, Würzburg, Germany

Recently, phase-coherent heat transport in superconducting tunnel junctions has received great interest. On the one hand, it allows for the realization of caloritronic circuits [1]. On the other hand, it can serve as a probe of fundamental properties of topological quantum matter [2]. Here, we investigate heat transport in superconductor-topological insulator-superconductor (S-TI-S) hybrid junctions perpendicular to the direction of phase bias. We demonstrate that the thermal conductance is quantized for a phase difference $\phi = \pi$. This arises directly from the existence of gapless Majorana modes which propagate along the S-TI interfaces. In contrast, we find a strong suppression of thermal conductance for $\phi \neq \pi$ due to the opening of a gap in the Andreev bound state spectrum.

[1] F. Giazotto and M. J. Martinez-Perez, Nature 492, 401 (2012)
[2] B. Sothmann and E. M. Hankiewicz, Phys. Rev. B 94, 081407 (2016)

TT 41: Unconventional Superconductors

Time: Wednesday 15:00–19:00 Location: HSZ 201

Invited Talk TT 41.1 Wed 15:00 HSZ 201

Probing unconventional superconductivity using the field dependent magnetic penetration depth — •Joseph A. Wilcox — H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, United Kingdom

In the field of unconventional superconductivity, one of the key efforts has been to investigate the momentum space structure of the superconductor energy gap due to its close relation to the underlying pairing mechanism. The temperature dependence of the magnetic penetration depth $\lambda(T)$ has long been used to perform such investigations and, in-particular, to identify the presence or absence of gap nodes. However, in certain cases it is not possible to distinguish between different scenarios that could give rise to the same observed behaviour, e.g. gap nodes with small amounts of impurities and large gap anisotropy with very deep gap minima, but no nodes.

A solution to this issue is that the temperature dependence of the magnetic penetration depth should change in the presence of a weak magnetic field. This effect was searched for extensively in cuprates but was not clearly observed, possibly because of other competing effects. Here we show that the magnetic field dependence of λ is strongly enhanced in low-T_c unconventional superconductors and that $\lambda(B,T)$ can be used as a tool with which to distinguish nodal pairing states from those where there is a small residual gap. We show data for $CeCoIn_5$ and LaFePO which show the effect of a nodal gap and for KFe_2As_2 which is consistent with a small but finite gap.

TT 41.2 Wed 15:30 HSZ 201

Sr_2RuO_4 under uniaxial pressure along the c-axis — •Fabian Jerzembeck[1], Alexander Steppke[1], Dmitry Sokolov[1], Naoki Kikugawa[2], Helge Rosner[1], Andrew Mackenzie[1,3], and Clifford Hicks[1] — [1]Max Planck Institute for Chemical Physics of Solids — [2]National Institute for Material Science, Tsukuba, Ibaraki — [3]School of Physics and Astronomy, University of St. Andrews

The unconventional superconductor Sr_2RuO_4 has been extensively studied under in-plane uniaxial pressure. a-axis pressure deforms one of the Fermi surfaces elliptically, so that at a compressive strain of $\varepsilon_{xx} = -0.44$ %, one of the Fermi surfaces undergoes a Lifshitz transition at a single point in k-space, dramatically altering the low-temperature electronic properties. Here, we investigate the consequences of pressure along the c-axis. c-axis pressure causes charge transfer from the d_{xz} and d_{yz} to the d_{xy}-orbital, resulting in an expansion of the main Fermi surface and finally in Lifshitz transitions at the X and Y points simultaneously. DFT calculations suggest that this occurs at $\varepsilon_{zz} \approx -2.5$ %. We present data for strains up to -2 %, finding that, surprisingly, T_c decreases even as the density of states increases.

TT 41.3 Wed 15:45 HSZ 201

Muon spin relaxation studies of time reversal symmetry breaking superconductivity in Sr_2RuO_4 by the application of uniaxial pressure — •Shreenanda Ghosh[1], Vadim Grinenko[1,2], Rajib Sarkar[1], Felix Brückner[1], Jean-Christophe Orain[3], Artem Nikitin[3], Joonbum Park[4], Mark Barber[4], Naoki Kikugawa[5], Jake Bobowski[6,7], Dmitry Sokolov[4], Takuto Miyoshi[6], Matthias Elender[3], Yoshiteru Maeno[6], Andrew Mackenzie[4], Hubertus Luetkens[3], Clifford Hicks[4], and Hans-Henning Klauss[1] — [1]IFMP, Technische Universität Dresden — [2]IFW, Dresden — [3]Paul Scherrer Institute, Switzerland — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [5]National Institute for Material Science, Japan — [6]Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan — [7]University of British Columbia, Kelowna, Canada

After more than two decades of extensive research, the idea regarding the symmetry of the superconducting order parameter of Sr_2RuO_4 is still lacking a consensus. One key prediction for Sr_2RuO_4, a splitting of the superconducting and time-reversal symmetry breaking(TRSB) transitions under uniaxial pressure have not been observed. Here, we report a large stress-induced splitting between the onset temperatures of superconductivity and TRSB transitions observed by muon spin relaxation (μSR) measurements on Sr_2RuO_4 placed under uniaxial pressure. In order to perform these technically challenging experiments, a customized uniaxial pressure cell was developed, which will be introduced.

TT 41.4 Wed 16:00 HSZ 201

Nematicity and checkerboard order in the surface layer of $\mathbf{Sr_2RuO_4}$ — •Carolina A. Marques[1], Luke C. Rhodes[1], Veronica Granata[2], Rosalba Fittipaldi[2], Antonio Vecchione[2], Andreas W. Rost[1], and Peter Wahl[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife KY16 9SS, United Kingdom — [2]CNR-SPIN, UOS Salerno, Via Giovanni Paolo II 132, Fisciano, I-84084, Italy.

Superconductivity in strongly correlated systems is often found near exotic electronic phases, such as antiferromagnetism and electronic nematicity. These phases can be highly sensitive to minor changes in the crystal structure, induced by doping or strain. In the unconventional superconductor Sr_2RuO_4, a 6° rotation of the RuO_6 octahedra at the surface seems to suppress its superconducting state and, additionally, pushes a van Hove singularity below the Fermi energy.

Using ultra-low temperature Scanning tunnelling microscopy (STM), we study the low energy electronic properties of the reconstructed surface of Sr_2RuO_4. Our measurements show clear signatures of C4 symmetry breaking, together with the appearance of a checkerboard order. This order is associated with a peak in the tunnelling spectrum, which splits in a magnetic field, revealing a charge nature. Tight binding calculations show that a nematic order parameter coexisting with a modulation of the charge-density reproduces the observed low energy density of states. Understanding the underlying physics at this surface provides a new platform to study the strongly correlated phases of Ruthenate materials.

TT 41.5 Wed 16:15 HSZ 201

Stabilizing even-parity chiral superconductivity in $\mathbf{Sr_2RuO_4}$ — Han G. Suh[1], Henri Menke[2], Philip M. R. Brydon[2], Carsten Timm[3], •Aline Ramires[4,5,6], and Daniel F. Agterberg[1] — [1]Department of Physics, University of Wisconsin, Milwaukee, WI 53201, USA — [2]Department of Physics and MacDiarmid Institute for Advanced Materials and Nanotechnology, University of Otago, P.O. Box 56, Dunedin 9054, New Zealand — [3]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Dresden, 01187, Germany — [5]ICTP-SAIFR, International Centre for Theoretical Physics, South American Institute for Fundamental Research, Sao Paulo, SP, 01140-070, Brazil — [6]Instituto de Fisica Teorica, Universidade Estadual Paulista, Sao Paulo, SP, 01140-070, Brazil

Sr_2RuO_4 has long been thought to host a spin-triplet chiral p-wave superconducting state. However, the singlet-like response observed in recent Knight shift measurements casts serious doubts on this pairing state. The available experimental results seem to point towards an even-parity chiral superconductor, a pairing state which has been systematically neglected given the quasi-2D electronic structure of Sr_2RuO_4. Here we show how the orbital degree of freedom can encode the two component nature of the E_g order parameter, allowing for an s-wave orbital-antisymmetric spin-triplet state which can be stabilized by Hund's coupling.

TT 41.6 Wed 16:30 HSZ 201

Direct observation of a uniaxial stress-driven Lifshitz transition in $\mathbf{Sr_2RuO_4}$ — •Edgar Abarca Morales[1,2], Veronika Sunko[1,2], Igor Markovic[1,2], Mark Barber[1], Dijana Milosavjlevic[1], Federico Mazzola[2], Dmitry Sokolov[1], Helge Rosner[1], Clifford Hicks[1], Philip King[2], and Andrew Mackenzie[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, 01187, Dresden, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, UK

Application of uniaxial pressure has recently been shown to more than double the transition temperature of the unconventional superconductor Sr_2RuO_4, leading to a peak in T_c versus strain whose origin is still under debate. Here we develop a simple and compact method to apply large uniaxial pressures in a way compatible with angle-resolved photoemission. We directly visualise how uniaxial stress drives a Lifshitz transition of the γ-band Fermi surface, pointing to the key role of strain-tuning its associated van Hove singularity to the Fermi level in mediating the peak in T_c. Our measurements provide stringent constraints for theoretical models of the strain-tuned electronic structure evolution of Sr_2RuO_4. Furthermore, our experimental approach opens the door to future studies of strain-tuned phase transitions where large pressure cells or piezoelectric-based devices may be difficult to implement.

15 min. break.

TT 41.7 Wed 17:00 HSZ 201

Uniaxial stress dependence of the critical temperature of $\mathbf{YBa_2Cu_3O_{6.67}}$ — •Clifford Hicks[1], Mark Barber[1], Marcin Konczykowski[2], Bernhard Keimer[3], and Andrew Mackenzie[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany — [2]École Polytechnique, Paris, France — [3]Max-Planck-Institut für Festkörperforschung

We use piezoelectric-based uniaxial pressure apparatus and GaAs/AlGaAs-based susceptometers to measure the stress dependence of the critical temperature of $YBa_2Cu_3O_{6.67}$. T_c of the unstressed material is 65 K, and with compression along the a axis T_c decreases steadily. At a pressure of 1 GPa, long-correlation-length charge density wave order appears, and strong competition between this order and superconductivity causes a rapid suppression of T_c.

TT 41.8 Wed 17:15 HSZ 201

Spiral magnetic order in high-T_c cuprates - a ground state candidate at high magnetic fields — •Johannes Mitscherling, Pietro Maria Bonetti, Demetrio Vilardi, and Walter Metzner — Max Planck Institute for Solid State Research, Stuttgart

The normal state beneath the superconducting dome determines the fluctuations that govern the anomalous properties of cuprate superconductors in a wide range of their phase diagram. Recent experiments at very high magnetic fields shed new light on the phenomenology of the high field ground state: A drastic change in the carrier density at the onset of the pseudogap observed in various cuprate compounds, thermodynamic signatures of a quantum critical point at this doping and, very recently, NMR and ultrasound experiments indicated glassy antiferromagnetic order up to the pseudogap onset.

We present incommensurate spiral magnetic order as a potential ground state candidate at high magnetic fields [1,2]. Previous theoretical work suggests that suppression of superconductivity leads to such a ground state [3]. We present quantitative results for magnetic order in the Hubbard model at strong coupling using dynamical mean-field theory [4]. We show that experimental signatures as the Fermi arcs, nematicity and a drastic drop in both the DC conductivity and the Hall number can be understood within this framework.

[1] A. Eberlein *et al.*, PRL **117**, 187001 (2016)
[2] J. Mitscherling *et al.*, PRB **98**, 195126 (2018)
[3] H. Yamase *et al.*, PRL **116**, 096402 (2016)
[4] P. M. Bonetti *et al.*, in prep.

TT 41.9 Wed 17:30 HSZ 201

A hydrodynamical description for magneto-transport in the strange metal phase of cuprates — Andrea Amoretti[1,2], •Martina Meinero[1,3], Daniel Brettan[2], Federico Caglieris[4], Enrico Giannini[5], Christian Hess[4], Bernd Buechner[4], Nicodemo Magnoli[1,2], and Marina Putti[1,3] — [1]DIFI-Università di Genova, via Dodecaneso 33, 14146 Genova, Italy — [2]INFN-Sezione di Genova, via Dodecaneso 33, 16146 Genova, Italy — [3]CNR-SPIN, corso Perrone 24, 16152 Genova, Italy — [4]Leibniz IFW Dresden, Helmholtz str. 20, 10169 Dresen, Germany — [5]University of Geneva, 24 Quai Ernst Ansermet, 1211 Geneva, Switzerland

High temperature superconductors are strongly coupled systems which present a complicated phase diagram with many coexisting phases. This makes it difficult to understand the mechanism which generates their singular transport properties. Hydrodynamics, which mostly relies on the symmetries of the system without referring to any specific microscopic mechanism, constitutes a promising framework to analyze these materials. In this paper we show that in the strange metal phase of the cuprates, a whole set of transport coefficients are described by a universal hydrodynamic framework once one accounts for the effects of quantum critical charge density waves. We corroborate our theoretical prediction by measuring the DC transport properties of Bi-2201 close to optimal doping, proving the validity of our approach. Our argument can be used as a consistency check to understand the universality class

governing the behavior of high temperature cuprate superconductors.

TT 41.10 Wed 17:45 HSZ 201

The source of spontaneous currents in BTRS superconductors — •V. Grinenko[1,2], S. Ghosh[1], R. Sarkar[1], F. Brückner[1], H. Luetkens[3], K. Kihou[4], C.H. Lee[4], P. Chekhonin[1,2], W. Skrotzki[1], R. Hühne[2], K. Nielsch[2], S.-L. Drechsler[2], V.L. Vadimov[5], M.A. Silaev[6], P. Volkov[7,8], I. Eremin[7], J. Park[9], M.E. Barber[9], N. Kikugawa[10], D.A. Sokolov[9], J.S. Bobowski[11,12], T. Miyoshi[11], Y. Maeno[11], A. P. Mackenzie[9,13], C. Hicks[9], and H.-H. Klauss[1] — [1]TU Dresden — [2]IFW Dresden — [3]PSI, Switzerland — [4]AIST, Japan — [5]IPM, Russia — [6]University of Jyväskylä, Finland — [7]Ruhr-Universitat Bochum — [8]Rutgers University — [9]MPI CPFS — [10]NIMS, Japan — [11]Kyoto University — [12]University of British Columbia — [13]University of St. Andrews

Recently, the superconductivity that breaks time-reversal symmetry (BTRS) attracts a lot of attention in the scientific community. However, there is no general agreement among the researches whether the evadible experimental data provide convincing support for the theoretical predictions. In particular, the nature of the spontaneous currents in the BTRS state remains mysterious. Here, we verify the proposal that spontaneous currents in the BTRS superconducting state appear due to spatial inhomogeneities of the superconducting order parameter. We study the effect of disorder on the strength of the spontaneous currents in the BTRS state in two superconducting systems: Sr_2RuO_4 and $Ba_{1-x}K_xFe_2As_2$. Our available data indicates that non-magnetic impurities indeed affect noticeably the strength of the spontaneous magnetization measured by muon spin rotation/relaxation technique.

TT 41.11 Wed 18:00 HSZ 201

Field-induced change of the superconducting state in the locally non-centrosymmetric heavy fermion $CeRh_2As_2$ — •Javier Landaeta, Seunghyun Khim, Daniel Hafner, Jacinta Banda, Manuel Brando, Robert Küchler, Christoph Geibel, and Elena Hassinger — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

$CeRh_2As_2$ is a new heavy fermion superconductor with a $CaBe_2Ge_2$-type crystalline structure, which lacks inversion symmetry locally at the Ce site. A weak phase transition is observed in the specific heat at T_0=0.4 K with possibly quadrupolar origin and below T_c= 0.27 K the material becomes superconducting. Here, we present a comprehensive study of the low temperature AC magnetic susceptibility in a single crystal of $CeRh_2As_2$ up to 15 T. We did not detect any additional transition above T_c, supporting that the specific heat anomaly might be caused by a quadrupolar order. The superconducting upper critical field is strongly anisotropic with $\mu_0 H_{c2} = 13$ T for $B \parallel c$ and $\mu_0 H_{c2} = 2$ T for $B \perp c$, which exceed the Pauli limit. The large H_{c2} and their anisotropy are reminiscent of non-centrosymmetric superconductors such as $CePt_3Si$, $CeRhSi_3$, $CeIrSi_3$. What makes $CeRh_2As_2$ stand out is its unique superconducting phase diagram with a pronounced kink at 4 T for $B \parallel c$ reproducible in heat capacity, resistivity and AC susceptibility measurements. Moreover, isothermal AC susceptibility and magnetostriction reveal a sharp phase transition inside the superconducting phase at 4 T independent of temperature. Therefore, two different superconducting states exist for $B \parallel c$ in $CeRh_2As_2$.

TT 41.12 Wed 18:15 HSZ 201

Uranium-based superconducting materials — •Eteri Svanidze — Max Planck Institute for Chemical Physics of Solids

A rather large number of uranium-based materials are exotic - they show complex magnetic orders, coexistence of superconductivity with magnetism, enhanced effective electron masses, quantum critical behavior, and topological states [1-3]. All of these peculiar phenomena are thought to arise from electrons' dual nature, which is also believed to lie at the origin of high-temperature superconductivity. From a condensed matter point of view, the most intriguing uranium-based materials are in fact superconductors - UBe13, URu2Si2, and UPt3. In this talk, I will provide a brief historic overview of superconductivity in uranium-based systems, and address several pertinent questions: Is superconductivity in uranium-based materials always unconventional? Why are superconducting temperatures in uranium-based compounds so low, compared to other compounds, based on actinide or lanthanide elements? Is there a way to pinpoint crystallographic motifs, which are favorable for the emergence of superconducting state? I will then provide a number of empirical features that should be targeted in the search for new uranium-based superconductors [4].

[1] J. C. Griveau and É. Colineau, Comptes Rendus Phys. 15, 599 (2014)
[2] B. D. White et al., Phys. C Supercond. its Appl. 514, 246 (2015)
[3] H. R. Ott and Z. Fisk, Encycl. Inorg. Bioinorg. Chem. (2018)
[4] E. Svanidze, Handbook Phys. Chem. Rare Earths 56, 163 (2019)

TT 41.13 Wed 18:30 HSZ 201

Low-Temperature Phase of the $Cd_2Re_2O_7$ Superconductor: Ab initio Phonon Calculations and Raman Scattering — •Reinhard K. Kremer[1], Konrad J. Kapcia[2], Andrzej Ptok[2], Przemysław Piekarz[2], Fereidoon S. Razavi[3], Maureen Reedyk[3], Mojtaba Hajialamdari[3], and Andrzej M. Oleś[4] — [1]MPI für Festkörperforschung, Stuttgart, Germany — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland — [3]Dep. of Physics, Brock University, St. Catharines, Canada — [4]Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland

Using an *ab initio* approach, we report a phonon soft mode in the tetragonal structure described by the space group $I4_122$ of the 1 K $5d$ superconductor $Cd_2Re_2O_7$. It induces an orthorhombic distortion to a crystal structure described by the space group $F222$ which hosts the superconducting state. This new phase has a lower total energy than the other known crystal structures of $Cd_2Re_2O_7$. Comprehensive temperature dependent Raman scattering experiments on isotope enriched samples, $^{116}Cd_2Re_2{}^{18}O_7$, not only confirm the already known structural phase transitions but also allow us to identify a new characteristic temperature regime around $\sim$ 80 K, below which the Raman spectra undergo remarkable changes with the development of several sharp modes and mode splitting. Together with the results of the *ab initio* phonon calculations we take these observations as strong evidence for another phase transition to a novel low-temperature crystal structure of $Cd_2Re_2O_7$.

TT 41.14 Wed 18:45 HSZ 201

Local spin susceptibility in the FFLO state of an all-organic conductor — •S. Molatta[1,2], H.H. Wang[3], G. Koutroulakis[3], J.A. Schlueter[4], S.E. Brown[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 and Astronomy, UCLA, Los Angeles, USA — [4]Materials Science Division, Argonne National Laboratory, Argonne, USA

The phenomenology of the superconducting Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state, initially proposed in 1964, was experimentally confirmed in several organic conductors during the last years. A spatial modulation of the superconducting order parameter and spin susceptibility, caused by a strong population imbalance of a multi-component Fermi liquid, is a hallmark of the FFLO state. We report on recent results of ^{13}C nuclear magnetic resonance (NMR) measurements of the material β''-$(ET)_2SF_5CH_2CF_2SO_3$, which probe the inhomogeneous spatial distribution of the static and dynamic spin susceptibility across the transition from normal into the FFLO state. The NMR results reveal a low-temperature onset and increase of the inhomogeneous spectral line broadening and related superconducting gap amplitude. Further, increased spin fluctuations in the regime of the thermodynamic phase boundary indicate a complex interplay of FFLO superconductivity, reduced dimensionality, and inter-plane coherence.

TT 42: Correlated Electrons: f-Electron Systems and Heavy Fermions 2

Time: Wednesday 15:00–17:45 Location: HSZ 204

TT 42.1 Wed 15:00 HSZ 204

Low-Temperature Properties of the Non-Centrosymmetric Heavy-fermion Compound $CeAl_2$ — •Christian Oberleitner, Alexander Regnat, Christian Franz, Jan Spallek, Georg Benka, Michael Petrov, Marc Wilde, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

Heavy-fermion compounds exhibit many unexpected low-temperature properties like unconventional superconductivity, non-Fermi liquid behavior or negative magnetoresistance. In this work, we report a comprehensive study of the non-centrosymmetric heavy-fermion compound $CeAl_2$ with T_N = 3.8K. The metallurgical characterization by Laue x-ray scattering and powder x-ray diffraction shows the excellent crystalline quality, which is confirmed by very high RRR values. Subsequently, magnetization, specific heat, torque magnetometry, resistivity, and Hall-effect measurements down to 200mK and up to 14T were carried out. The low-temperature measurements in the antiferromagnetic regime show complex magnetic behavior. Presumably, the Hall-effect cannot be explained by a superposition of anomalous and normal Hall-effect, which suggests a topological contribution.

TT 42.2 Wed 15:15 HSZ 204

Field-angle resolved magnetic excitations as a probe of hidden-order symmetry in CeB_6 — •Pavlo Y. Portnichenko[1], Alireza Akbari[2], Stanislav E. Nikitin[3], Alistair S. Cameron[1], Natalya Yu. Shitsevalova[4], Igor Radelytskyi[5], Astrid Schneidewind[5], Zita Hüsges[6], Jianhui Xu[6], Alexandre Ivanov[7], Jean-Michel Mignot[8], Peter Thalmeier[3], and Dmytro S. Inosov[1] — [1]TU Dresden, Germany — [2]APCTP Pohang, Korea — [3]MPI-CPfS Dresden, Germany — [4]IMPS, Kiev, Ukraine — [5]JCNS, Jülich, Germany — [6]HZB, Berlin, Germany — [7]ILL, France — [8]LLB, France

The heavy-fermion compound CeB_6 and its La-diluted alloys are among the best-studied realizations of the long-range multipolar phases, often referred to as "hidden order". Previously the hidden order in phase II was identified as primary antiferroquadrupolar and field-induced octupolar order. Here we present a combined experimental and theoretical investigation of collective excitations in the phase II of CeB_6. Inelastic neutron scattering in fields up to 16.5 T reveals a new high-energy mode above 14 T in addition to the low-energy magnetic excitations. The experimental dependence of their energy on the magnitude and angle of the applied magnetic field is compared to the results of a multipolar interaction model. We show that the rotating-field technique at fixed momentum can complement conventional INS measurements of the dispersion at constant field and holds great promise for identifying the symmetry of multipolar order parameters and the details of inter-multipolar interactions.

TT 42.3 Wed 15:30 HSZ 204

Topology in Magnetic Phases of SmB_6 — •Moritz M. Hirschmann, Huimei Liu, Andreas P. Schnyder, and Giniyat Khaliullin — Max Planck Institute for Solid State Research, Stuttgart, Deutschland

The heavy fermion compound SmB_6 is well known to be a Kondo insulator. Whereas its paramagnetic state was found to be topological, an analysis of the magnetic phases emerging in high-pressure SmB_6 considering its f-quartet ground state is still lacking. The exact magnetic order is yet unknown, therefore we discuss the two most likely magnetic structures, A-type and G-type, as well the high-field limit. We offer topological features as an experimental starting point to determine the magnetic order. With this in mind we present Dirac nodal lines for the A-type structure and Dirac points for the G-type structure. To investigate the topological properties we describe the mixed valence samarium sites with a tight-binding model and incorporate the effect of an internal magnetization. Our discussion includes symmetry arguments, Berry phases and the resulting surface states.

TT 42.4 Wed 15:45 HSZ 204

A Resonant Inelastic X-ray Scattering investigation of the 4f states in SmB_6 — •Andrea Amorese[1,2], Oliver Stockert[2], Kurt Kummer[3], Nicholas Brookes[3], Maurits Haverkort[4], Peter Thalmeier[2], Liu Hao Tjeng[2], and Andrea Severing[1] — [1]University of Cologne, Germany — [2]MPI-CPfS, Dresden, Germany — [3]ESRF, Grenoble, France — [4]University of Heidelberg, Germany

The crystal-field (CF) splitting of the $^6H_{5/2}$ Hund's rule ground state of Sm^{3+} in the strongly correlated topological insulator SmB_6 has been determined with high resolution resonant inelastic x-ray scattering (RIXS) at the Sm M_5 edge. The valence selectivity of RIXS allows isolating the crystal-field-split excited multiplets of the Sm^{3+} ($4f^5$) configuration from those of Sm^{2+} ($4f^6$) in intermediate valent SmB_6. We find that the quartet Γ_8 ground state and the doublet Γ_7 excited state are split by Δ_{CF} = 20±10meV. Considering this as an upper limit for the 4f bandwidth gives an extremely large mass renormalization from the band structure value, which can be linked to the small coefficient of fractional parentage for the hopping of the 4f electrons. The tiny band width complies with the small value of the gap and may be used to put constraints to the energies of the topological surface states. Financial support of the DFG under grant SE-1441/4-1 is acknowledged.

TT 42.5 Wed 16:00 HSZ 204

Partially Localized Phases in 5f Systems — •Bishal Poudel[1,2], Sébastien Burdin[1], and Gertrud Zwicknagl[2] — [1]LOMA UMR 5798, Université de Bordeaux, 33400, Talence, France — [2]Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany

We study a generalized multi-orbital Hubbard Hamiltonian as an effective model for 5f electrons in actinide compounds. Our model assumes a large spin-orbit interaction, and includes local correlations. In our model, we use jj-scheme to classify the electronic states and due to large spin-orbit interaction the multiplet states with j = 7/2 or higher are neglected.

Here, we generalize the previous calculations [1-3] performed for 5f electrons systems using a rotationally invariant slave boson method [4] within a mean-field approximation. We analyze the phase diagram of the system at zero temperature. Varying the strength and anisotropy of the effective non-interacting electronic bandwidths, we analyze the partial -orbitally selective- localization of f electrons as well as their magnetic ordering.

[1] G. Zwicknagl, and P. Fulde, J. Phys. Condens. Matter 15, S1911 (2003).
[2] D. V. Efremov, N. Hasselmann, E. Runge, P. Fulde, and G. Zwicknagl, Phys. Rev. B 69, 115114 (2004).
[3] F. Pollmann, and G. Zwicknagl, Phys. Rev. B 73, 035121 (2006).
[4] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, Phys. Rev. B 76, 155102 (2007)

TT 42.6 Wed 16:15 HSZ 204

Spectroscopic investigation of UFe_2Si_2, URu_2Si_2, UNi_2Si_2, and UPd_2Si_2: from Pauli paramagnetism to antiferromagnetism via the hidden order state. — Andrea Amorese[1,2], Martin Sundermann[1,2], Andrea Marino[2,3], Maurits Haverkort[4], Liu Hao Tjeng[2], and •Andrea Severing[1] — [1]University of Cologne, Germany — [2]MPI-CPfS, Dresden, Germany — [3]Politecnico di Milano, Milano, Italy — [4]Heidelberg University, Heidelberg, Germany

We have carried out hard x-ray photoelectron spectroscopy (HAXPES) measurements at the U 4f core level and non-resonant inelastic x-ray scattering (NIXS) at the U O4,5 edge of UT_2Si_2 compounds that all form in the tetragonal ThCr2Si2 structure but exhibit different ground state properties: UFe_2Si_2 is a Pauli paramagnet; URu_2Si_2 is the famous hidden order compound of which the order parameter is still fiercely debated despite 30 years of intense experimental and theoretical studies [1]; UPd_2Si_2 and UNi_2Si_2 are antiferromagnets with TN well above 100 K and sizeable ordered magnetic moments. We have determined the degree of the 5f-electron localization (HAXPES) as well as the symmetry of the 5f ground state wave function (NIXS [2]) across these very different compounds. This enabled us to identify their systematics and to place them in an effective Doniach phase diagram.

Financial support of the DFG under grant SE-1441/5-1 is gratefully acknowledged.

[1] references in J.A. Mydosh and P.M. Oppeneer in Rev. Mod. Phys. 83, 1301 (2011) and in Phil. Magazine 94, 3642 (2014)
[2] M. Sundermann et al., PNAS 113, 13989 (2016)

15 min. break.

TT 42.7 Wed 16:45 HSZ 204

Metamagnetism in microstructured uranium mononitride — •S. Hamann[1,2], D. Gorbunov[1], T. Förster[1], M. König[2], A. V. Andreev[3], R. Troć[4], and T. Helm[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]MPI für Chemische Physik fester Stoffe, Dresden, Germany — [3]Institute of Physics, Academy of Sciences, Prague, Czech Republic — [4]W. Trzebiatowski Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wrocław, Poland

As in most $5f$ compounds, the origin of antiferromagnetism in uranium mononitride (UN) cannot be solely related to either itinerant or local behavior. While inelastic neutron scattering [1] and photoemission measurements [2] as well as bandstructure calculations suggest an itinerant nature, the recently discovered metamagnetic transition at 55 T [3] contradicts this picture. To investigate this spin-flop-like transition with transport measurements, we fabricated microstructures from single-crystalline UN using focussed ion beam technique. The gained resolution allows us to study the temperature and field-dependent Hall effect and longitudinal electrical transport in great detail.

[1] T. M. Holden *et al.*, Phys. Rev. B. **30**, 1 (1984)
[2] S. Fujimori *et al.*, Phys. Rev. B. **86**, 235108 (2012)
[3] K. Shrestha *et al.*, Scientific Reports **7**, 1 (2017)

TT 42.8 Wed 17:00 HSZ 204

Crystallographic structure and magnetism of UNi_4B — •Jannis Willwater[1], Stefan Süllow[1], Milan Klicpera[2], Michal Valiska[2], Vladimir Sechovsky[2], Bachir Ouladdiaf[3], and Hiroshi Amitsuka[4] — [1]IPKM, TU Braunschweig, Germany — [2]Department of Condensed Matter Physics, Charles University, Czech Republic — [3]Institut Laue-Langevin, France — [4]Department of Condensed Matter Physics, Japan

The frustrated intermetallic magnet UNi_4B has been reported to crystallize in a hexagonal crystallographic structure and to exhibit a peculiar type of partial magnetic order at low temperatures. Recently, synchrotron x-ray diffraction data have indicated that the structure is orthorhombic and not hexagonal. The best description of the crystal structure at 300 K was obtained with the space group 63 (*Cmcm*). In this situation, to understand the nature of the magnetic transitions at low temperature, it requires the determination of the low temperature crystallographic symmetry. Therefore, we have studied a ^{11}B enriched single crystal UNi_4B, here using elastic neutron scattering. In our experiment, various structural Bragg peaks forbidden for the *Cmcm* symmetry have been detected and indicate that the symmetry of the crystal structure is even lower. From fits to our data, we have obtained the best description of the structure with the orthorhombic space group 25 (*Pmm2*). Further we have detected various magnetic Bragg peaks and established their temperature dependence.

TT 42.9 Wed 17:15 HSZ 204

Terahertz conductivity of heavy-fermion systems from time-resolved spectroscopy — •C.-J. Yang[1], S. Pal[1], F. Zamani[2], K. Kliemt[3], C. Krellner[3], O. Stockert[4], H. v. Löehneysen[5], J. Kroha[2], and M. Fiebig[1] — [1]ETH Zürich, Switzerland — [2]University of Bonn, Germany — [3]Goethe-University Frankfurt, Germany — [4]MPI CPfS Dresden, Germany — [5]KIT Karlsruhe, Germany

Ultrafast, phase-sensitive terahertz (THz) spectroscopy has recently been introduced as a novel tool to investigate the quasiparticle (QP) dynamics across the quantum phase transition in heavy-fermion compounds [1,2]. The incident THz pulse with a spectral range of 0–3 THz creates collective intraband excitations within the heavy band as well as resonant interband transitions between the hybridizing heavy and light parts of the conduction band. The latter break the Kondo singlet and thus lead to a time-delayed echo-like response [1,2]. By contrast, the intraband excitations leave the heavy quasiparticles intact and are expected to be Fermi-liquid Drude response. Our time-resolved phase-sensitive measurements of the electric field response enables us to separate both types of excitations by their delay time and to derive their individual contributions to the THz optical conductivity. While the Kondo-breaking interband transitions create no Drude peak, the intraband excitations recover the Drude response as expected. It is thus possible to separate strongly and weakly correlated electronic contributions to the optical conductivity.

[1] C. Wetli *et al.*, Nat. Phys. **14**, 1103 (2018)
[2] S. Pal *et al.*, PRL **122**, 096401 (2019)
[3] C.-J. Yang *et al.*, under prep. (2019)

TT 42.10 Wed 17:30 HSZ 204

Resonant X-Ray Emission Spectra: Effects of the Final-State Core Hole — •Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

The resolution of the x-ray absorption spectroscopy is fundamentally limited by the life-time broadening of the core hole created in the absorption event. When the absorption is detected by monitoring a particular core-to-core emission process of filling the created hole (for instance, the 3d → 2p transition in the case of lanthanide L edges), the broadening is reduced and it is determined by a considerably longer life time of the shallower 3d hole remaining in the final state [1]. This is not always the whole story – there can be a sizable exchange interaction between the final-state core hole and some partially filled valence shell (this would be the 4f shell in the lanthanide example). The exchange interaction causes multiplet splitting that reduces the resolution again and potentially even introduces spurious features to the deduced absorption spectra. I will discuss these effects theoretically using the atomic model and the Anderson impurity model. I will show under which simplifying conditions the many-body part of the problem reduces to evaluation of a propagator of the final-state core hole, a quantity that is measured by the x-ray photoemission.

[1] K. Hamalainen, D. P. Siddons, J. B. Hastings, L. E. Berman, Phys. Rev. Lett. **67**, 2850 (1991).

TT 43: Frustrated Magnets - Strong Spin-Orbit Coupling 2 (joint session TT/MA)

Time: Wednesday 15:00–17:45 Location: HSZ 304

TT 43.1 Wed 15:00 HSZ 304

Magnetic frustration in fcc lattices — •Veronika Fritsch[1], Christina Baumeister[1], F. Maximilian Wolf[1], Johanna Oefele[1], Jens-Uwe Hoffmann[2], Manfred Reehuis[2], and Oliver Stockert[3] — [1]EP 6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

A face-centered cubic (fcc) lattice is inherently prone to magnetic frustration, since it is build from a network of edge-sharing tetrahedra. Up to now most studies were performed on insulating systems. We have investigated various metallic systems with neutron diffraction experiments, where the magnetic Ho-ions form an fcc lattice: $HoInCu_4$ and $HoCdCu_4$ [1] as well as $HoInAg_2$ and $HoInAu_2$. All compounds exhibit long-range magnetic order with different propagation vectors, which can be understood within a simple J_1/J_2 model [2]. Furthermore we found diffuse scattering dependent on the degree of frustration of the samples.

[1] V. Fritsch *et al.*, arXiv:1907.09885 [cond-mat.str-el]
[2] P. W. Anderson, Phys. Rev. **79**, 705 (1950).

TT 43.2 Wed 15:15 HSZ 304

The evolution of magnetic frustration in $HoInAg_{2-x}Au_x$ — •Johanna Oefele[1], Oliver Stockert[2], Philipp Gegenwart[1], and Veronika Fritsch[1] — [1]EP6, Electronic Correlations and Magnetism, Augsburg University, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

While the intermetallic compounds $HoInAg_2$ and $HoInAu_2$ share the same face-centered cubic crystal structure and are isoelectronic, the magnetic properties significantly deviate from each other. $HoInAg_2$ is strongly frustrated as evidenced by its thermodynamic properties and a large frustration parameter. In contrast the $HoInAu_2$ system shows no signs of magnetic frustration. In order to explore the transition from the frustrated to the non-frustrated system we synthesised the substitution series $HoInAg_{2-x}Au_x$.

In this talk I will present the crystal growth and the susceptibility, specific heat and the resistivity measurements on our polycrystalline samples. The effective paramagnetic moments extracted from the magnetic susceptibility coincide with the value expected for free Ho^{3+}. From the specific heat the entropy was calculated confirming the presence of magnetic frustration in $HoInAg_2$. With increasing substitution of Ag with Au the Néel temperature is monotonically increasing, while the frustration vanishes.

TT 43.3 Wed 15:30 HSZ 304

Short range spin ice type correlations of Kagome spin ice HoAgGe by diffuse neutron scattering — •Kan Zhao and Philipp Gegenwart — Experimentalphysik VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86159 Augsburg, Germany

Spin ices are exotic phases of matter characterized by frustrated spins obeying local ice rules that minimize the number of spatially isolated magnetic monopoles, in analogy with the electric dipoles in water ice. In two dimensions, one can similarly define ice rules for in-plane Ising-like spins arranged on a kagome lattice, which require each triangle plaquette to have a single monopole, and can lead to a variety of unique orders and excitations.

With P-62m structure, Ho sites of HoAgGe in the ab plane form a distorted kagome lattice. According to magnetometry, thermodynamic measurements, elastic neutron scattering and Monte Carlo simulations, we establish HoAgGe as the unique crystalline system to realize the kagome spin ice state [1].

The short range spin ice type correlations, have been predicted as one characteristic feature of classical kagome spin ice model. Thus, we conducted the diffuse scattering for HoAgGe above the long range magnetic order temperature. And clear diffuse scattering pattern is obtained, which is consistent with that of Monte Carlo simulations based on a classical spin model consisting of Ising-like in-plane spins on the 2D distorted kagome lattice of HoAgGe [1].

[1] Zhao, Kan et al. Submitted (2018)

TT 43.4 Wed 15:45 HSZ 304

New phases in the Shastry-Sutherland compound NdB_4 discovered by high-resolution dilatometry — •Rahel Ohlendorf[1], Sven Spachmann[1], Daniel Brunt[2], Oleg Petrenko[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Department of Physics, University of Warwick, UK

We report detailed thermal expansion and magnetostriction studies on NdB_4 single crystals in magnetic fields up to 15 T. The system can be mapped on a Shastry-Sutherland model implying magnetically frustrated orthogonal dimers of Nd-moments. Accordingly, a sequence of unusual magnetic phases has been reported [1]. At $B = 0$ T these phases are associated with the evolution of antiferromagnetic (afm) order at $T_1 = 17.2$ K and two incommensurate afm phases at $T_2 = 7.0$ K and $T_3 = 4.8$ K. All transitions are associated with pronounced anomalies in the thermal expansion coefficients which enables studying the phase boundaries in external magnetic fields, here applied along the crystallographic [001]- and [110]-axis, respectively. Our data confirm previously reported phase boundaries and show, e.g., that the nature of the phase transition $T_2(B)$ changes from continuous to discontinuous. In addition, for each field direction our data evidence novel phases not reported before. The phase diagram is discussed based on the anomalies in the thermal expansion and magnetostriction data and the respective uniaxial pressure dependencies.

[1] Ryuta Watanuki et al 2009 J. Phys.: Conf. Ser. 150 042229

15 min. break.

TT 43.5 Wed 16:15 HSZ 304

Energy dynamics in the Kitaev quantum spin liquid at finite temperature and momentum — •Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106, Braunschweig, Germany

The role of finite temperature and momentum in the energy dynamics of the two-dimensional Kitaev spin-model on the honeycomb lattice are studied. Fractionalization of magnetic moments into mobile Majorana matter and a static $\mathbb{Z}_2$ gauge field lead to a continuum of energy density modes comprising two channels. Thermal flux excitations, which act as an emergent disorder, strongly affect the dynamical energy susceptibility. Above the flux proliferation temperature, coherent energy propagation is modified into a quasi hydrodynamic density relaxation, the temperature and momentum dependence of which is analyzed. Results from the low-temperature homogeneous gauge and a mean-field treatment of thermal gauge fluctuations, valid at intermediate and high temperatures are considered.

TT 43.6 Wed 16:30 HSZ 304

Raman spectrum of two particle excitations in the Kitaev-Heisenberg bilayer — •Erik Wagner and Wolfram Brenig — Institute for Theoretical Physics, Technical UniversityBraunschweig, Braunschweig, Germany

We study the Raman response of a honeycomb Kitaev spin-model with (an-)isotropic intralayer exchange $J_{x,y,z}$, coupled by additional interlayer Heisenberg exchange J to form a bilayer. Starting from the limit of decoupled dimers we use a perturbative continuous unitary transformation (pCUT), based on the flow equation method, to perform series expansion on the Hamiltonian and the Raman operator to analyze the spectrum. In particular we consider the groundstate energy and one particle dispersion up to 9th order in $J_{x,y,z}$ as well as the two particle interactions and spectrum up to 8th order. Results for the Raman response as well as (anti-)bound states will be presented versus anisotropy and for various bilayer-stackings.

TT 43.7 Wed 16:45 HSZ 304

Excitonic Magnetism at the intersection of Spin-orbit coupling and crystal-field splitting — Teresa Feldmaier[1], Pascal Strobel[1], Michael Schmid[1,2], Philipp Hansmann[3], and •Maria Daghofer[1] — [1]FMQ, Universität Stuttgart, Germany — [2]IQST, Stuttgart and Ulm, Germany — [3]MPI-CPfS, Dresden, Germany

Excitonic magnetism involving superpositions of singlet and triplet states is expected to arise for two holes in strongly correlated and spin-orbit coupled t_{2g} orbitals. However, uncontested material examples for its realization are rare. Applying the Variational Cluster Approach to the square lattice, we find for weak spin-orbit coupling stripy spin antiferromagnetism combined with stripy orbital order without a crystal field and checkerboard spin antiferromagnetism when crystal field favors the xy orbital. Strong spin-orbit coupling leads to excitonic antiferromagnetism that can coexist with substantial orbital polarization. We then address the specific example of Ca_2RuO_4 using *ab initio* modeling and conclude it to realize excitonic magnetism despite its pronounced orbital polarization.

TT 43.8 Wed 17:00 HSZ 304

Influence of spin-orbit coupling onto thermodynamic and dynamic properties of d^5- and d^4-systems — •Jan Lotze and Maria Daghofer — University of Stuttgart, Functional Matter and Quantum Technologies, Pfaffenwaldring 57, 70569 Stuttgart

We investigate the two-dimensional, spin-orbit coupled, three-band Hubbard model in the d^5 and d^4 configuration at finite temperature by means of the variational cluster approximation. Thermodynamic (magnetization, specific heat) and dynamic (DOS, spectral function) properties are presented. We investigate the influence of cluster size and symmetry on the Néel temperature T_N and on spectra.

We find that the DOS of the d^5-system supports the picture of a system between clear Slater- and Mott-scenarios and that the orbital degrees of freedom remain quenched even for temperatures above T_N. The d^4-system is already insulating at very high temperatures. Both a crystal field and spin-orbit coupling (SOC) lead to antiferromagnetic order at low temperature, but the finite-T properties differ markedly: Without SOC, the onsite states defining the local moments do not change substantially with $T > T_N$. In the presence of SOC, in contrast, weight in the onsite singlet favored by SOC increases markedly when T is lowered towards T_N. This is in agreement with X-ray reporting changes to the orbital character at temperatures above T_N.

TT 43.9 Wed 17:15 HSZ 304

Nonlinear spin-wave theory for the Heisenberg-Kitaev model in a magnetic field — •Pedro M. Cônsoli[1,2], Lukas Janssen[2], Matthias Vojta[2], and Eric C. Andrade[1] — [1]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [2]Institut für Theoretische Physik, TU Dresden, Dresden, Germany

The exact solution of Kitaev's honeycomb model and the ensuing realization that it gives rise to chiral Majorana edge modes in a small and properly oriented magnetic field sparked an intense search for a physical mechanism capable of replicating such a system in real materials. This missing link was provided by Khaliullin and Jackeli, who showed that an interplay between crystal field effects and strong spin-orbit coupling originates the Kitaev interaction along with a Heisenberg exchange in a class of Mott insulators. Hence, the Heisenberg-Kitaev

Hamiltonian became a minimal model to describe Kitaev materials and was subsequently studied in much detail. Still, several questions related to effects of external perturbations remain unanswered.

Here, we discuss the physics of the Heisenberg-Kitaev model in the presence of a magnetic field applied along two different directions: [100] and [111], for which an intricate classical phase diagram has been reported. In both settings, we employ spin-wave theory for a number of ordered phases to compute magnetization curves and phase boundaries in next-to-leading order in $1/S$, with S being the spin size. In this way, we show that quantum corrections substantially modify the phase diagram. Finally, we compare our spin-wave theory results to exact diagonalization calculations performed on a 24-site cluster.

TT 43.10 Wed 17:30 HSZ 304

How spin-orbital entanglement depends on the spin-orbit coupling in a Mott insulator — •Dorota Gotfryd[1,2], Ekaterina M. Paerschke[3,4], Andrzej M. Oles[2,5], and Krzysztof Wohlfeld[1] — [1]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Institute of Physics, Jagiellonian University, Lojasiewicza 11, PL-30348 Krakow, Poland — [3]Department of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA — [4]Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria — [5]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The concept of spin-orbital entanglement plays a crucial role in understanding various phases and exotic ground states in a broad class of materials, including orbitally ordered materials and spin liquids. We investigate how this entanglement depends on the value of the relativistic spin-orbit coupling. To this end, we numerically diagonalise spin-orbital model with the 'Kugel-Khomskii' exchange supplemented by the on-site spin-orbit coupling. While for small spin-orbit coupling the ground state resembles the vanishing spin-orbit coupling case, for large spin-orbit coupling it can either show negligible spin-orbital entanglement or can evolve to a highly entangled state with completely distinct properties, described by an effective model. The presented range of spin-orbit coupling is relevant not only for 5d but also for 3d or some of the 4d transition metal oxides.

TT 44: Quantum Chaos (joint session DY/TT)

Time: Wednesday 15:00–19:00 Location: HÜL 186

Invited Talk TT 44.1 Wed 15:00 HÜL 186

Supersymmetric Polarization Anomaly in Photonic Discrete-Time Quantum Walks — •Sonja Barkhofen[1], Lennart Lorz[1], Thomas Nitsche[1], Christine Silberhorn[1], and Henning Schomerus[2] — [1]Applied Physics, University of Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom

Quantum anomalies lead to finite expectation values that defy the apparent symmetries of a system. These anomalies are at the heart of topological effects in electronic, photonic, and atomic systems, where they result in a unique response to external fields but generally escape a more direct observation. Here, we implement an optical-network realization of a discrete-time quantum walk, where such an anomaly can be observed directly in the unique circular polarization of a topological midgap state. We base the system on a single-step protocol overcoming the experimental infeasibility of earlier multistep protocols. The evolution combines a chiral symmetry with a previously unexplored unitary version of supersymmetry. Having experimental access to the position and the coin state of the walker, we perform a full polarization tomography and provide evidence for the predicted anomaly of the midgap states. This approach opens the prospect to dynamically distill topological states for quantum information applications.

TT 44.2 Wed 15:30 HÜL 186

Corrected perturbation theory for transverse-electric whispering-gallery modes in deformed microdisks — •Manuel Badel and Jan Wiersig — Postfach 4120, D-39016 Magdeburg, Germany

The perturbation theory by Ge et al. [Phys. Rev. A 87, 023833 (2013)] for transverse-electric polarized modes in weakly deformed microdisks omits terms related to the variation of the normal derivative of the magnetic field along the boundary. We show that these terms are necessary to accurately describe microdisks with a strongly winding boundary. In particular, it is demonstrated that the corrected perturbation theory allows one to describe the counterintuitive phenomenon of Q-factor enhancement due to weak boundary deformation, exemplified by the microflower cavity. Good agreement of the corrected perturbation theory with full numerical results is observed.

TT 44.3 Wed 15:45 HÜL 186

Controlling chaos in the quantum regime using adaptive measurements — •Jessica Eastman[1,2,3], Stuart Szigeti[1], Joseph Hope[1], and André Carvalho[3] — [1]Department of Quantum Science, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601, Australia — [2]Centre for Quantum Computation and Communication Technology (Australian Research Council), Griffith University, Brisbane, Queensland 4111, Australia — [3]Centre for Quantum Dynamics, Griffith University, Brisbane, Queensland 4111, Australia

The continuous monitoring of a quantum system strongly influences the emergence of chaotic dynamics near the transition from the quantum regime to the classical regime. Here we present a feedback control scheme that uses adaptive measurement techniques to control the degree of chaos in the driven-damped quantum Duffing oscillator. This control relies purely on the measurement backaction on the system, making it a uniquely quantum control, and is only possible due to the sensitivity of chaos to measurement. We quantify the effectiveness of our control by numerically computing the quantum Lyapunov exponent over a wide range of parameters. We demonstrate that adaptive measurement techniques can control the onset of chaos in the system, pushing the quantum-classical boundary further into the quantum regime.

TT 44.4 Wed 16:00 HÜL 186

Microstar cavities: An alternative concept for the confinement of light — •Julius Kullig[1], Xuefeng Jiang[2], Lan Yang[2], and Jan Wiersig[1] — [1]Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany — [2]Department of Electrical and Systems Engineering, Washington University in St. Louis, St. Louis, USA

We report on a novel concept to confine light in a microcavity. In contrast to traditional approaches we exploit neither total internal reflection nor a photonic band gap. Our approach is rather based on the perfect transmission of light at Brewster's angle. Thus, in a properly designed star-shaped cavity light rays can sequentially leave and reenter the cavity along a periodic orbit without loss of intensity. Accordingly, in the wave dynamics long-lived optical modes arise with fascinating and unique properties.

TT 44.5 Wed 16:15 HÜL 186

Investigations on the spectral density of kicked spin chains — •Felix Meier, Daniel Waltner, Petr Braun, and Thomas Guhr — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Deutschland

We study the semiclassical description of locally interacting spin chains whose individual constituents are identical to the kicked-top model. The magnetic field inducing the periodically applied kicks is chosen so that the model is quantum mechanically non-integrable for all possible spin representations. The classical analog of the spin chain is a collection of coupled Bloch vectors, whose dynamics is described stroboscopically. The corresponding classical phase space features highly mixed behavior with regular and chaotic motion occuring simultaneously. We investigate the structure of the quantum spectral density for different particle numbers and system parameters, which send the classical analog through a number of bifurcations.

TT 44.6 Wed 16:30 HÜL 186

Many-Body Densities of States on Quantum Graphs — •Adrian Seith[1], Gregor Tanner[2], Stephen Creagh[2], Klaus Richter[1], and Juan-Diego Urbina[1] — [1]Institut für Theoretische

Physik, Universität Regensburg, Universitätsstraße 31 D-93053 Regensburg — [2]School of Mathematical Sciences, University of Nottingham, University Park, Nottingham, NG7 2RD, UK

We study the bulk density of states in non-interacting many-body systems on a quantum graph, a one-dimensional network of connected bonds on which the wave function is a solution of the one-dimensional Schrödinger equation.

In [1], Kottos & Smilansky derived a trace formula for the spectrum of a one-particle quantum graph using a secular equation and a transfer operator that describes the dynamics of the system. In [2], Bolte & Kerner show that the DOS of a many-body quantum graph follows an asymptotic Weyl law. We derive an explicit expression of the many-particle DOS on quantum graphs for distinguishable and indistinguishable particles and extend Smilansky's transfer operator approach to many-body systems using Bogomolny's formalism [3] so that we can give a geometric interpretation of many-body quantum graphs and the principle of indistinguishability and pave the way to include interaction effects.

[1] T. Kottos, U. Smilansky. Annals of Physics, Vol. 274 (1999)
[2] J. Bolte, J. Kerner. Journal of Mathematical Physics 55, (2014)
[3] E. B. Bogomolny. Nonlinearity, Vol. 5 (1992)

TT 44.7 Wed 16:45 HÜL 186

New insights on the semiclassical study of many-body interference in Fermionic Fock space: a path integral approach — •Wolfgang Hogger, Juan-Diego Urbina, Falk Bruckmann, and Klaus Richter — Universität Regensburg

A long standing goal of quantum chaos is to establish the classical limit of Fermionic fields and to follow the corresponding semiclassical program. Following Gutzwiller, we propose to apply the stationary phase approximation to the coherent state path integral for bosons on a lattice and transforming a Fermionic system into the latter by subsequent use of Jordan-Wigner transformation and Schwinger-boson mapping. However, it was shown by Wilson and Galitzki in PRL 106, 110401 (2011) how the coherent state path integral breaks down for the Bose-Hubbard model and simple spin systems. Since the issues with the partition function path integral for the aforementioned systems were solved by Bruckmann and Urbina in arXiv:1807.10462v1 through dualization (a known method from lattice quantum field theories), the correct perturbative expansion is now correctly reproduced and one can obtain a path integral for the propagator as well. As a second key ingredient, thanks to a novel transformation in the spirit of Jordan-Wigner providing an exact map from many Fermionic degrees of freedom to a single large spin, we now obtain also a well-defined classical limit. Combining these two insights, a semi-classical theory of generic Fermi-Hubbard models is finally constructed and applied to some simple examples.

15 min. break.

TT 44.8 Wed 17:15 HÜL 186

Geometry of complex instability in four-dimensional symplectic maps — •Jonas Stöber[1,2] and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

In four-dimensional symplectic maps complex instability of periodic orbits is possible, which cannot occur for the two-dimensional case. We investigate the transition from stable to complex unstable dynamics of a fixed point under parameter variation. The change in the geometry of regular structures is visualized using three-dimensional phase-space slices and in frequency space using the example of two coupled standard maps. The chaotic dynamics is studied using escape time plots and two-dimensional invariant manifolds associated with the complex unstable fixed point. Based on a normal-form description, we investigate the underlying transport mechanism by visualizing the escape paths and the long-time confinement in the surrounding of the complex unstable fixed point. Consequences for the quantum wave-packet dynamics are illustrated.

TT 44.9 Wed 17:30 HÜL 186

Quantum signatures of separatrix crossing: self-trapping in high dimensional Bose-Hubbard systems — •Mathias Steinhuber[1], Steven Tomsovic[2], Remy Dubertrand[1], Klaus Richter[1], and Juan-Diego Urbina[1] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, Washington 99164-2814, USA

We generalize the concept and phenomenology of self-trapping in the integrable Bose-Hubbard dimer into systems with non-integrable mean-field dynamics by relating it with crossing of separatrices. To this end, we construct a mapping of site-periodic solutions to find a sub-manifold of integrable dynamics in the non-integrable phase space. This new and powerful concept allows us to analytically explain the numerical observation of a massive transition in the stability properties of mean-field solutions found by Tomsovic in [1]. We also show how this mapping has extensions and generalizations to higher dimensions, opening a door for analytical understanding beyond state of the art numerics, and obtain the Lyapunov spectra of site-periodic fix points, their stabilities and bifurcations. Last we show some quantum signatures of these morphology changes in the classical phases space focusing primarily on the self-trapping transition.

[1] Tomsovic, S. Complex saddle trajectories for multidimensional quantum wave packet and coherent state propagation: application to a many-body system. Phys. Rev. E 98, 023301 (2 Aug. 2018)

TT 44.10 Wed 17:45 HÜL 186

What is the structure of chaotic resonance eigenfunctions? — •Roland Ketzmerick[1,2], Konstantin Clauss[1], Felix Fritzsch[1], and Arnd Bäcker[1,2] — [1]TU Dresden, Institut für Theoretische Physik — [2]MPI für Physik komplexer Systeme, Dresden

While chaotic eigenfunctions in closed systems are uniformly distributed according to the quantum ergodicity theorem, they show fractal structures in systems with escape. This structure depends crucially on the decay rate of the resonance eigenfunction. It is semiclassically quite well understood for quantum maps with full [1] and partial [2] escape. Here we present the extension to billiard systems, in particular the famous three-disk system (full escape) and the dielectric limaçon billiard relevant for optical microcavities (partial escape).

[1] K. Clauß, M. J. Körber, A. Bäcker, and R. Ketzmerick, Phys. Rev. Lett. **121**, 074101 (2018).
[2] K. Clauß, E. G. Altmann, A. Bäcker, and R. Ketzmerick, Phys. Rev. E **100**, 052205 (2019).

TT 44.11 Wed 18:00 HÜL 186

A PT-symmetric kicked top — Steve Mudute-Ndumbe and •Eva-Maria Graefe — Imperial College London, UK

A PT-symmetric version of the kicked top is introduced to study the interplay of quantum chaos with loss and gain. The classical dynamics arising from the quantum dynamics of the angular momentum expectation values are derived and analysed in some detail. Further, the statistics of the (complex) eigenvalues of the quantum system are investigated.

TT 44.12 Wed 18:15 HÜL 186

Towards universal Hong-Ou-Mandel correlations in topological insulators — •Andreas Bereczuk[1], Juan Diego Urbina[1], Barbara Dietz[2], Jack Kuipers[3], Cosimo Gorini[1], and Klaus Richter[1] — [1]Institut of Theoretical Physics, University Regensburg, Germany — [2]School of Physical Science and Technology, Lanzhou University, China — [3]Department of Biosystems Science and Engineering (BSSE), ETH Zurich, Switzerland

The indistinguishable-distinguishable transition for 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 universal correlations of the scattering matrix entries at different energies enter. We present here a consistent semiclassical, numerical and Random Matrix Theory (RMT) analysis of this correlators together we a progress report on its experimental realization in a microwave billard. With this results at hand, we propose a HOM setup with cavities as complex beam splitters and edge states instead of waveguides to observe universal HOM correlations in a topological insulators (TI).

[1] C. K. Hong, Z. Y. Ou and L. Mandel, Phys. Rev. Lett. 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 44.13 Wed 18:30 HÜL 186

The Conditioned Real Ginibre Ensemble and PT-Symmetric

Quantum Chaos — •Simon Malzard[1], Steve Mudute-Ndumbe[1], Roman Riser[2], Joshua Feinburg[2], and Eva-Maria Graefe[1] — [1]Imperial College London, London, UK — [2]University of Haifa, Haifa, Israel

In Hermitian systems the universality of spectral fluctuations described by the standard Gaussian ensembles is one of the most pronounced fingerprints of chaos in a quantum system. With the recent intense interest in non-Hermitian PT-symmetric systems, it is a natural question whether there are PT-symmetric random matrix ensembles yielding similar universality classes. One candidate for PT-symmetric systems with P^2=1 and T^2=1 which display quantum chaos is the real Ginibre ensemble. Eigenvalues of real Ginibre matrices are real or occur in complex conjugate pairs. The spectral properties of the real Ginibre matrices depend crucially on the number of real eigenvalues. Hence, when studying the eigenvalue distributions and level spacings of PT-symmetric quantum chaotic systems, one should make comparisons to an ensemble of real Ginibre matrices conditioned to have the corresponding number of real eigenvalues. Here we present a numerical method to produce samples of real Ginibre matrices conditioned to have a particular number of real eigenvalues.

TT 44.14 Wed 18:45 HÜL 186

Rate of decoherence and entanglement growth in coupled kicked rotors — •Sanku Paul[1] and Arnd Bäcker[2,1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden 01187, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, Dresden 01069, Germany

The classical-quantum correspondence of a pair of coupled kicked rotors is investigated. In this interacting system, one rotor acts as an environment to the other. This leads to the emergence of decoherence with classical-like behavior at large times. This classical-like behavior is characterized by normal diffusion in energy space and interestingly, it is preceded by an intermediate dynamical localization for weak interactions. It is observed that these different rates of energy diffusion are associated with different regimes of decay of coherence, in particular showing exponential and power-law behavior. We show that the observed decoherence is related to distinct rates of entanglement entropy growth between the rotors which is described by an initial power-law followed by logarithmic growth.

TT 45: Skyrmions III (joint session MA/TT)

Time: Wednesday 15:00–18:30 Location: POT 6

TT 45.1 Wed 15:00 POT 6

Noncommutative geometry and the anomalous Hall effect in chiral spin textures — •Fabian R. Lux[1], Frank Freimuth[1], Stefan Blügel[1], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany

We demonstrate that the anomalous Hall effect (AHE) in chiral magnetic textures can naturally be described in the language of Alain Connes' noncommutative geometry which provides it with a deep geometrical interpretation. For periodic magnetic structures, the formalism reduces to the well-known Kubo-Bastin equations, but its applicability extends to all aperiodic cases in general. Under the assumption of a slowly varying texture, we derive the first order correction to the conventional AHE which is linear in the gradients of the magnetization texture [1]. This chiral Hall effect is neither proportional to the net magnetization nor to the emergent magnetic field that is responsible for the topological Hall effect and thus introduces an interesting twist in the interpretation of experimental data.

We acknowledge funding from Deutsche Forschungsgemeinschaft (DFG) through SPP 2137 "Skyrmionics".

[1] F. R. Lux *et al.*, arXiv:1910.06147 (2019)

TT 45.2 Wed 15:15 POT 6

Magnetic force microscopy investigation of spin textures in the ferromagnetic semimetal $\mathbf{Fe_2Sn_3}$ — •Markus Altthaler[1,2], Erik Lysne[2], Erik Roede[2], Mohamed Kassem[1], Vladimir Tsurkan[1], Lilian Prodan[1], Stephan Krohns[1], Dennis Meier[2], and István Kézsmárki[1] — [1]Universität Augsburg, Germany — [2]Norwegian University of Science and Technology (NTNU)

Recently, Fe_3Sn_2 has been reported to exhibit a giant anomalous Hall effect [1] as well as a topological electronic structure [2] and to host magnetic skyrmions [3]. Unlike common skyrmion hosts, this material has inversion symmetry, therefore, the skyrmions do not emerge due to the Dzyalohinskii-Moriya interaction. Z. Hou et al. [3] suggested that both uniaxial magnetic anisotropy competing with long-range dipolar forces and exchange frustration due to the Kagome lattice play a significant role in the formation of skyrmions at room temperature in this compound. Our goal was to specify in more detail the driving force of skyrmion formation. In MFM studies performed on the surface of bulk Fe_3Sn_2 crystals we did not find stripe domains, instead a dendrite pattern, which indicates the lack of magnetic spirals in bulk samples. On the other hand, we found stripe domains in thin lamellae in zero magnetic field which transform to a bubble (skyrmion) lattice in modest magnetic fields. This together with the thickness dependence of the spiral wavelength implies that the uniaxial anisotropy competing with dipolar interactions is the origin of modulated magnetic states in Fe_3Sn_2. [1] L. Ye et al., Nature **555** (2018), 638; [2] J.-X. Yin et al., Nature **562** (2018), 91; [3] Z. Hou et al., Adv. Mater. (2017), 1701144

TT 45.3 Wed 15:30 POT 6

Stability and dynamics of in-plane Skyrmions — •Venkata Krishna Bharadwaj[1], Ricardo Zarzuela[1], Kyoung-Whan Kim[2], Jairo Sinova[1,3], and Karin Everschor-Sitte[1] — [1]Johannes Gutenberg-University, Mainz — [2]Center for Spintronics, Korea Institute of Science and Technology, South Korea — [3]Institute of Physics Academy of Sciences of the Czech Republic, Cukrovarnická 10, 162 00 Praha 6, Czech Republic

In this work [1] we analyze skyrmions in in-plane magnets. Through symmetry analysis, we offer possible material candidates to observe these skyrmions and also provide the phase diagram of such crystal systems. In addition, we determine their stability and properties, taking into account the crystal symmetries of the materials. Using micromagnetic simulations we show that in-plane skyrmions can be produced via two mechanisms, namely: i) the 'blowing bubbles' technique, i.e the creation of skyrmions due to current flow through constricted geometries and ii) shedding of skyrmions from a magnetic impurity driven by spin-transfer torques, analogues to their out-of-plane counterparts. Furthermore, we study the spin-orbit torques driven skyrmion dynamics both analytically and through micromagnetic simulations. Our results also indicate the possibility of designing the racetrack for in-plane skyrmions, which are promising candidates for memory applications. [1]R. Zarzuela, V.K. Bharadwaj, K-W. Kim, J. Sinova, K. Everschor-Sitte, arXiv:1910.00987 (2019)

TT 45.4 Wed 15:45 POT 6

First-principles prediction of in-plane magnetic skyrmions: a topological spin-texture for high-storage density — •Flaviano José dos Santos, Markus Hoffmann, Manuel dos Santos Dias, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany

Magnetic skyrmions competitive in information technology should be small to allow a high storage density. However, the dipole-dipole interaction (DDI) effectively impedes the miniaturization of skyrmions embedded in thin films and multilayers with typically out-of-plane magnetization. We predict from first-principles the existence of in-plane magnetic skyrmions in a Co monolayer on W(110). The magnetization of Co exhibits an in-plane easy axis, a geometry in which the DDI contributes to reducing the size of such topological spin textures. We discuss the various properties of these particles and list the mechanisms causing their stabilization. Due to the in-plane easy axis of the magnetization, mirror symmetry is preserved enabling the existence of antiskyrmions being degenerate in energy with skyrmions. This makes Co/W(110) a strong candidate for prospective devices, such as skyrmion/antiskyrmion racetracks [3].
We acknowledge funding from EU Horizon 2020 via ERC-consolidator Grant No. 681405-DYNASORE and DARPA TEE program through grant MIPR (#HR0011831554) from DOI. — Refs.: [1] Vidal-Silva *et*

al., J. Magn. Magn. Mater. **443**, 116 (2017); [2] Büttner *et al.*, Sci. Rep. **8**, 4464 (2018); [3] Moon *et al.*, arXiv:1811.12552 (2018).

TT 45.5 Wed 16:00 POT 6

Skyrmion lattice formation — •Thomas Winkler, Jakub Zázvorka, Nico Kerber, Klaus Raab, Florian Dittrich, Yuqingh Ge, Peter Virnau, and Mathias Kläui — Johannes Gutenberg Universität Mainz, Staudinger Weg 7, 55128 Mainz

Magnetic skyrmions are highly interesting magnetic spin structures and potential candidates for next generation computing devices due to their topology based stability [1,2]. There has been much work on the individual static and dynamic properties of skyrmions. However, their collective behavior is not yet well explored in particular in multilayer stacks with interfacial DMI. We have stabilized a skyrmion lattice in a single stack of Ta(5)/Co20Fe60B20(0.9)/Ta(0.08)/MgO(2)/Ta(5), and found that statistical order parameters can be varied by a change of the In-plane field and the temperature. The 2d skyrmion ensemble typically forms a liquid phase, but we also observe the emergence of hexagonal order for high densities. Using experimentally obtained parameters, coarse-grained numerical simulations are performed by modelling skyrmions as repulsive soft disks [3] to explain the results.

[1] Finocchio, G., Büttner, F., Tomasello, R., Carpentieri, M. & Kläui, M. Magnetic skyrmions: from fundamental to applications. J. Phys. D. Appl. Phys. 49, 423001 (2016). [2] Fert, A., Reyren, N. & Cros, V. Magnetic skyrmions: advances in physics and potential applications. Nat. Rev. Mater. 2, 17031 (2017). [3] S. Kapfer, S., Krauth, W. Soft-disk melting: From liquid-hexatic coexistence to continuous transitions. Physical Review Letters 114, 035702 (2015)

TT 45.6 Wed 16:15 POT 6

The effects of disorder on hysteresis loops in chiral magnets — David Cortes[1], Marijan Beg[1], Hans Fangohr[1,2], Tom Lancaster[3], Peter Hatton[3], Thorsten Hesjedal[4], and •Ondrej Hovorka[1] — [1]University of Southampton, UK — [2]European XFEL GmbH, Schenefeld, Germany — [3]Durham University, UK — [4]Oxford University, UK

In this talk we investigate the effect of random pinning sites on magnetization behaviour in systems with Dzyaloshinskii-Moriya interaction (DMI). We consider a standard classical spin Hamiltonian with Heisenberg exchange and DMI energy terms, and model the disorder through statistical Gaussian distribution of anisotropy. We first develop a mean-field model which allows to compute systematically and efficiently the magnetisation versus field hysteresis loops for variable temperature, and can be used for computing qualitative thermodynamic phase diagrams to guide computationally costly Monte-Carlo simulations. We show that as the standard deviation of the anisotropy distribution increases, relative to the strength of exchange interaction and DMI, the nature of the reversal modes observed along a typical hysteresis loop changes in a certain temperature window. Namely, in 'clean' systems with narrow anisotropy distribution, the reversal proceeds through the appearance of skyrmion lattices at low external fields, while in 'dirty' systems with broad anisotropy distribution, the reversal is through the nucleation of individual or small groups of skyrmions. We systematically quantify this effect and discuss its broader implications for applications.

TT 45.7 Wed 16:30 POT 6

Tuning the topology flip of magnetic skyrmions by an in-plane magnetic field — Florian Muckel[1], Stephan von Malottki[2], Christian Holl[1], Benjamin Pestka[1], Marco Pratzer[1], Pavel F. Bessarab[3], Stefan Heinze[2], and •Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany — [3]University of Iceland, Reykjavík, Iceland and ITMO University, St. Petersburg, Russia

Topological protection of magnetic skyrmions on a discrete lattice manifests itself in an energy barrier that can be overcome by local heating, for example by a tunneling electron. Here we use spin polarized scanning tunneling microscopy at 7 K to probe the current induced collapse of magnetic skyrmions in the Pd/Fe bilayer on Ir(111) as a function of the in-plane magnetic field $B_{\|}$ .The collapse rate caused by single hot electrons is tuned by four orders of magnitude via $B_{\|}$. We aim a more detailed understanding of the skyrmion collapse mechanism by locally mapping the collapse rate and deduce a change from a radially symmetric shrinkage of the skyrmion [1] towards a zipper-like Chimera collapse mechanism predicted by theory [2].

[1] Bessarab et. al. Comp. Phys. Comm. 196, (2015). [2] Meyer et. al. Nat. Commun. 10, (2019)

15 min. break.

TT 45.8 Wed 17:00 POT 6

Observation of unusual magnetic response at topological defects in FeGe — •Mariia Stepanova[1,2], Erik Lysne[1,2], Peggy Schoenherr[3], Jan Masell[4], Laura Köhler[5], Achim Rosch[6], Naoya Kanazawa[7], Yoshinori Tokura[4,7], Markus Garst[5,8], Alireza Qaiumzadeh[2], Arne Brataas[2], and Dennis Meier[1,2] — [1]NTNU, Trondheim, Norway — [2]QuSpin, NTNU, Trondheim, Norway — [3]ETH Zurich, Zürich, Switzerland — [4]RIKEN, Wako, Japan — [5]Technische Universität Dresden, Dresden, Germany — [6]Universität zu Köln, Köln, Germany — [7]University of Tokyo, Tokyo, Japan — [8]Karlsruhe Institute of Technology, Karlsruhe, Germany

Lamellar textures do not just arise in liquid crystals and biological systems, they are also observed in helimagnets. Analogous to cholesteric liquid crystals, chiral magnets possess a periodic layered structure and form different types of non-trivial topological defects. Using magnetic force microscopy (MFM) on the near-room temperature helimagnet FeGe, we resolve disclinations and dislocations with nonzero topological winding number, as well as three fundamental types of helimagnetic domain walls. Interestingly, in addition to their non-trivial structure, all topological defects in FeGe exhibit an unusual MFM response, which is not observed in regions with perfect lamellar-like order. This magnetic signature is similar to the so-called "lines of flare" in cholesteric liquid crystals, suggesting local variations in magnetic susceptibility. We investigate the origin of the magnetic signature of the topological defects and discuss the possibility to use the local MFM response as a read-out signal in device applications.

TT 45.9 Wed 17:15 POT 6

Band structure tuning of a skyrmion lattice with giant topological Hall effect — •Leonie Spitz[2], Max Hirschberger[1], Shang Gao[1], Taro Nakajima[1], Christian Pfleiderer[2], Takahisa Arima[1,3], and Yoshinori Tokura[1] — [1]RIKEN Center for Emergent Matter Science, 2-1 Hirosawa, Wakoshi, Saitama 351-0198, Japan — [2]Physik-Department, Technical University of Munich, 85748 Garching, Germany — [3]Department of Advanced Materials Science, University of Tokyo, Kashiwa, Chiba 277-8561, Japan

A skyrmion lattice accompanied by a large topological Hall effect was found for the centrosymmetric frustrated triangular lattice magnet Gd_2PdSi_3 [1]. In contrast to non-centrosymmetric compounds, the skyrmion spin-vortices reported for Gd_2PdSi_3 can not be stabilized by the Dzyaloshinskii-Moriya interaction, but rather by frustration and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [2-4]. The nanometer-scale size of the skyrmions in Gd_2PdSi_3 is a further novelty and may give rise to a very large emergent magnetic field B_{em}.

The project to be presented aims at a deeper understanding of the emergence of the giant topological Hall effect in Gd_2PdSi_3. In an extensive study we investigated the effect of isoelectronic doping on the topological Hall effect, the magnetic structure, and the band structure of the system.

[1] T. Kurumaji, et al., Science 365, 914-918 (2019) [2] T. Okubo, et al., Phys. Rev. Lett. 108, 017206 (2012) [3] A. O. Leonov, et al., Nat. Commun. 6, 8275 (2015) [4] S. Hayami, et al., Phys. Rev. B 95, 224424 (2017)

TT 45.10 Wed 17:30 POT 6

Nanoscale magnetic resonance imaging at room temperature using single spins in diamond — •Tetyana Shalomayeva[1], Jianpei Geng[1], Qi-Chao Sun[1], Rainer Stöhr[1], Stuart Parkin[2], and Jörg Wrachtrup[1,3] — [1]3rd Institute of Physics, University of Stuttgart — [2]Max Planck Institute of Microstructure Physics — [3]Max Planck Institute for Solid State Research

Due to the significant development of compounds hosting skyrmions at ambient conditions [1] the need of the quantitative real-space imaging of the magnetic textures is high nowadays. As an atomic-sized magnetic field sensor we use the point lattice defect in diamond, which consists of carbon vacancy and substitutional nitrogen atom (NV centre). For the scanning probe experiments single NV centre is integrated into the monolithic nanopillar, which plays the role of the sharp end of the AFM tip.

In this contribution we demonstrate the scanning probe measurement of the magnetic helical structure on the surface of thin Mn1.4Pt0.9Pd0.1Sn lamella via off-axial fluorescence quenching at room temperature and further numerical extraction of B-field.

[1] A.K. Nayak et al. Nature 548, 561-566 (2017)

TT 45.11 Wed 17:45 POT 6

Real-Space Imaging of the low-temperature Skyrmion phase in Cu2OSeO3 by Magnetic-Force-Microscopy — •Gerald Malsch[1], Peter Milde[1,2], Dmytro Ivaneiko[1], Christian Pfleiderer[3], Helmuth Berger[4], and Lukas Eng[1,2] — [1]Institute of Applied Physic, TU Dresden, 01187 Dresden, Germany — [2]ct.qmat: Würzburg-Dresden Cluster of Excellence - EXC 2147, TU Dresden, Germany — [3]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [4]Institut de Physique de la Matière Complexe, EPFL, 1015 Lausanne, Switzerland

Both small-angle neutron scattering measurements (SANS) and theoretical calculations indicate that there might exist additional skyrmion phases in Cu2OSeO3 in addition to its high-temperature phase, found at very low temperatures (LT) and only for magnetic fields applied along the <100> direction. These phases are usually hidden beneath a metastable tilted conical phase, but can be revealed by modulating the applied magnetic field.

Here we present a Magnetic-Force-Microscopy (MFM) analysis monitoring this LT skyrmion phase in real space. We find the LT skyrmion lattice to nucleate in micrometer-sized domains that coexist with tilted conical domains during the annealing process. Moreover, individual skyrmion domains are rotated relative to each other, resulting exactly in the ring-shaped halo as measured by SANS or REXS on a multidomain Cu2OSeO3 crystal.

TT 45.12 Wed 18:00 POT 6

Magnetic anisotropy in the itinerant helimagnet MnSi — •Schorsch Michael Sauther[1], Michelle Hollricher[1], Vivek Kumar[1], Andreas Bauer[1], Markus Garst[2], Dirk Grundler[3], Christian Pfleiderer[1], and Marc Andreas Wilde[1] — [1]Phys.-Dept. E51, TU München — [2]TFP, KIT, Karlsruhe — [3]LMGN, IMX, STI, EPF Lausanne

We report torque magnetometry in Manganese silicide (MnSi). In our experiments, we employ different implementations of cantilever magnetometry 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 of τ displays distinct oscillations with differently pronounced extrema im compliance with an effective Landau potential for the magnetization. This minimal model allows us to extract the anisotropy constant directly from the $\tau(\phi)$ curve. We study its dependence on field magnitude and temperature in the vicinity of the material's modulated phases and discuss our results in the context of complementary experiments [1,2].

[1] A. Bauer *et al.*, Phys. Rev. B **95**, 024429 (2017)
[2] T. Adams *et al.*, Phys. Rev. Lett. **121**, 187205 (2018)

TT 45.13 Wed 18:15 POT 6

Quantitative magnetic force microscopy investigation of magnetic features in the biskyrmion hosting hexagonal Mn33Ni33Ga33 magnet — •N. Puwenberg[1,2], C. F. Reiche[3], P. Devi[4], U. Burkhardt[4], C. Felser[4], M. Sharma[1,2], T. Mühl[1], and B. Büchner[1,2] — [1]IFW Dresden, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]University of Utah, Salt Lake City, USA — [4]MPI CPfS, Dresden, Germany

We present quantitative magnetic force microscopy maps and distance dependent force spectroscopy measurements of the potentially biskyrmion hosting compound Mn33Ni33Ga33 employing an in-house fabricated custom-designed force sensor. Our magnetic sensing element is based on an iron-filled carbon nanotube attached to the free end of a super-flexible cantilever. Using a high aspect ratio magnetic nanowire offers a well-defined magnetic moment with a monopole-like magnetic stray-field characteristics at the nanowire's end, enabling the opportunity to easily quantify the magnetic stray-field on the sample surface. Our measurements were conducted in a single pass non-contact hybrid imaging mode. It features a direct sensing of the perpendicular magnetic stray-field component by measuring the normal cantilever deflection whilst a tip-sample distance control is realized by exploiting an AC bias driven flexural cantilever oscillation. Furthermore, the distance-dependency of the magnetic field and field gradient measured in the vicinity of individual magnetic features is fitted to simple magnetic models to make predictions about feature type, size and extension into the bulk's perpendicular third dimension.

TT 46: Poster Session: Frustrated Magnets, Quantum Magnets, Charge Order and Complex Oxids

Time: Wednesday 15:00–19:00 Location: P2/2OG

TT 46.1 Wed 15:00 P2/2OG

Manipulation of charge density waves in transition metal dichalcogenides by strain and adsorbates — •F. Cossu[1], I. Di Marco[1], and A. Akbari[1,2] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang, Korea

Interest in transition metal dichalcogenides (materials consisting of van der Waals bonded layers) has been revived due to relatively recent access to synthesis of few layers, where their characteristic structure may result in massive symmetry breaking, which lead to exotic properties in the electronic structure. Collective phases such as superconductivity and charge density waves (CDW), which may be conventional in the bulk, could in principle become unconventional in single layers. Therefore, understanding the mechanisms of emergence of these electronic phases and how they change upon external fields or doping is of great interest. Since the symmetry of the CDW induces the symmetry of the superconducting gap, it is interesting to investigate instances of symmetry change. In $NbSe_2$, charge density waves are incommensurate and follow a triangular modulation 3×3, in the bulk and in single layers. However, zones where the modulation has a stripe character have been observed in single layers. By means of ab-initio calculations, we investigate the possible scenarios beneath the occurrence of the stripe phase. In addition, adsorption by transition metals induces a hierarchy change and a reduction of the symmetry in CDW; it may be argued that, due to the nature of the adsorbate, spin-orbit effect may dominate the nature of the collective excitations.

TT 46.2 Wed 15:00 P2/2OG

Influence of inhomogeneous orderings on charge transport in a Falicov-Kimball heterostructure — •Rudolf Smorka, Martin Žonda, and Michael Thoss — Albert-Ludwigs-Universität Freiburg i. Br., Deutschland

The spinless Falicov-Kimball model outside the particle-hole symmetric point exhibits different stable inhomogeneous charge orderings. Among these are well-known charge stripes and a variety of orderings with phase separated domains, which influence the charge transport through the correlated electron system significantly. In this work, we will show these effects by investigating a heterostructure, where the Falicov-Kimball model on a finite two-dimensional lattice is located between two non-interacting semi-infinite leads. We use a combination of nonequilibrium Green's functions techniques with a sign-problem-free Monte Carlo method for finite temperatures, and simulated annealing technique for the ground state, to address steady-state transport through the system. Our study shows that different ground-state phases of the central system can lead to simple metallic-like or insulating charge transport characteristics, but also to more complicated current-voltage dependencies reflecting a multi-band character of the transmission function. As temperature is increased, there is a tendency towards formation of transient phases before the system reaches a disordered phase. This leads to nontrivial temperature dependencies of transmission function and charge current.

TT 46.3 Wed 15:00 P2/2OG

Microscopic Dynamics during Charge-Glass Formation in θ-(BEDT-TTF)$_2$TlZn(SCN)$_4$ — •Tim Thyzel[1], Tatjana Thomas[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

Organic charge-transfer salts allow for a systematic examination of strong electron-electron correlation in reduced dimensions. The θ-$(ET)_2X$ salts, which consist of alternating layers of conducting organic molecules $(ET)_2$ and insulating anions X, exhibit charge ordering in the conducting layers below a characteristic temperature. However, the phase transition of the electronic system to this ordered state can be avoided by rapid cooling [1]. Then, a glass-like state emerges due to the geometric frustration of the conducting lattice, which acts against the formation of long-range order. We study the system θ-$(ET)_2TlZn(SCN)_4$, whose lattice is more anisotropic, and thus less frustrated, than that of other θ-phase compounds. Therefore, rather high cooling rates of at least 50 K/min are required to force a transition to the charge-glass state [2]. We achieve these cooling rates using a voltage pulse method recently shown [3] to be capable of rates in excess of 1000 K/min. Resistance fluctuation spectroscopy is then employed to gain insights into the deceleration of microscopic dynamics at the liquid-glass transition [4].

[1] Adv. Mater. 29, 1601979
[2] Science 357, 1381-1385
[3] Phys. Rev. B 90, 195150
[4] Crystals 8, 166

TT 46.4 Wed 15:00 P2/2OG

Strain-induced metal-to-insulator transitions in spinel oxide thin films — •Tim Schweizer[1,2], Ulrike Niemann[1,2], Dennis Huang[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

Spinel compounds with underlying pyrochlore lattice are known playgrounds for geometric frustration. In particular, LiV_2O_4 has attracted considerable attention due to its unconventional heavy fermion phase, which emerges at low temperatures in the absence of localized f electrons [1]. Recent studies have shown that metallic LiV_2O_4 can be driven into an insulating, charge-ordered state by applying epitaxial strain in the thin-film limit. Such an observation hints at the role of charge frustration and quantum criticality in the heavy fermion phase of LiV_2O_4. Using pulsed laser deposition, we studied thin films of LiV_2O_4 (strained and unstrained), and compared them with thin films of the distorted spinel AlV_2O_4, where a charge-ordered state was previously reported in powder samples [2].

[1] C. Urano et al., Phys. Rev. Lett. 85, 1052 (2000)
[2] K. Matsuno et al., JPS Journal, 70, 1456-1459 (2001)

TT 46.5 Wed 15:00 P2/2OG

Emergence and stability of spin-valley entangled quantum liquids in Moiré heterostructures — •Dominik Kiese, Finn Lasse Buessen, Ciaran Hickey, Simon Trebst, and Michael M. Scherer — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Moiré heterostructures with nearly flat bands have recently been established as a new playground for strongly-correlated electron physics. The precise nature of the correlated states is yet to be understood through the application of quantum many-body methods. Essential traits of phenomenological models for Moiré heterostructures include a hexagonal superlattice, a two-valley structure, as well as extended Hubbard and Hund's interaction terms. Taking a strong-coupling perspective, these features result in generalized Heisenberg models with separate spin and valley degrees of freedom. Here, the combination of geometric frustration and enhanced quantum fluctuations may inhibit the formation of conventional magnetic order. We study such extended spin-valley Heisenberg models using functional RG methods and find rich phase diagrams exhibiting stable realms of quantum spin-valley liquid behavior. We further show that even for purely antiferromagnetic couplings, ferromagnetic order may emerge in an extensive parameter regime. We discuss the relevance of our results for trilayer graphene on hexagonal boron nitride and twisted double bilayer graphene.

TT 46.6 Wed 15:00 P2/2OG

Lifshitz Transitions in Neutral Fermi Surfaces — •Vaishnavi Jayakumar and Ciaran Hickey — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

In his seminal 1960 paper, I. M. Lifshitz predicted the existence of a transition where the Fermi surface of a metal changes its topology, as a Van Hove singularity crosses the Fermi energy. These "Electronic Topological Transitions", or "Lifshitz transitions" , leave a strong imprint on thermodynamic and transport observables, and have since been observed in a variety of metals.

Here, we examine the consequences of a Lifshitz transition in a neutral Fermi surface, i.e. a metal of fermionic quasiparticles that are charge neutral. Such an exotic Fermi surface can arise in strongly correlated systems, with a paradigmatic example being the spinon Fermi surface of a U(1) quantum spin liquid.

We discuss the unique signatures of Lifshitz transitions in neutral metals, and compare and contrast them with the conventional electronic case. Similarly, we also discuss the recently classified multicritical Lifshitz transitions and their potential experimental fingerprints in spinon Fermi surface states.

TT 46.7 Wed 15:00 P2/2OG

Quasi-molecular electronic structure of the spin-liquid candidate $Ba_3InIr_2O_9$ revealed by RIXS — Alessandro Revelli[1], •Marco Magnaterra[1], Marco Moretti Sala[2], Giulio Monaco[3], Jan Attig[4], Alexander Tsirlin[5], Tusharkanti Dey[1,5], Philipp Gegenwart[5], Tobias Fröhlich[1], Petra Becker[6], Maria Hermanns[7], Paul H. M. van Loosdrecht[1], Daniel I. Khomskii[1], Jeroen van den Brink[8], and Markus Grüninger[1] — [1]II. Physikalisches Inst., Universität zu Köln — [2]Dip. di Fisica, Politecnico di Milano, Italy — [3]Dip. di Fisica, Università di Trento, Italy — [4]Inst. fur Theoretische Physik, Universität zu Köln — [5]Experimental Physics VI, University of Augsburg — [6]Abt. Kristallographie, Inst. fur Geologie und Mineralogie, Universitat zu Köln — [7]Dep. of Physics, Stockholm University, Sweden — [8]Inst. for Theoretical Solid State Physics, IFW Dresden

We address the electronic structure of the mixed-valent iridate $Ba_3InIr_2O_9$ by means of resonant inelastic x-ray scattering (RIXS). Previously, it has been discussed as a promising candidate for quantum spin-liquid behavior [1]. It exhibits $Ir^{4.5+}$ ions in face-sharing IrO_6 octahedra forming Ir_2O_9 dimers. RIXS unravels a rich excitation spectrum below about 1.5eV. The observation of a pronounced sinusoidal RIXS interference pattern unambiguously demonstrates the quasi-molecular orbital character of the electronic states. Three t_{2g} holes are delocalized over a dimer, establishing $Ba_3InIr_2O_9$ as a cluster Mott insulator with a quasi-molecular j_{dim}=1/2 ground state.

[1] Dey et al., PRB 96, 174411 (2017).

TT 46.8 Wed 15:00 P2/2OG

Investigation of the thermodynamic effects of electron-nucleus interactions in pyrochlores — •J. Gronemann[1,2], T. Gottschall[1], C. Salazar[1], J. Hornung[1], T. Herrmannsdörfer[1], A. Islam[3], V. Anand[3], B. Lake[3,4], H. Kaneko[5], H. Suzuki[6], and J. Wosnitza[1,2] — [1]HLD-EMFL, HZDR, Dresden, Germany — [2]Inst. f. Festkörper- und Materialphysik, TU Dresden, Germany — [3]Helmholtz-Zentrum Berlin, Germany — [4]Inst. f. Festkörperphysik, TU Berlin, Germany — [5]Dep. of Quantum Matter, Hiroshima Univ., Japan — [6]Dep. of Physics, Kanazawa Univ., Japan

We have investigated selected pyrochlore compounds in order to study possible nuclear magnetic contributions to the formation of their magnetic ground states and unconventional excitations. For that we focused on $Ho_2Ti_2O_7$ and $Pr_2Hf_2O_7$. Both are representatives for the occurence of spin-ice behavior.^{165}Ho and ^{141}Pr are isotopically pure elements and have large hyperfine enhanced nuclear magnetic moments. The non-spherical ^{165}Ho nuclei, in addition, carry large electric quadrupole moments. For this reason, these two pyrochlore compounds are well suited to determine possible nuclear magnetic influence. Our specific heat and ac susceptibility data measured at 0.06 K to 10 K suggest a formation of a complex $\vec{F} = \vec{J}+\vec{I}$ coupled ground state which is further modified by electrical field gradients. The ground state F multiplets of $Ho_2Ti_2O_7$ and $Pr_2Hf_2O_7$, in consequence, are accompanied by a total entropy which is significantly larger than the one of a purely electronic CEF ground state doublet and in particular larger than the Pauling residual entropy.

TT 46.9 Wed 15:00 P2/2OG

ESR investigations of disorder effects in organic spin-liquid compounds — •Björn Miksch[1], John A. Schlueter[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, Illinois 60439-4831 and National Science Foundation, Alexandria, Virginia 2223, USA

Although many low temperature properties of the organic spin-liquid candidate κ-$(ET)_2Cu_2(CN)_3$ have been studied experimentally, a comprehensive description is still difficult. Disorder effects have been recently suggested to provide an explanation for the intriguing magnetic and thermodynamic properties. In this study we present electron spin resonance measurements performed with conventional spectrometers as well as with our on-chip approach. This allows us to cover temperatures from 300 K to the mK regime in a broad range of magnetic fields. The results indicate the presence of local moments at very low temperatures supporting the importance of disorder for the low temperature magnetic state.

TT 46.10 Wed 15:00 P2/2OG

Thermodynamic investigations of the quantum-spin-liquid candidate $Ca_{10}Cr_7O_{28}$ — •Ulrich Tutsch[1], Christian Thurn[1], Christian Balz[2,3,4], Bella Lake[3,4], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt am Main, Germany — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Tennessee, USA — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [4]Institut für Festkörperphysik, Technische Universität Berlin, Germany

A quantum-spin-liquid (QSL) is characterized by a coherent and highly entangled ground state without any long-range spin order. One strategy for the realization of such a state is the use of geometrical frustration, as, e.g., encountered in $Ca_{10}Cr_7O_{28}$ with its distorted spin-1/2 kagome bilayer structure. Previous studies have failed to detect any sign of long-range magnetic order in this compound down to 19 mK, its spins staying entirely dynamic. Here, we present low-temperature (40 mK$\leq T \leq$1.7 K) data of the specific heat C and the thermal expansion α for $Ca_{10}Cr_7O_{28}$ at various magnetic fields B up to 12 T [1]. No indications for a phase transition are observed. Instead, a kink-like structure is revealed around 0.5 K, resembling a crossover rather than a phase transition. Both quantities, $C(T)$ and $\alpha(T)$, are significantly affected by already small magnetic fields (<1 T) although a field of about 12 T is needed to open a gap in the magnetic excitation spectrum. These experimental findings support the quantum-spin-liquid hypothesis for $Ca_{10}Cr_7O_{28}$ and promise interesting physics.

[1] J. Sonnenschein *et al.*, Phys. Rev. B **100**, 174428 (2019)

TT 46.11 Wed 15:00 P2/2OG

Nonlocal correlations in the metallic phase of the Kagome Hubbard model — •Josef Kaufmann[1,4], Klaus Steiner[1,2], Andrej Lehmann[3], Daniel Hirschmeier[3], Alexander Lichtenstein[3], Richard Scalettar[2], Karsten Held[1], and Oleg Janson[4,1] — [1]TU Wien — [2]UC Davis — [3]Universität Hamburg — [4]IFW Dresden

In recent years the geometrically frustrated Kagome lattice has been in the focus of many model studies. However, most of them were done in the context of the Heisenberg model, whose ground state is believed to be a spin-liquid. Much less is known about the parent Hubbard model, which includes both electron hopping and local Coulomb repulsion on equal footing. Therefore it is very difficult obtain even approximate solutions.

A very successful approximation is made in the dynamical mean-field theory, where one obtains an auxiliary impurity model. To overcome its inherent restriction to local correlations, we employ the dynamical vertex approximation [1], the dual fermion approach [2], and determinant quantum Monte Carlo [3].

As a result, we obtain sizable non-local components in the self-energy. The effect of geometrical frustration becomes manifest in the magnetic structure factor, which is essentially independent of temperature at low temperatures.

[1] A. Toschi et al., PRB 75, 045118 (2007)
[2] A. N. Rubtsov et al., PRB 79, 045133 (2009)
[3] S. R. White et al., PRB 40, 506 (1989)

TT 46.12 Wed 15:00 P2/2OG

Frustrated quantum magnetism in the Kondo lattice on the zig-zag ladder — •Cassian Plorin, Lena-Marie Woelk, Matthias Peschke, and Michael Potthoff — I. Institut für Theoretische Physik, Fachbereich Physik, Universität Hamburg

We study the phase diagram of the one-dimensional Kondo lattice model with nearest-neighbor hopping t_1 and next-nearest-neighbor hopping t_2 at half-filling using matrix-product-states techniques. Of particular interest is the interplay between geometric frustration, antiferromagnetic ordering of the localized spins, and the Kondo effect.

It is shown that t_2 can induce various magnetic phases such as spin dimerization, quasi-long-range spin-spiral order and short-range incommensurate spin-spiral order – strongly depending on the Kondo exchange coupling J_K. In the strong-J_K regime, the appearance of short-range magnetic order can be explained by perturbative techniques.

The same model but with classical localized spins is investigated as well. Here, we find a qualitatively similar ground-state phase diagram.

In addition we discuss the spin-only Kondo-necklace model on the zig-zag ladder, which can be seen as an effective theory of the correlated Kondo lattice in the $U \to \infty$ limit. Here, the intriguing question is how the critical point of the J_1-J_2 spin chain affects the phase diagram and whether or not this is linked to the $U = 0$ Kondo lattice.

TT 46.13 Wed 15:00 P2/2OG

The repulsive interactions of the elastic quantum strings. — •Xue-Feng Zhang — Department of Physics, Chongqing University, Chongqing, 401331, China

The elastic quantum string is the quantum topological defects exist not only in the high-Tc superconductivity [1], but also in the frustrated system, such as the hard-core boson on the Kagome lattice [2,3], anisotropic triangular lattice [4] and spin half Ising model with long range interaction in the transverse magnetic field [5]. In this work, we study the repulsive interaction between effective closed strings defined on the bonds of the titled square lattice. By using the large-scale high accuracy exact diagonalization (ED) (error less than 10^{-28}), we find the effective repulsive interactions between the strings are approximately exponential decaying with form $V(r) \approx \exp(-kr^2)$, where r is the distance between strings.

[1] B-X Zheng, et. al, Science **358**, 1155 (2017)
[2] X.-F. Zhang, and S. Eggert, Phys. Rev. Lett. **111**, 147201 (2013)
[3] X.-F. Zhang, Y.-C. He, S. Eggert, R. Moessner, and F. Pollmann Phys. Rev. Lett. **120**, 115702 (2018)
[4] X.-F. Zhang, S.-J. Hu, A. Pelster and S. Eggert Phys. Rev. Lett. **117**, 193201 (2016)
[5] Z. Zhou, Z. Yan, D.-X. Liu, Y. Chen and X.-F. Zhang ongoing work

TT 46.14 Wed 15:00 P2/2OG

Improved EPR spectroscopy on single molecular magnets — •Michael Schulze[1], Daniel Schroller[1], Gheorghe Taran[1], Eufemio Pineda[2], Mario Ruben[2], Christoph Sürgers[1], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut, KIT, Karlsruhe — [2]Institut für Nanotechnologie, KIT, Karlsruhe

The quantum nature and large magnetic anisotropies in lanthanide-based single molecular magnets (SMMs) provides potential for interesting applications in quantum computing and information storage. The development of the micro-SQUID technique provides a tool for high-resolution magnetization measurements of SMM single crystals from the mK-range up to several Kelvin. EPR spectroscopy, where different spin states are excited by resonant absorption of radio frequency radiation, serves as a powerful extension of the micro-SQUID technique to gain further insight into the magnetic properties of SMMs. This project strives to improve various features of this combined setup, such as higher coupling strenghts, better thermalization, and coherent spin manipulation of SMMs.

TT 46.15 Wed 15:00 P2/2OG

Electrical read out of the nuclear spin in Tb_2Pc_3 triple decker — •Luca Kosche[1,2], Philipp Schneider[2], Christoph Sürgers[2], Franck Balestro[3], and Wolfgang Wernsdorfer[1,2,3] — [1]Institut für Nanotechnologie, KIT, Germany — [2]Physikalisches Institut, KIT, Germany — [3]Institut Néel, CNRS Grenoble, France

Single-molecular magnets (SMMs) have emerged as an excellent link between the two disciplines of spintronics and molecular electronics. Their ultimate small size, excellent single spin characteristics, and long coherence times at low temperatures make them promising candidates for fundamental quantum operations. In this project we investigate three terminal transistors comprising a SMM trapped in a nanometer sized gap coupled to a back gate thereby forming a quantum dot. The gap is achieved by electromigration of a gold junction fabricated by shadow evaporation. Recent low-noise electrical transport measurements enable the read out of the four nuclear spin states of a single terbium ion in a $TbPc_2$ double decker [1]. Here we pursue to investigate more complex multi-state systems such as the Tb_2Pc_3 triple decker to investigate the interactions between the two terbium nuclear spins.

[1] C. Godfrin et al. ACS Nano 11, 3984 (2017)

TT 46.16 Wed 15:00 P2/2OG

Mean-field study of the magnetocaloric effect in a quasi-one-

dimensional bimetallic compound — •Maheshwor Tiwari and Andreas Honecker — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Understanding the nature of all possible ground states, in particular, field-induced phases of antiferromagnets, represents an important first step towards understanding their thermodynamic properties, and in particular the magnetocaloric effect. $MnNi(NO_2)_4(en)_2$, en = ethylenediamine, contains ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. Here a self-consistent mean-field calculation of the corresponding mixed-spin model with antiferromagnetic exchange between the chains, single ion anisotropy (D), and Zeeman coupling to a magnetic field parallel to the easy axis gives rise to an antiferromagnetic state and a spin-flop transition. We construct the full phase diagram in the H-T plane and discuss the different magnetic states. The antiferromagnetic interchain coupling gives rise to a low ordering temperature and a low saturation field that promise interesting magnetocaloric properties, as we verify by computation of the thermodynamic properties of the model in a magnetic field.

TT 46.17 Wed 15:00 P2/2OG

Quantum magnetism in copper sulfates and selenates — Maria Rosner[1], Marcus Schmidt[2], Yurii Prots[2], •Helge Rosner[2], Dijana Milosavljevic[2], and Andreas Leithe-Jasper[2] — [1]Cambridge University, Homerton College, Hills Road CB2 8PH Cambridge — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Copper sulfates and selenates, quantum magnets exhibiting magnetic spin 1/2 copper sites, show a large variety of crystal structures depending on the amount of crystal water, ranging from water free compounds to up to five water molecules per Cu spin. The different amount of crystal water has a surprisingly strong influence on the magnetic properties of the different species. Here, we present a detailed study of the structure property relation for this compound family based on microscopic grounds.

TT 46.18 Wed 15:00 P2/2OG

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 the thermal conductivity of a two-dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of a homogeneous magnetic and a spatially confined electric field. The former alters the Zeeman energy and the latter the Dzyaloshinskii-Moriya interaction. Both affect the spin-canting which controls the heat flow.

For the magnetic field, we use non-linear spin wave theory and a Kubo approach to evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon decay for finite fields and temperature. We use a real-space approach to spin wave theory for the spatially confined electric field. Results for the heat conductivity as a function of the temperature, the strength of the external field, and shape of the electric-field gated region are presented. Semi-quantitative estimates for attainable variations of the heat conductivity in the context of spincaloric applications are included.

TT 46.19 Wed 15:00 P2/2OG

Temperature evolution of molecular-reorientation modes in CuPOF — •D. Opherden[1,2], C. P. Landee[3], F. Bärtl[1,2], R. Stern[4], I. Heinmaa[4], 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 — [4]Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present a detailed ^{31}P-NMR spectroscopy and relaxometry study of molecular rotations in the metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF). Here, a freezing of the PF_6 rotation modes is revealed by a step-like increase of the temperature-dependent linewidth, accompanied by broad maxima of the longitudinal and transverse nuclear spin relaxation rates. An analysis based on the Bloembergen, Purcell, and Pound theory quantifies the related activation energies E_a/k_B as 250 and 1400 K. The according characteristic correlation times of the local-field fluctuations, caused by the molecular rotation, are $\tau_0 = 20$ and 3 ps. Further, the second and fourth spectral moment of the ^{31}P absorption line were calculated for a rigid lattice, as well as for different types of PF_6 molecular-reorientation modes. The very good agreement between the experimental angular dependences of the second spectral moment and our numerical calculations clarifies the relevant symmetry axes of the PF_6 rotation modes in the different temperature regimes.

TT 46.20 Wed 15:00 P2/2OG

Low Energy Spin Excitations of $LiFePO_4$ — •Johannes Werner[1], Christoph Neef[1], Sergei Zvyagin[2], Alexey Ponomaryov[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Spin excitations in single crystalline antiferromagnetic $LiFePO_4$ have been investigated by high-frequency electron spin resonance studies in static and pulsed fields up to 50 T. Several resonance branches are observed, which can be associated with the antiferromagnetic resonance (AFMR) modes as well as with single-ion-like excitations of iron ions at the lithium position (i.e., antisite disorder). Pulsed-field ESR experiments in magnetic fields parallel to the easy b-axis clearly show closing of the AFM gap at the spin-reorientation transition at 32 T, previously observed by pulsed magnetisation measurements [1]. The pronounced curvature of the AFM resonance mode cannot be explained in a conventional two-sublattice mean field model. In addition to the AFMR branches, a less intense linear resonance branch is observed in pulsed fields. Its extrapolated zero field splitting fits well to an excitation which a recent neutron study [2] associates to a single-ion-like transition between excited (i.e., non-ground state) CF-split states. Our data however exclude this scenario but we attribute it to the presence of antisite disorder.

[1] J. Werner et al. PRB 99.21: 214432 (2019)
[2] Y. Yiu et al PRB 95.10: 104409 (2017)

TT 46.21 Wed 15:00 P2/2OG

Angular dependence of the Raman scattering intensity of optical phonons in rare-earth germanate pyrochlore single crystals — •Christian Röder[1,2], Nathan Leubner[2], Mathis Antlauf[3], Takashi Taniguchi[4], Marcus Schwarz[3], Edwin Kroke[3], and Jens Kortus[2] — [1]TU Bergakademie Freiberg, Institute of Applied Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [3]TU Bergakademie Freiberg, Institute of Inorganic Chemistry, D-09599 Freiberg, Germany — [4]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044 Japan.

Rare-earth (RE) pyrochlores are one of the most interesting groups of materials to study geometrically frustrated magnetism. In this work, the vibrational properties of RE germanates (RE = Er, Ho, Dy, Tb) of pyrochlore structure were studied by Raman scattering at room temperature. The phonon assignment in the case of similar pyrochlores such as titanates, zirconates or stannates is still debated in literature. Angular dependent Raman measurements were performed in backscattering geometry using single crystals of $Ho_2Ge_2O_7$ and $Dy_2Ge_2O_7$. The observed Raman scattering intensity as function of the azimuthal angle reveals a unique behavior for each phonon mode symmetry. The experimental results are complemented by theoretical simulations of the Raman scattering intensity allowing for an unambiguous assignment of the phonon mode symmetry.

This work was financially supported by German Research Foundation within SFB 1143.

TT 46.22 Wed 15:00 P2/2OG

Combined experimental and theoretical study of $Pr_{0.5}Sr_{0.5}MnO_3$ thin films under tensile strain — •Lokamani Lokamani[1,2], Changan Wang[1], Matthias Zschornak[1,4], Ulrich Kentsch[1], Peter Zahn[1], Bangmin Zhang[3], Shengqiang Zhou[1], and Sibylle Gemming[1,4] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [2]Department of Information Services and Computing, HZDR, Germany — [3]Department of Materials Science and Engineering, National University of Singapore, Singapore — [4]Institute of Physics, TU Chemnitz, Germany

Perovskites manganites with the general chemical formula $A_{1-x}B_xMnO_3$ are known to exhibit interesting electronic and magnetic properties, which can be further modified by varying the in-plane and out-of-plane lattice parameters. In this poster, we report a transition from insulator to metal in $Pr_{0.5}Sr_{0.5}MnO_3$ epitaxial thin films by using He ion irradiation. With increasing fluence, the out-of-plane (c-axis) lattice constant expands continuously by defect creation. Although the defect density tends to increase the resistivity, irradiated films show metallic behaviour at low temperature. We also present a comparison using density functional theory including Hubbard-U corrections to account for strongly localized Mn d- and Pr f-electrons.

TT 47: Poster Session Correlated Electrons 2

Time: Wednesday 15:00–19:00 Location: P2/3OG

TT 47.1 Wed 15:00 P2/3OG

DMRG study of a Kagome strip with two types of site spins — •Felix Liedeker[1], Nedko Ivanov[1,2], and Jürgen Schnack[1] — [1]Universität Bielefeld, Fakultät für Physik — [2]Institute of Solid State Physics, Bulgarian Academy of Sciences

We study the quantum phase diagram and the low-lying excited states of a Heisenberg kagome strip containing two types of site spins and different exchange constants for the nearest-neighbor exchange bonds by means of the density matrix renormalization group (DMRG). Geometrically, this system is a cut out from the kagome lattice, so that a cluster of five spins repeats along the chain. In particular we study non-trivial phases apart from the standard ferromagnetic and ferrimagnetic phases.

TT 47.2 Wed 15:00 P2/3OG

Properties of effective potentials obtained within the Localisation Landscape Theory of random potentials — •Sebastian Luhn and Erich Runge — Technische Universität Ilmenau, Institut für Physik, 98693 Ilmenau

Anderson Localisation is the leading paradigm for localisation in random potentials, e.g. due to interface roughness and alloy disorder in semiconductor heterostructures. The so-called Localisation Landscape Theory of S. Mayboroda et al. maps disordered potentials to a family of much smoother "effective potentials", whose minima are likely candidates for localized states. We study these effective potentials for 1D Gaussian random distributed atom chains via numerical simulations and approximate analytical expressions. In particular we compare the distributions of extrema and the spatial correlation of the effective Potential to the properties of the original potential.

TT 47.3 Wed 15:00 P2/3OG

RPA as exact high-density limit of 1D correlated electrons — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [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]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab) - 144 011, India — [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 $\epsilon_f \sim p_f^\beta$ 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 calculated analytically and the ground-state energy is presented exactly in the high-density and Coulomb limit. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] arXiv:1909.09331

TT 47.4 Wed 15:00 P2/3OG

Thermal expansion and magnetostriction studies on $CoTiO_3$ — •Marco Hoffmann[1], Kaustav Dey[1], Sven Spachmann[1], Rabindranath Bag[2], Surjeet Singh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]IISER Pune, Maharashtra, India

The $S=3/2$ compound $CoTiO_3$ crystallizes in the ilmenite-type structure which belongs to the R-3 space group. In particular, it features a strong magnetoelectric coupling. Recent discovery of Dirac magnons [1] in this compound motivates further research on the interplay of electronic, magnetic and structural degrees of freedom. We have grown high-quality single crystals by means of the optical floating-zone method and have studied magnetisation, magnetostriction, thermal expansion and specific heat of $CoTiO_3$. Pronounced anomalies in the thermal expansion coefficients at the phase transitions evidence strong magnetoelastic coupling. The magnetic phase diagram evidences a spin-reoriented phase at low magnetic fields indicating small anisotropy within the *ab*-plane. Grüneisen scaling reveals the relevant energy scales of the ordering phenomena and the structural changes at the phase boundaries are discussed.

[1] Bo Yuan et al., arXiv:cond-mat/1907.02061v1

TT 47.5 Wed 15:00 P2/3OG

Strain engineering of the Mott material $LaTiO_3$ — •Berengar Leikert[1], Julia Küspert[1], Martin Stübinger[1], Matthias Schmitt[1], Judith Gabel[2], Tien-Lin Lee[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg — [2]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE

3d transition metal oxides exhibit fascinating phenomena - absent in conventional semiconductors - like Mott insulating behaviour due to pronounced electron-electron interactions. The field of Mottronics dreams of harnessing the phase transition between the correlated metal and the Mott insulating phase of such strongly correlated materials for novel electronic devices.

We have recently demonstrated that the prototypical Mott insulator $LaTiO_3$ can undergo the band filling controlled Mott transition if it is chemically p-doped by excess oxygen during thin film growth by pulsed laser deposition [1]. Here we report on the influence of epitaxial strain. By using different substrates ($GdScO_3$, $DyScO_3$, $LaAlO_3$) we should be able to tune $LaTiO_3$ in the generic phase diagram (correlation strength versus band filling) from the Mott insulating phase towards the correlated metal phase [2]. Our goal is, exploiting strain and doping, to find an optimal spot in the phase diagram close to the boundary of the phase transition, where one might be able to trigger the phase transition with moderate electric fields.

[1] Scheiderer et al., Adv. Mater. 30, 1706708 (2018)
[2] Dymkowski et al. Phys. Rev. B 89, 161109 (2014)

TT 47.6 Wed 15:00 P2/3OG

Dielectric and Fluctuation (Noise) Spectroscopy as Complements Tools to Study Slow Dynamics in Electronic Systems with Frustration — •Giuseppe Cantarella, Merlin Mitschek, Benjamin Kammerbauer, Tatjana Thomas, and Jens Müller — Institute of Physics, Goethe University, Frankfurt (Main), Germany

The fluctuation-dissipation-theorem (FDT) quantifies the relation between the response of a system to external perturbations and its fluctuations at thermal equilibrium. In general the FDT connects the noise power spectral density (PSD) of a system with the dissipative part of susceptibility, χ''. As a consequence, in dielectric system like e.g. glasses, one can measure boths sides of the FDT equation and independently check the validity of the FDT [1]. Our aim is to explore a connection between the dielectric properties of a molecular Mott insulator and the conductance noise PSD, which often shoes a $1/f$ - type behaviour. As a test system, we chose the spin-liquid [2] candidate κ-$(BEDT\text{-}TTF)_2Cu_2(CN)_3$, which is a dimer Mott insulator on a frustrated triangular lattice that exhibits anomalous dielectric relaxations which resemble that of relaxor ferroelectric materials with quantum electric dipoles. In this work, we present first results of complementary dielectric susceptibility and current noise measurements.

[1] Phys. Rev. Lett. **107**, 095701 (2011) [2] Phys. Rev. B **82**, 125119

TT 47.7 Wed 15:00 P2/3OG

Drastic change of the charge carrier dynamics at the Mott metal-insulator transition in κ-$(BETS)_2Mn[N(CN)_2]_3$ — •Yassine Agarmani[1], Tatjana Thomas[1], Mark Kartsovnik[2], Nataliya Kushch[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaft, Germany — [3]Institute of Problems of Chemical Physics, Russian Academy of Sciences, Russia

The quasi-two-dimensional organic conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ combines strong electronic correlations with magnetic properties dominated by the presence of magnetic Mn^{2+} ions in the insulating polymeric anion layers. The system undergoes a superstructure transition near 102 K, presumably of structural origin, and a metal-insulator transition at $T_{\rm MI} \sim 30\,\rm K$ likely associated with a Mott instability [1,2]. In order to investigate the dynamical properties of the charge carriers, fluctuation (noise) spectroscopy has proven to be a successful method by measuring the time-dependent fluctuations of a sample's resistance [3]. In this compound the normalized noise power spectral density shows a broad maximum at $\sim 100\,\rm K$ and a dramatic increase below $T_{\rm MI}$. The increase is accompanied by non-Gaussian fluctuations indicated by time-dependent noise spectra. In contrast, above $T_{\rm MI}$ there is a good agreement with a simple model assuming independent fluctuators allowing to determine characteristic energies. We discuss our results in light of the possibilities of electronic ferroelectricity, recently observed in a number of dimer-Mott insulators.

[1] JACS 130, 7238 [2] PRB 82, 155123 [3] Crystals 8, 166

TT 47.8 Wed 15:00 P2/3OG

Magnetic phase diagram of Li_2FeSiO_4 — •Ahmed ElGhandour[1], Martin Jonak[1], Waldemar Hergett[1], Sven Spachmann[1], Mahmoud Abdel-Hafiez[1,2], Johannes Werner[1], Sven Sauerland[1], Nadejda Bouldi[3], Maurits Haverkort[3], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute of Physics, Heidelberg University, Germany — [2]Faculty of Science, Physics Department, Fayoum University, Egypt — [3]Institut für Theoretische Physik, Heidelberg University, Germany

Li_2FeSiO_4 single crystals of *Pmnb*-structure exhibit tetrahedrally coordinated Fe^{2+}-ions in high-spin configuration and quasi-2D magnetic substructures. The anisotropy gap $\Delta = 2.9$ meV implies significant anisotropy as compared to the antiferromagnetic dominant in-plane couplings along the crystallographic *a*- and *c*-directions, i.e., 1.0 and 3.6 meV, respectively. Notably, long-range AFM order evolving at $T_{\rm N} = 17$ K is nearly completely suppressed by magnetic fields of 16 T. While, at higher magnetic fields additional phases appear which extend to 35 T and around 15 K. In addition to the unusual magnetic phase diagram, short-range correlations at least up to $T \approx 110$ K are discussed with respect to short-range magnetic order and low-energy orbital excitations within the low-lying e_g-orbitals.

TT 47.9 Wed 15:00 P2/3OG

Ultrafast dynamics in transition-metal dichalocogenide $IrTe_2$ — •Amrit R Pokharel[1], Meng Yang[2], You Guo Shi[2], Tao Dong[1], and Jure Demsar[1] — [1]Uni Mainz, Germany — [2]Institute of physics, CAS, China

Layered transition-metal dichalocogenide $IrTe_2$ undergoes a structural phase transition to a(1/8, 0, 1/8) modulated state at T_c 280 K, followed by a transition to a(1/5, 0, 1/5) lattice modulated phase around 170 K. The low temperature modulated phase is further accompanied by the emergence of superconductivity below 2 K. Upon warming, the low temperature (1/5, 0, 1/5) lattice modulated phase persist up to T_c 280 K without entering into the (1/8, 0, 1/8) modulated state. The structural phase transitions are accompanied by sharp jumps in resistivity, indicating a complex electronic modulation entangled with structural phase transition. Despite the extensive studies, origins of the structural phase transitions and possible non-thermal light induced phase transitions remain elusive. We study the carrier relaxation dynamics and collective modes in different phases of $IrTe_2$ utilizing time-resolved pump-probe spectroscopy. Upon cooling below 280 K we observe the emergence of A1g modes at 1.28 THz and 2.17 THz. Upon further cooling through 170 K the 2.17 THz mode is dramatically reduced and new modes appear near 2.52 THz. On warming up from liquid-He temperatures the low frequency phonon modes remain unchanged up to 280 K, without entering the intermediate phase. These observations suggest the coherent phonon spectroscopy to be a sensitive tool to probe the symmetry breaking phase transitions.

TT 47.10 Wed 15:00 P2/3OG

Theoretical study of designer Hubbard models — •David Mikhail and Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

There has been tremendous progress towards engineering of tuneable two-dimensional Hubbard models in Si:P systems using scanning tunnelling microscopy (STM). STM placement allows for localization of dopants with atomic-scale precision. Motivated by these recent experimental developments, we theoretically study low-dimensional phosphorus lattices in the framework of the Hubbard model. We numerically calculate local properties of the dopants like the local density of states as well as local correlations of spin and charge. These features are experimentally accessible through scanning tunnelling spectroscopy measurements. Additionally, we investigate electronic transport properties which can be measured in standard experiments. Atomically engineered nanostructures represent promising candidates for quantum many-body simulators of strongly correlated fermionic systems, which are known to exhibit exotic physics such as high-Tc superconductivity and topological phases. The discussed Si:P systems constitute a competitive alternative to cold atoms in optical lattices as for the former much lower temperature scales can be reached.

TT 47.11 Wed 15:00 P2/3OG

Electronic structure and dynamical properties of KO_2 — •Dorota Gotfryd[1,2], Olga Sikora[3], Andrzej Ptok[3], Andrzej M. Oles[2,4], Krzysztof Wohlfeld[1], and Przemyslaw Piekarz[3] — [1]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [2]Institute of Physics, Jagiellonian University, Lojasiewicza 11, PL-30348 Krakow, Poland — [3]Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342 Krakow, Poland — [4]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Here we investigate the possible mechanisms behind the insulating properties of the strongly correlated superoxide KO_2. The intermediate monoclinic C2/c phase with O_2 molecules rotated by about 20 deg from the high-temperature tetragonal structure reported in experiments is here examined by means of density functional theory and lattice dynamics. We identify a soft phonon leading to the new stable distorted phase of C2/c symmetry and analyse its structural properties. Comparison of the electronic structure of KO_2 in the tetragonal and monoclinic phases reveals the insulating mechanism in the monoclinic phase: while only the joint efforts of large on-site Coulomb and small spin-orbit interactions are able to open a small charge gap in the tetragonal phase, in the monoclinic phase perturbing GGA+U by the small spin-orbit coupling moves KO_2 from weak to strong Mott-insulator regime. This indicates an important role of the interplay between Coulomb and on-site spin-orbit interactions as well as pronounced lattice distortions in formation of the insulating phase.

TT 47.12 Wed 15:00 P2/3OG

LDA+DMFT Approach to Resonant Inelastic X-Ray Scattering in Correlated Materials — •Mathias Winder[1], Atsushi Hariki[1], and Jan Kuneš[1,2] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We present a computational study of *L*-edge resonant inelastic x-ray scattering (RIXS) in 3*d* transition-metal (TM) oxides: NiO; $RNiO_3$; Fe_2O_3; $SrCoO_3$, $LaCoO_3$ and $LiCoO_2$; $LaCuO_3$ and $NaCuO_2$ [1]. We apply exact diagonalization to a material specific Anderson impurity model with a by DMFT obtained hybridization function. In contrast to other available methods, this approach enables us to describe simultaneously localized (*d*-*d*) and delocalized (unbound electron-hole pair) excitations in the RIXS spectra. Our calculated results reproduce well the experimental data and RIXS can be used as a tool to study material-specific hybridization between x-ray excited TM ion and low-energy states.

[1] A. Hariki, M. Winder, and J. Kuneš, Phys. Rev. Lett. **121**, 126403 (2018)

TT 47.13 Wed 15:00 P2/3OG

Interplay of electronic structure, magnetic state, and lattice stability in iron oxides under extreme conditions — •Ivan Leonov — M.N. Mikheev Inst. of Metal Physics, Yekaterinburg, Russia — NUST 'MISiS', Moscow, Russia

The theoretical understanding of iron oxides is of fundamental importance for modeling the properties and evolution of the Earth's interior. Here, we employ the DFT+DMFT method to determine the electronic structure, magnetic state, and structural phase stability of paramagnetic hematite Fe_2O_3 and pyrite-type FeO_2. Our results reveal a complex interplay between electronic correlations and the lattice in these compounds under extreme conditions. In particular, in the vicinity of a pressure-induced Mott transition Fe_2O_3 exhibits a series of complex electronic, magnetic, and structural transformations, which are accompanied by a site-selective collapse of local magnetic moments and delocalization of the Fe 3*d* electrons. Our results for structural optimization of FeO_2 within DFT+DMFT show that FeO_2 is a metal and that the oxidation state of Fe is equal to nearly 3+. In contrast to the previous claims, we found no noticeable oxygen-oxygen bonding in FeO_2 to at least 180 GPa (no evidence for the O_2 dimerization), implying that the oxidation state of oxygen in pyrite-type FeO_2 is 1.5- due to the oxygen-to-iron negative charge transfer. Our calculations of the relative phase stability of FeO_2 and Fe_2O_3 reveal that FeO_2 is unstable below ∼40 GPa. In agreement with experiment, it is found to decompose into Fe_2O_3 with release of oxygen, suggesting the importance of iron oxides in oxygen cycling between Earth's reservoirs.

TT 47.14 Wed 15:00 P2/3OG

Exploring quasi-molecular orbitals in iridates by cluster RIXS calculations — •Jan Attig[1], Maria Hermanns[2], and Markus Grüninger[3] — [1]Institut für Theoretische Physik, Universität zu Köln, Germany — [2]Stockholm University, Sweden — [3]II. Physikalisches Institut, Universität zu Köln, Germany

In recent years, the spin-orbit assisted Mott-insulating behavior of many iridate compounds has been established as a rich playground for quantum magnetism and novel phases of matter, since control in the compound structure allows to tune the subtle interplay of Hubbard interaction, spin-orbit coupling and hopping. In particular it has been shown that for Ir_2O_9 dimers in $Ba_3CeIr_2O_9$, the electronic structure consists of quasi-molecular orbitals on those dimers, which can be probed by observing a double-slit like interference pattern in resonant inelastic X-ray scattering (RIXS) [1].

Here, we present an approach that allows systematic investigation of quasi-molecular orbitals in various iridate compounds by calculation of the respective RIXS signatures from exact diagonalization (ED). We present ED calculations of the electronic structure on individual clusters of IrO_6 octahedra, as well as their RIXS spectrum. Our calculations are performed by an effective, numerical framework which is implemented on a dynamical level within the programming language Julia. This framework allows us to investigate sytems with adjustable geometry, varying number of IrO_6 octahedra, as well as different number of electrons within the system.

[1] A. W. Sleight, *Phys. C* **514**, Revelli et al., Science Advances 2019, 5: eaav4020

TT 47.15 Wed 15:00 P2/3OG

Hard-core bosonic dynamical mean-field study on melting of excitonic dispersion in $LaCoO_3$ — •Atsushi Hariki[1], Ru-Pan Wang[2], Andrii Sotnikov[1,3], Keisuke Tomiyasu[4], Davide Betto[5], Nicholas B. Brookes[5], Yohei Uemura[2], Mahnaz Ghiasi[2], Frank M. F. de Groot[2], and Jan Kuneš[1,6] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Debye Institute for Nanomaterials Science, Utrecht University, Universiteitsweg 99, 3584 CG Utrecht, The Netherlands — [3]Akhiezer Institute for Theoretical Physics, NSC KIPT, Akademichna 1, 61108 Kharkiv, Ukraine — [4]Department of Physics, Tohoku University, Aoba, Sendai 980-8578, Japan — [5]European Synchrotron Radiation Facility, 71 Avenue des Martyrs, CS40220, F-38043 Grenoble Cedex 9, France — [6]Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Praha 8, Czechia

We study excitonic nature of the spin-state transition in $LaCoO_3$. Based on Co L_3-edge resonant inelastic x-ray scattering (RIXS) data, we construct an effective bosonic model which describes (i) intermediate-spin (S=1, IS) excitons propagating on a low-spin (S=0) background and (ii) a high-spin (S=2, HS) state as tightly-bound two IS excitons. The effective model is solved at finite temperatures by means of hard-core bosonic dynamical mean-field theory (HB-DMFT). The RIXS data across the spin-state transition around 100K reveals melting of the IS excitonic dispersion. The HB-DMFT analysis of the RIXS data points out a novel picture of the HS state as bi-exciton dressed by virtual fluctuations HS↔IS+IS.

TT 47.16 Wed 15:00 P2/3OG

Electronic properties of strongly correlated ruthenates — •Neda Riahisamani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425, Germany

We study the electronic properties of strongly correlated ruthenates by using the LDA+DMFT method. We construct materials-specific models for the t_{2g} bands via maximally localized Wannier functions. We solve the DMFT quantum impurity problem adopting as solver the weak coupling continuous-time Quantum Monte Carlo approach, in the implementation of Refs. [1, 2, 3]. Results will be discussed.

[1] E. Gorelov, M. Karolak, T. O. Wehling, F. Lechermann, A. I. Lichtenstein, E. Pavarini, Phys. Rev. Lett. **104**, 226401 (2010)
[2] G. Zhang, E. Gorelov, E. Sarvestani, E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)
[3] E. Sarvestani, G. Zhang, E. Gorelov, E. Pavarini, Phys. Rev. B **97**, 085141 (2018)

TT 47.17 Wed 15:00 P2/3OG

Response functions for correlated systems with LDA+DMFT — •Julian Musshoff[1,2] 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

Response functions are essential to compare theoretical calculations with experiments. For strongly correlated systems the calculation of the associated two-particle Green functions remains challenging, however. The state-of-the-art approach is the LDA+DMFT method. Here we adopt this technique; we use the strong-coupling continuous-time quantum Monte Carlo approach as the quantum impurity solver. Our massively-parallel general implementation [1,2] allows us to calculate response functions in different efficient polynomial bases. We will present recent results on the magnetic and orbital ordering mechanism in K_2CuF_4 [2]. In addition, we will discuss the application to layered cuprates, with and without doping.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, *Phys. Rev. B* **87**, (2013) 195141
[2] J. Musshoff, G. Zhang, E. Koch, E. Pavarini, *Phys. Rev. B* **100**, (2019) 045116

TT 47.18 Wed 15:00 P2/3OG

Generic phase diagram of quantum dimer model on square lattice — Zheng Yan[1,2], •Zheng Zhou[1], Olav Syljuasen[3], Junhao Zhang[1], Tianzhong Yuan[1], Jie Lou[1,4], and Yan Chen[1,4] — [1]Department of Physics and State Key Laboratory of Surface Physics, Fudan University, Shanghai 200438, China — [2]Department of Physics, The University of Hong Kong, Hong Kong, China — [3]Department of Physics, University of Oslo, P. O. Box 1048 Blindern, N-0316 Oslo, Norway — [4]Collaborative Innovation Center of Advanced Microstructures, Nanjing 210093, China

Constraint is an important property in low-energy physics, but it also bring a lot of difficulties for numeric calculation. The quantum dimer model is a low-energy description of many spin models, but its phase diagram is still controversial, even on the square lattice. In this article, we focus on the square lattice quantum dimer model and give a unified conclusion about its phase diagram which reconciles conflicting results given in the literature. With our newly developed sweeping cluster method, we studied the phase diagram of the almost full parameter space by introducing the definition of pair correlation function and other supporting evidence to distinguish the mixed phase from the columnar phase with high precision. In particular, we find that the ground state corresponds to the mixed phase for a vast parameter region.

TT 47.19 Wed 15:00 P2/3OG

Artificial Neural Networks Ansatz for Quantum Integrable Models — •Dennis Wagner[1,2], Andreas Klümper[1], and Jesko Sirker[2] — [1]Begische Universität Wuppertal — [2]University of Manitoba

Computing wave functions of quantum many-body systems is in general an exponentially hard problem. However, wave functions are required to calculate correlation functions. To approximate these wave functions, Artificial Neural Networks (ANN) have been considered.

In our work we investigate why this specific wave function ansatz seems to be useful for certain integrable models and how it can be improved. Furthermore, we try to get a deeper insight into quasi-local charges and compute dynamic correlation functions effectively.

TT 47.20 Wed 15:00 P2/3OG

Higher order auxiliary field quantum Monte Carlo methods — •Florian Goth and Fakher Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

The auxiliary field method QMC method has been a workhorse of solid state physics for a long time and has found its most recent implementation in the ALF package. The utilization of the Trotter-Suzuki decomposition to decouple the interaction from the non-interacting Hamiltonian makes this method inherently second order in terms of the imaginary time slice. We show the necessary generalizations to enable higher orders in ALF and perform numerical comparisons with other second order methods as well as methods of higher order.

TT 47.21 Wed 15:00 P2/3OG

Orbital differentiation in Hund metals — •Fabian B. Kugler[1], Seung-Sup B. Lee[1], Manuel Zingl[2], Hugo U. R. Strand[2], Andreas Weichselbaum[3], Gabriel Kotliar[4], Antoine Georges[2], and Jan von Delft[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Flatiron Institute - Simons Foundation, USA — [3]Brookhaven National Laboratory, USA — [4]Rutgers University, USA

Orbital differentiation is a common theme in multi-orbital systems, yet a complete understanding of it is still missing. Here, we focus on three-orbital Hubbard models to describe the t_{2g} bands of materials such as ruthenates and iron-based superconductors, and provide results of unprecedented accuracy by using the numerical renormalization group as real-frequency impurity solver for dynamical mean-field theory. First, we consider a minimal model for orbital differentiation, where a crystal field shifts one orbital in energy, and describe the various phases with dynamic correlation functions. Upon approaching the orbital-selective Mott transition, we find a strongly suppressed spin-coherence scale and uncover the emergence of a singular Fermi liquid and interband doublon-holon excitations. Then, we apply our method to the paradigmatic material Sr_2RuO_4 in a real-materials framework. We illustrate distinctive Hund-metal features and provide theoretical evidence for a Fermi-liquid scale of about 25 Kelvin.

TT 47.22 Wed 15:00 P2/3OG

Energy Gap in Strongly Correlated Hubbard Clusters—Comparing Green Functions and DMRG — •Sönke Hese[1], Jan-Philip Joost[1], Niclas Schlünzen[1], Claudio Verdozzi[2], Peter Schmitteckert[3], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]Lund University, Sweden — [3]HQS Quantum Simulations, Germany

The (Fermi–)Hubbard model is a key system in the theory of strongly correlated electrons in solids. While the exact solution of the Hubbard Hamiltonian is known to possess a spin-symmetric ground state, in the mean-field approximation magnetic instabilities can, for on-site interactions beyond a critical U_c, induce the spontaneous breaking of spin symmetry leading to stable spin-density waves [1]. Using a Green function approach with higher order corrections to the self-energy, namely second Born and GW, we observe a similar effect at considerably larger interactions. Further, we find that similar inhomogeneous solutions are also present in spin-restricted calculations. By comparing to exact DMRG data for the 1D chain we find that these symmetry-broken states produce reliable data for the spectral function including the size of the Mott gap.

[1] J.-P. Joost, A.-P. Jauho, M. Bonitz, Nano Letters (2019), DOI:10.1021/acs.nanolett.9b04075

TT 47.23 Wed 15:00 P2/3OG

Symmetric WDA — •Asbjorn Rasmussen[1,2], Jens Jorgen Mortensen[1], and Kristian Sommer Thygesen[1,2] — [1]Center for Atomic-Scale Materials Design, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [2]Center for Nanostructued Graphene, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

The Weighted Density Approximation (WDA) is an approximation to the exchange-correlation (xc) energy functional originally developed by D. J. Singh et al. and was shown to work well for a number of materials. WDA involves an approximation to the xc-hole that preserves the correct normalization, however the resulting pair-distribution is not symmetric. We expect that using a version of WDA that obeys the exact symmetry of the pair-distribution will generally improve results. In this work we implement a symmetric WDA using numerical techniques developed in the context of vdW functionals to calculate the non-local expressions efficiently.

TT 47.24 Wed 15:00 P2/3OG

Efficient ladder dual fermion calculations from a three-leg vertex — •Viktor Harkov[1,2], Angelo Valli[3], Alexander I. Lichtenstein[1], and Friedrich Krien[4] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]European X-Ray Free-Electron Laser Facility, 22869 Schenefeld, Germany — [3]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [4]Institut Jožef Stefan, Ljubljana, Slovenia

The calculation of the dynamical susceptibility within the dynamical mean-field theory requires the numerically expensive measurement of the vertex function of the auxiliary Anderson impurity model. We investigate an optimal parametrization of the vertex in terms of single-boson exchange (SBE). The approximation lowers the cost of ladder dual fermion calculations to a level comparable with the TRILEX approach.

TT 47.25 Wed 15:00 P2/3OG

The Chebyshev expansion as solver for the variational cluster approximation at finite temperature — •Jan Lotze and Maria Daghofer — University of Stuttgart, Functional Matter and Quantum Technologies, 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 to be tractable. An alternative approach is to expand the reference systems Green's function in Chebyshev polynomials [2].

Here, thermodynamic and dynamical properties of the one- and two-dimensional Hubbard model at finite temperature are presented to illustrate the Chebyshev expansion in comparison to the Lanczos method as solver of the reference system.

[1] M. Potthoff, 'Self-Energy-Functional Theory', in Strongly Correlated Systems - Theoretical Methods (Springer, 2012)
[2] A. Braun and Schmitteckert, Phys. Rev. B **90**, 165112 (2014)

TT 47.26 Wed 15:00 P2/3OG

Magneto transport in light tuned STO-based interfaces — •Roland Schäfer, Daniel Arnold, and Dirk Fuchs — Institut fürFestkörperphysik, KIT, Karlsruhe

Recently we have shown that light can be utilized to tune transport properties of strontium titanate based interfaces at low temperatures in a controlled manner [1]. The effect has been observed at the interface with lanthanum aluminate and aluminum oxide. Light exposure at temperatures below $T = 1\,\mathrm{K}$ leads to a persistent reduction of resistance. The reduction depends on exposure dose, can be as large as a factor of five, and is accompanied by a reduction of the superconducting transition temperature reminiscent of the overdoped side of the dome structure in back gate experiments. Persistent changes can be reverted by heating the samples to a moderate temperature of about $T \approx 15\,\mathrm{K}$.

Here we present and discuss magneto transport data. The well established band structure of the two dimensional electron gas at the surface is used to calculate the conductance tensor as function of the magnetic field by semiclassical transport theory. The theoretical results are compared to the experimental findings.

[1] D. Arnold et. al, APL **115**, 122601 (2019)

TT 47.27 Wed 15:00 P2/3OG

RKKY driven quenching of local moments in Kondo dominated multi impurity models and Kondo insulators — •Fabian Eickhoff and Frithjof Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, Dortmund

For a single spin $\vec{S}$ ferromagnetically coupled to a metallic host, the Kondo effect is absent and a spinful groundstate remains. However, if an additional Anderson-type impurity orbital O is added, such that antiferromagnetic RKKY interaction $J_{\mathrm{RKKY}}\vec{S}_O\vec{S}$ is generated, $\vec{S}$ will always be quenched at zero temperature. For $T_{\mathrm{K}}^{O} \gg J_{\mathrm{RKKY}}$, the quenching occurs below the temperature scale $\tilde{T} \propto \exp(-T_{\mathrm{K}}^{O}/J_{\mathrm{RKKY}})$ where $\langle\vec{S}_O\vec{S}\rangle \approx 0$ at all temperatures. Using a new type of approximation for the wide band limit, we demonstrate that such a RKKY driven quenching of local moments on a scale $\tilde{T}$ occurs in multi impurity Anderson Hamiltonians as well, requiring at least three impurity sites. We show, that the formation of local moments due to a single Kondo-hole, is a direct consequence of RKKY driven local moment quenching and associated with an exponentially suppressed $\tilde{T}$. This goes beyond the scope of well established two impurity physics and sheds some new light on emerging magnetic moments and their screening in multi-impurity models as well as in periodic systems.

TT 47.28 Wed 15:00 P2/3OG

Dynamical Effects in Topological Kondo Insulators — •Marvin Lenk and Johann Kroha — Physikalisches Institut and Bethe Center for Theoretical Physics, Universität Bonn, Germany

Topological Kondo insulators (TKIs) are a new class of topological insulators, emerging through the interplay of strong correlations and spin-orbit coupling [1]. In TKIs, the bulk is a narrow band insulator due to the appearance of a localized Kondo resonance near the Fermi level and its hybridization with the conduction band. Additionally, the strong spin-orbit coupling of the localized moments generates a non-local hybridization between the local moments and the conduction band, which results in a topologically nontrivial band structure and gapless surface states.

In the past, TKIs have been described predominantly by slave-boson mean-field (SBMF) calculations. Such static methods are unable to capture finite life-time effects of the heavy Kondo quasiparticles. It is therefore not possible to investigate physics at the boundaries, like the dynamical emergence of topological edge states, where SBMF calculations become uncontrolled. We design a spin-orbit coupled dynamical mean-field theory (cf. [2]) with an auxiliary-particle conserving approximation (cf. [3]) as an impurity solver. With this, we aim at calculating characteristic, observable quantities, like the surface conductivity, including life-time effects.

[1] M. Dzero et al., Phys. Rev. Lett. 104 (2010) 106408
[2] A. Georges, AIP Conference Proceedings 715, 3 (2004)
[3] J. Kroha and P. Wölfle, Acta Phys. Pol. 29 (12), 3781 (1998)

TT 47.29 Wed 15:00 P2/3OG

Electronic and magnetic properties of Co impurity in Cu Host — •Daria Medvedeva[1], Alexander Poteryaev[2], Jindřich Kolorenč[1], and Alexander Shick[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Institute of Metal Physics of the Russian Academy of Sciences, Yekaterinburg, Russian Federation

The electron correlations play a crucial role in understanding of quantum matter. The Kondo effect that originates from scattering of itinerant electrons by local moments and corresponding screening is a manifestation of these many-electron correlations. Realistic multi-orbital approaches have to be applied in order to explain the experimental properties of Kondo $3d$ impurities in the bulk [1] and at the surface [2]. We consider the solution of multi-orbital single impurity Anderson model (SIAM) making use of CT-QMC (CT-HYB) and Exact diagonalization (ED based on Lanczos) for the Co impurity in bulk Cu. The model is parametrized using LDA computed hybridization function, and the crystal field. Spectral functions calculated by the ED method are in good agreement with QMC. It is found that the ground state of the impurity model is a singlet for different occupations of the impurity d-shell, that is, the Co magnetic moment is screened by Cu conduction electrons.

[1] L. Joly et al. Phys. Rev. B 95, 041108(R) (2017)
[2] R. Mozara et al., Phys. Rev. B 97, 085133 (2018)

TT 47.30 Wed 15:00 P2/3OG

Restoring the continuum limit in the time-dependent numerical renormalization group approach — •Jan Böker and Frithjof Anders — TU Dortmund, Theoretische Physik II, Otto-Hahn-Straße 4, 44227 Dortmund

We analytically construct a set of additional reservoirs coupled to the Wilson chain to recover the original continuous coupling functions to a quantum impurity.

We present a hybrid time-dependent numerical renormalization group (TD-NRG) approach which combines an accurate NRG treatment of the non-equilibrium dynamics on the finite size Wilson chain with a Bloch-Redfield formalism to include the effect of the additional reservoirs. For the solution of the Lindblad-style master equations a Lanczos method is employed. Our proposed approach tackles the intrinsic shortcoming of the TD-NRG induced by the bath discretization with a Wilson parameter $\Lambda > 1$. The effects of conservation laws and charge reflections along the Wilson chain are damped due to dissipation into the reservoirs, and a correct thermalization even on longer timescales is reached. The presented hybrid TD-NRG approach is used to investigate the real-time nonequilibrium dynamics in fermionic quantum-impurity systems. An analytical solution of the resonant-level model (RLM) serves as a benchmark for the accuracy of the method which is then applied to non-trivial models, such as the interacting RLM and the single impurity Anderson model.

TT 48: Poster Session: Many Body Systems, Quantum Critical Phenomena

Time: Wednesday 15:00–19:00 Location: P2/4OG

TT 48.1 Wed 15:00 P2/4OG

Low temperature magnetoresistance and Hall effect measurements of $YbNi_4P_2$ — •William Broad[1], Sven Friedemann[1], Kristin Kliemt[2], and Cornelius Krellner[2] — [1]HH Wills Laboratory, University of Bristol, UK — [2]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a heavy-fermion Kondo-lattice metal with a very low ferromagnetic ordering temperature of 0.17 K. The transition temperature can be suppressed by partial substitution of As on the P site, leading to a quantum critical point (QCP). The rarity of such a QCP makes $YbNi_4P_2$ an important material to study for the understanding of ferromagnetic quantum criticality. Magnetoresistance and Hall effect data on $YbNi_4P_2$ are presented from low temperature dilution refrigeration measurements between 35 mK and 1 K. We have observed several Lifshitz transitions with a new orientation of the magnetic field in the ab plane, and discuss the anomalous Hall effect in the ferromagnetic state.

TT 48.2 Wed 15:00 P2/4OG

A.C. susceptibility investigations near quantum critical points on strongly correlated spin systems — •Paul Eibisch, Lars Postulka, Bernd Wolf, Ulrich Tutsch, Yeekin Tsui, Franz Ritter, Cornelius Krellner, and Michael Lang — Physikalisches Institut Goethe-Universität

Quantum phase transitions (QPT), i.e., phase transitions at $T = 0$ driven by the variation of a control parameter such as the magnetic field B, continue to be of high interest in condensed matter research. Above the quantum critical point (QCP) the system shows quantum critical behaviour which manifests itself in scaling behaviour of thermodynamic quantities and divergences in certain ratios of these quantities, the so-called Grüneisen parameters. In addition to signatures in these equilibrium properties, quantum criticality is expected to affect also the dynamic properties via a critical slowing down, i.e., the divergence of the correlation time at the QPT. Here we present a study of the a.c. susceptibility, including both the real- and imaginary-contributions, on the low-dimensional quantum spin systems $CuSO_4$ and Cs_2CuCl_4 both of which show B-induced quantum critical points in the field range $B \leq 10\,T$. At the critical fields for $T < 1\,K$ we find clear signals in the imaginary part, χ'' of the a.c. susceptibility, yielding a pronounced maximum at finite temperature. The position of these anomalies in the B-T-phase diagram suggests a quantum critical nature, i.e., changes in the spin dynamics on approaching the QCP.

TT 48.3 Wed 15:00 P2/4OG

Thermodynamic studies of field-induced quantum critical behaviour in the organic spin-dimer system $C_{28}H_{32}N_4O_2$ (BY310) — •Christian Thurn[1], Paul Eibisch[1], Lars Postulka[1], Ulrich Tutsch[1], Bernd Wolf[1], Yulia Borozdina[2,3], Martin Baumgarten[2], and Michael Lang[1] — [1]PI, Goethe Uni, Frankfurt/M., SFB/TR49, Deutschland — [2]MPI für Polymerforschung, Mainz, SFB/TR49, Deutschland — [3]MPI für biologische Kybernetik, Tübingen, Deutschland

Systems of interacting spin dimers provide suitable model systems for studying critical phenomena under well-controlled conditions. Prominent examples include the Bose-Einstein-condensation of triplons in 3D systems [1] or the Berezinskii-Kosterlitz-Thoules scenario in a 2D system [2]. Within this class of materials, spin-dimer systems based on organic radicals stand out due to the high degree of tunability with regard to both the interaction strength as well as the dimensionality. In this work we focus on the tolane-bridged imino-nitroxide radical $C_{28}H_{32}N_4O_2$ (BY310) [3]. In BY310 we find quantum-critical points at around 1.8 T and 4.3 T delimiting a B-induced ordered phase for

$T \leq 0.5\,\mathrm{K}$. We present results of thermal expansion α as well as magnetostriction λ measurements in the field range up to 5.5 T and for temperatures from 1.7 K down to 50 mK. The results are compared with results of the specific heat, the magnetocaloric effect and the ac-susceptibility.

[1] Giamarchi *et al.*, Nat. Phys. **4**, No 2, 198-204 (2008)
[2] Tutsch *et al.*, Nat. Commun. **5**, 5169 (2014)
[3] Borozdina *et al.*, J. Mater .Chem **5**, 9053-9065 (2017)

TT 48.4 Wed 15:00 P2/4OG

Quantitative analysis of the energy constant's effect on the performance of directed loop quantum Monte Carlo Algorithm — •Dong-Xu Liu and Xue-Feng Zhang — Department of Physics, Chongqing University, Chongqing, 401331, China

The efficiency and performance of the stochastic series expansion (SSE) with directed loop quantum Monte Carlo algorithm is not only related to the specific Hamiltonian, but also the implementation of the algorithm. As one tunable parameter of SSE, the shifted constant of the energy is demonstrated to affect the autocorrelation time and also the performance of the algorithm. In order to quantitatively analyze the effect of the energy constant, we defined the cost-function as $\tau_{int} \times T_{\mathrm{CPU}}$, where τ_{int} is auto-correction time and T_{CPU} is the CPU time costed by loop-updating process. The CPU time T_{CPU} has a good linear relationship with energy constant, because it will linearly increase the length of imaginary time. However, we discovered that auto-correction time shows a power-law decay and exponential decay behaviour with energy constant increased in one-dimensional spin-$\frac{1}{2}$ XY model and Heisenberg model, respectively. Then, we turn to analyze the effect of energy constant on the average length of loops. We demonstrated the average loop length is linearly related to the energy constant, however not proportional to the total energy. Finally, we discussed how to improve performance and also the accuracy of the correlation function by adjusting the energy constant.

TT 48.5 Wed 15:00 P2/4OG

Hierarchy of energy scales in an antiferromagnetic quantum critical metal: a Monte Carlo study — •Carsten Bauer[1], Yoni Schattner[2], Simon Trebst[1], and Erez Berg[3] — [1]University of Cologne, Germany — [2]Stanford University, USA — [3]The Weizmann Institute of Science, Israel

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 excitations on a Fermi surface. When driving a metal through a phase transition, this interplay can lead to a damping of the critical modes and can give rise to unconventional superconductivity, and "strange metal" behavior. It might therefore serve as a microscopic model for some of the rich physics of high-T_c materials.

Fortunately, certain classes of metallic quantum critical points can be analyzed by determinant quantum Monte Carlo as one can circumvent the notorious "sign problem" and retain polynomial efficiency. I will show numerically exact studies of two dimensional metals at the verge of an antiferromagnetic transition indicating Landau-damping of the order parameter fluctuations and a breakdown of Fermi liquid theory. I will further discuss the case of an (almost) locally nested Fermi surface, where T_c is strongly suppressed. Lastly, I will demonstrate that a machine learning technique dubbed "quantum loop topography" can be utilized to probe transport and identify the superconductivity transition in such a many-particle system.

TT 48.6 Wed 15:00 P2/4OG

Transport and Localization Phenomena in One-Dimensional Open Quantum Systems Simulated with Matrix Product States — •Manuel Katzer, Willy Knorr, Regina Finsterhoelzl, and Alexander Carmele — Institut fuer Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universitaet Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The discovery of disorder induced localization in the presence of interactions opened up a new field of research. We investigate the yet open question of phase transitions in transport and the conditions for the existence of many-body localization in different one dimensional open quantum systems in the presence of driving by an external bath. Here, we compare the model of a Heisenberg spin chain [1], where isotropic nearest-neighbor coupling shows negative differential conductivity and a transition from diffusive to subdiffusive transport with a chain of harmonic oscillators [2]. When these bosonic oscillators interact with a Kerr nonlinearity, higher-order excitations are suppressed and thus state-filling effects start to dominate. For large nonlinearities, this eventually results in a transport behaviour quite similar to the spin chain. In order to simulate larger chain lengths, the systems are simulated in a MPS approach [3] or via QMC in order to investigate the role of finite size effects and to get closer to a possible regime for many body localization effects.

[1] Droenner and Carmele, Phys. Rev. B **96**, 184421 (2017)
[2] Huber and Rabl, Phys. Rev. A **100**, 012129 (2019)
[3] Prosen, Phys. Rev. Lett. **106**, 217206 (2011)

TT 48.7 Wed 15:00 P2/4OG

Entanglement, spectra and Floquet engineering of topological many-body localized systems — •Kevin S.C. Decker[1], Dante Kennes[2,3], Jens Eisert[4], and Christoph Karrasch[1] — [1]Technische Universität Braunschweig, Institut für Mathematische Physik, Mendelssohnstraße 3, 38106 Braunschweig, Germany — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, 52056 Aachen, Germany — [3]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [4]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Many-body localized systems in which interactions and disorder come together defy the expectations of quantum statistical mechanics: They do not thermalize when undergoing non-equilibrium dynamics. In this work, we numerically address how topological features interplay with many-body localized phases as well as the nature of the transition between a topological and a trivial state within the latter. We also show how second-order Floquet engineering can be employed to realize systems in which many-body localization coexists with topological properties in a driven system. This allows one to implement and dynamically control a symmetry protected topologically ordered qubit even at high energies, overcoming the road block that the respective states cannot be prepared as ground states of nearest-neighbor Hamiltonians.

TT 48.8 Wed 15:00 P2/4OG

Interacting bosons in an optical cavity: fluctuation effects — •Alla Bezvershenko, Florian Lange, and Achim Rosch — University of Cologne, Germany

We consider a chain of interacting bosonic atoms coupled to the field of an optical cavity with imperfect mirrors. In such a non-equilibrium open quantum system, temperature in the usual sense is not defined. In the conventional, theoretical mean-field approach, only the mean-field contribution of the coupling between the cavity field and the bosonic degrees of freedom is considered. We argue, however, that fluctuations beyond mean field theory are essential to obtain the effective temperature and, therefore, also the correct value of the mean-field for the atomic subsystem. Our approach is valid in a regime where the thermalization rates of the atomic system are larger than the rates of energy transfer between atoms and light.

TT 48.9 Wed 15:00 P2/4OG

Combining dynamical quantum typicality and numerical linked cluster expansions — •Jonas Richter and Robin Steinigeweg — University of Osnabrück, Germany

We demonstrate that numerical linked cluster expansions (NLCE) yield a powerful approach to calculate time-dependent correlation functions for quantum many-body systems in one dimension. As a paradigmatic example, we study the dynamics of the spin current in the spin-1/2 XXZ chain for different values of anisotropy, as well as in the presence of an integrability-breaking next-nearest neighbor interaction. For short to intermediate time scales, we unveil that NLCE yields a convergence towards the thermodynamic limit already for small cluster sizes, which is much faster than in direct calculations of the autocorrelation function for systems with open or periodic boundary conditions. Most importantly, we show that the range of accessible cluster sizes in NLCE can be extended by evaluating the contributions of larger clusters by means of a pure-state approach based on the concept of dynamical quantum typicality (DQT). Even for moderate computational effort, this combination of DQT and NLCE provides a competitive alternative to existing state-of-the-art techniques, which may be applied in higher dimensions as well.

[1] J. Richter and R. Steinigeweg, Phys. Rev. B 99, 094419 (2019).

TT 48.10 Wed 15:00 P2/4OG

Non-equilibrium dynamics of photo-induced triplons — •Hossam Tohamy and Maria Daghofer — University Stuttgart, Institute for Functional Matter and Quantum Technologies, Pfaffenwaldring 57, 70569 Stuttgart, Germany

We study the non-equilibrium dynamics of photo-induced triplons in periodically driven Mott insulators. Strong spin-orbit coupling in these systems favors a ($J = 0$) singlet ground state while magnetic superexchange favors ($J = 1$) triplet excited states. Triplons are excitations from singlet to triplet states.

We numerically simulate a pump-probe experiment for a 1D spin-orbital Hubbard model using the Lanczos exact diagonalization method. For certain laser pulse excitation frequencies and interaction parameters in the spin-orbital Hubbard model, we find that induced triplet states show antiferromagnetic (AFM) correlations. Both the strength of the triplet moment and the modulation of the AFM pattern depend on the laser excitation frequency, pulse width, and amplitude.

TT 48.11 Wed 15:00 P2/4OG

Irreversible real-time dynamics of quantum, classical and quantum-classical spin systems — •Leon Mixa and Michael Potthoff — I. Institute of Theoretical Physics, Department of Physics, Universität Hamburg

Macroscopic irreversibility of the time evolution of interacting many-body systems is a necessary condition for thermalisation. For classical systems, the corresponding loss of information on the initial state is due to non-linear dynamics with exponential sensitivity to small perturbations resulting in chaotic behaviour. A closed quantum system, on the other hand, is described by linear unitary dynamics. Recent ideas for quantum irreversibility conceptually build on the eigenstate-thermalisation-hypothesis and on specific measures such as out-of-time order correlators or observable echos, see e.g. [1].

Here, we consider a one-dimensional nonintegrable quantum-spin model, i.e., the Kondo necklace model with anisotropic (XY) local "Kondo" coupling to local quantum spins, and, in a first step, confirm the results of Ref. [1]. We then study the corresponding model with quantum spins replaced by classical spins and find thermalisation driven by classically chaotic motion. Our main goal is to classify the intermediate situation, namely the quantum-classical hybrid model where only the local spins are treated classically. We systematically study observable echos, Lyapunov exponents and other measures.

[1] M. Schmitt and S. Kehrein, Phys. Rev. B 98, 180301(R) (2018)

TT 48.12 Wed 15:00 P2/4OG

Fast Nonequilibrium Green Functions simulations with GW selfenergies — •Christopher Makait, Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — Institut für Theoretische Physik und Astrophysik, CAU Kiel, Germany

The Nonequilibrium Green Functions (NEGF)[1] method is a powerful tool to compute time-dependent expectation values of single-particle observables in correlated quantum many-body systems. Its unfavorable N_t^3-scaling with propagation time N_t could be reduced to N_t^2 by introduction of the Generalized Kadanoff–Baym Ansatz (GKBA)[2]. Recently, an exact time-local (N_t^1) reformulation of the GKBA, the G1–G2 scheme [3,4], has been found for various self energies, which makes this method viable for long time simulations.

In a general basis the G1–G2 scheme has a computationally expensive scaling with basis size (N_b^5–N_b^6). For the uniform electron gas (UEG) however, we found an advantageous $N_b^3 N_t^1$ scaling for both second-order and GW selfenergies, which makes this scheme particularly interesting for this system. Here, we present first results of the application of the G1–G2 scheme to the UEG.

[1] L. P. Kadanoff, G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962)
[2] P. Lipavský, V. Špička, B. Velický, *Phys. Rev. B*34, 6933 (1986)
[3] N. Schlünzen, Jan-Philip Joost, Michael Bonitz, *submitted*, arXiv:1909.11489 [cond-mat.str-el]
[4] M. Bonitz, *Quantum Kinetic Theory* (Springer, 2016)

TT 49: Topolectric Circuits and Quantum Hall Systems

Time: Wednesday 17:15–19:00 Location: HSZ 103

TT 49.1 Wed 17:15 HSZ 103

Re-entrant Topological Defect Mode in a PT-Symmetric Circuit — •Alexander Stegmaier[1], Tobias Helbig[1], Tobias Hofmann[1], Stefan Imhof[1], Lee Ching Hua[2], and Ronny Thomale[1] — [1]Institute of Theoretical Physics I, University of Würzburg, Germany — [2]National University of Singapore, Singapore

Systems obeying PT-symmetry are a special case in non-Hermitian physics where real eigenvalue spectra can still emerge. They usually exhibit a phase diagram with different regimes of symmetry conservation or spontaneous symmetry breaking in their eigenstates. We examine a localized zero-energy defect mode within a PT-symmetric SSH chain that disappears and re-emerges at different PT phase transitions and present an exhaustive explanation for this phenomenon. Our theoretical findings are confirmed by eigenstate measurements for different gain/loss profiles in an electrical circuit implementation.

TT 49.2 Wed 17:30 HSZ 103

Reciprocal skin effect and its realization in a topolectrical circuit — •Tobias Helbig[1], Tobias Hofmann[1], Ching Hua Lee[2,3], Frank Schindler[4], Titus Neupert[4], Martin Greiter[1], and Ronny Thomale[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Department of Physics, National University of Singapore, Singapore 117542 — [3]Institute of High Performance Computing, A*STAR, Singapore 138632 — [4]Department of Physics, University of Zurich, 8057 Zurich, Switzerland

The non-Hermitian Skin effect heralds the start of a new paradigm in synthetic metamaterial research. The newly established notion of the Skin effect requires specifically tailored gain and loss in combination with a necessary breaking of reciprocity. In this talk we extend this viewpoint and present a model which shows extensive eigenmode localization for open boundaries despite preserving reciprocity. In contrast to non-reciprocal implementations of the Skin effect, which require an external supply of energy, this model can be realized by using exclusively passive components. We experimentally demonstrate this novel phenomenon in a passive RLC circuit network. The reciprocal Skin effect suggests itself for realization in a plethora of metamaterial platforms with limited availability of active components.

[1] T. Hofmann et al. , arXiv: 1908.02759 (2019)

TT 49.3 Wed 17:45 HSZ 103

The Chern state in electric circuits — •Hendrik Hohmann[1], Tobias Helbig[1], Tobias Hofmann[1], Alexander Stegmaier[1], Ching Hua Lee[2,3], Martin Greiter[1], and Ronny Thomale[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Department of Physics, National University of Singapore, Singapore 117542 — [3]Institute of High Performance Computing, A*STAR, Singapore 138632

Topolectrical circuits present themselves as a versatile platform to investigate topological states of matter realized in a classical environment. Among them, the Chern insulator is commonly viewed as the most fundamental one, because it solely relies upon its non-trivial band topology and does not require additional symmetries. The combined breaking of reciprocity and time-reversal symmetry (TRS) as well as minimizing dissipation effects signify the central challenges of a Chern state realization in classical setups. In a passive realization, the breaking of TRS can be circumvented by creating a doubled copy of Chern bands [V. Albert et al., Phys. Rev. Lett. 114, 173902]. In contrast, the inclusion of active components allows for a nontrivial topological band structure in direct analogy to the Haldane model [T. Hofmann, T. Helbig et al., Phys. Rev. Lett. 122, 247702]. The hallmark of the active Chern state realization is its support of unidirectionally propagating voltage modes at its boundary.

TT 49.4 Wed 18:00 HSZ 103

Observation of the non-Hermitian skin effect in topolectric circuits — •Tobias Hofmann[1], Tobias Helbig[1], Stefan Imhof[2], Tobias Kiessling[2], Ching Hua Lee[3,4], Martin Greiter[1], and Ronny Thomale[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg — [2]Physikalisches Institut und Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg — [3]Department of Physics, National University of Singapore, Singapore, 117542 — [4]Institute of High Performance Computing, A*STAR, Singapore, 138632

A contemporary frontier of metamaterial research is the challenge non-Hermitian systems pose to the established characterization of topological matter. There, one of the most relied upon principles is the bulk-boundary correspondence (BBC). In Hermitian systems energy eigenvalues and eigenstates exhibit a perturbatively small change as the boundary conditions are modified from periodic to open. The framework of BBC captures the emergence of protected surface states at the boundary of a system with nontrivial bulk topology. In this talk, we present a periodic circuit network, where gain and loss conspire with the violation of reciprocity to affect this principle dramatically and result in the non-Hermitian Skin effect: upon switching from periodic to open boundary conditions, the spectrum changes drastically and all eigenstates localize at one boundary. We experimentally observe this phenomenon for the first time.

[1] T. Helbig et al., arXiv:1907.11562 (2019)

TT 49.5 Wed 18:15 HSZ 103

"Energy stacks" of Quantum Hall transitions in dirty surfaces of topological superconductors — Björn Sbierski[1], •Jonas Karcher[2,3,4], and Matthew Foster[4,5] — [1]Department of Physics, University of California, Berkeley, CA 94720, USA — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]Institut für Theorie der Kondensierten Materie Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [4]Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA — [5]Rice Center for Quantum Materials, Rice University, Houston, Texas 77005, USA

Normally QHPT states occur only at isolated energies; accessing them therefore requires fine-tuning of the electron density or magnetic field. In this work we show that QHPT states can be realized throughout an energy continuum, i.e. as an "energy stack" of critical states wherein each state in the stack exhibits QHPT phenomenology. The stacking occurs without fine-tuning at the surface of a class AIII topological phase, where it is protected by U(1) and time-reversal symmetries. Criticality is diagnosed by comparing numerics to universal results for the longitudinal Landauer conductance and multifractality at the QHPT. Results are obtained from an effective 2D surface field theory and from a bulk 3D lattice model. We demonstrate that the stacking of QHPT states is a robust phenomenon that occurs for AIII topological phases with both odd and even winding numbers. The latter conclusion may have important implications for the still poorly-understood logarithmic conformal field theory believed to describe the QHPT.

TT 49.6 Wed 18:30 HSZ 103

Microscopic theory of fractional excitations in gapless bilayer quantum Hall states: semi-quantized quantum Hall states — •Tobias Meng — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Recent experiments in quantum Hall bilayer systems have revealed a new strongly correlated state: the semi-quantized quantum Hall state. This state arises in a bilayer quantum Hall system with strong interlayer-interactions, has a quantized Hall resistance and vanishing longitudinal resistance, while at the same time featuring a gapless sector that allows this state to exist for a continuum of filling factors. In this talk, I will explain what a semi-quantized quantum Hall state is, and use a coupled-wire construction to predict possible future experiments in the already existing experimental platforms.

TT 49.7 Wed 18:45 HSZ 103

Thermal Hall effect in a Bulk Quantum Hall System $EuMnBi_2$ — •Mohammad Pakdaman[1], Jan Bruin[1], Claus Muehle[1], Xinglu Que[1], Yosuke Matsumoto[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, University of Tokyo, Japan — [3]c Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

The recent observation of a quantum Hall effect in $EuMnBi_2$ is attracting a lot of attention since it is a rare example of quantum Hall physics in a bulk material. Here, the largely suppressed coupling between 2D electron layers is a key. Moreover, the 2D electrons are understood to have a Dirac dispersion, which may help explain their low carrier density and high mobility. In this study, diagonal and nondiagonal thermal conductivity of $EuMnBi_2$ were measured down to 90 mK up to the field range of 14 T. We report a strong thermal Hall effect and a field dependent thermal conductivity that carries signatures of both electronic and magnetic origins. Possible origin and signatures of quantization will be discussed in the talk.

TT 50: Many-Body Localization

Time: Wednesday 18:00–19:00 Location: HSZ 204

TT 50.1 Wed 18:00 HSZ 204

Many-body localization from a one-particle perspective in the disordered 1D Bose-Hubbard model — •Miroslav Hopjan and Fabian Heidrich-Meisner — Institute for Theoretical Physics, University of Göttingen, Germany

We numerically investigate 1D Bose-Hubbard chains with onsite disorder by means of exact diagonalization. Consistent with previous studies, we observe signatures of transition from the ergodic to the many-body localized (MBL) regime when increasing the disorder strength or energy density. Apart form the entanglement entropy as a conventional but indirect measure for the ergodic-MBL transition we utilise the one-particle density matrix (OPDM) to characterize the system [1]. We show that the natural orbitals (the eigenstates of OPDM) are extended in the ergodic phase and real-space localized when one enters into the MBL phase. Furthermore, the distributions of occupancies of the natural orbitals as well as the diagonal part of OPDM (i.e., the site occupancies) can be used as measures of Fock-space localization in the respective basis [2]. Moreover, the full distribution of the densities of the physical particles provides a one-particle measure for the detection of the ergodic-MBL transition which could be directly accessed in experiments with ultra-cold gases.

[1] S. Bera, H. Schomerus, F. Heidrich-Meisner and J.H. Bardarson, PRL 115, 046603 (2015).
[2] M. Hopjan and F. Heidrich-Meisner, in preparation.

TT 50.2 Wed 18:15 HSZ 204

Dynamics of spin chains in the presence of long-range interactions — •Sebastian Wenderoth[1], Seelam Rajagopala[1], Nathan Ng[2], Michael Kolodrubetz[3], Eran Rabani[2], and Michael Thoss[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Freiburg, Germany — [2]Department of Physics and Chemistry, University of California, Berkeley, California, United States — [3]Department of Physics, The University of Texas at Dallas, Richardson, Texas, United States

In many-body localized (MBL) systems local observables do not equilibrate under unitary quantum dynamics and, therefore, these systems cannot be described within the framework of quantum statistical mechanics. Usually, the MBL phase is studied in locally interacting systems with static disorder e.g. a disordered Ising chain with nearest neighbour interactions. [1] Here, we study a disordered Ising chain in which all spins couple to a central d-level system (qudit), which induces spin flip interactions. Employing the multilayer multiconfiguration time-dependent Hartree approach [2,3], we are able to simulate the dynamics of large spin chains in a numerically exact way. Using this approach, we examine dynamical signatures of the localized and thermalizing phases at much larger system sizes than those achievable with exact diagonalization, consistent with having converged to the thermodynamic limit.

[1] A. Pal *et al.*, Phys. Rev. B **82**, 174411 (2010).
[2] O. Vendrell *et al.*, J. Chem. Phys. **134**, 044135 (2011).
[3] H. Wang *et al.*, J. Chem. Phys. **119**, 1289 (2003).

TT 50.3 Wed 18:30 HSZ 204

Entanglement dynamics of a one-dimensional many-body-localized system coupled to a bath — •Elisabeth Wybo, Michael Knap, and Frank Pollmann — Department of Physics, Technische Universität München, James-Franck-Strasse 1, D-85748 Garching, Germany

In isolated, interacting and strongly disordered quantum systems thermalization may break down, leading to a novel many-body localized phase. However, this special phase will be destroyed if the system is not well isolated from the environment. We investigate how many-body localization is destroyed in systems that are weakly coupled to a Markovian environment. In particular, we study entanglement probes like the negativity in quench setups, and determine their typical scaling. To this aim we use both tensor-network and exact-Krylov techniques.

TT 50.4 Wed 18:45 HSZ 204

Dynamical quantum phase transitions and many-body localization in spin chains with quasiperiodic fields — •Leonardo Benini[1], Piero Naldesi[2], Rudolf Roemer[1,3], and Tommaso Roscilde[4] — [1]University of Warwick, Coventry, U.K. — [2]Université Grenoble-Alpes, LPMMC and CNRS, Grenoble, France — [3]Université de Cergy-Pontoise, Institut d'Études Avancées, and LPT, Cergy-Pontoise, France — [4]Université de Lyon, Ens de Lyon, Université Claude Bernard and CNRS, Lyon, France

We study dynamical properties of many-body localized systems through the lens of dynamical quantum phase transitions (DQPTs) theory. We explore the quench dynamics of a one-dimensional Heisenberg model with quasi-periodic on-site magnetic fields, investigating the emergence of singularities in the return rate of the Loschmidt echo both in the strong MBL regime and close to criticality. Quenching from an initially ordered Néel state, we show the appearance of a sequence of DQPTs deep in the MBL phase, periodically distributed along the real-time axis. We then establish a connection between the non-analytic behavior of the dynamical free energy and the oscillations of the spin imbalance. A second quench protocol, which investigates the non-equilibrium dynamics of the system initialized in its ground-state, provides additional insights on the emergence of DQPTs associated with the MBL phase. We develop an experimentally viable criterion to discern between the ergodic and the MBL phase exploiting non-analyticities of the Loschmidt free energy in the short-time dynamics.

TT 51: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Wednesday 18:00–19:00 Location: HSZ 304

TT 51.1 Wed 18:00 HSZ 304

Efficient steady state solver for charge transport through single-molecule junctions — •Christoph Kaspar and Michael Thoss — Albert-Ludwigs-Universität, Freiburg, Germany

The steady state is a fundamental property used to describe the non-equilibrium transport of electrons through single-molecule devices. Its rigorous computation requires highly accurate methods such as the hierarchical quantum master equation approach [1,2]. This method gives access to the systematic inclusion of higher-order contributions resulting in the generalization of perturbative master equation approaches. The major disadvantage of calculating the steady state with this method is the excessive requirement of computational resources, e.g. needed for increasing strength of molecule-lead coupling or many molecular degrees of freedom [3,4]. In this contribution, we present an iterative approach enabling the efficient computation of the steady state for the transport through single-molecule junctions. Besides reducing the required computational time, the main benefit is a drastically decreased memory compared to conventional propagation schemes. We demonstrate the efficiency of our iterative approach on the scenario of a single-molecule junction with many system degrees of freedom.

[1] Jin *et al.*, J. Chem. Phys. **128**, 234703 (2008)
[2] Schinabeck *et al.*, Phys. Rev. B **94**, 201407R (2016)
[3] Hou *et al.*, J. Chem. Phys. **142**, 104112 (2015)
[4] Zhang *et al.*, J. Chem. Phys. **147**, 044105 (2017)

TT 51.2 Wed 18:15 HSZ 304

Low temperature single molecule transport measurements on fullerenes — •Alexander Strobel[1,2], Filip Kilibarda[1,2], Elke Scheer[2], and Artur Erbe[1,2] — [1]Helmhotz Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]University of Konstanz, Faculty of sciences, 78457 Konstanz, Germany

Molecular electronics offers a novel approach, for scaling traditional 3D electronics down to nanoscale dimensions in a quasi 1D system. This approach offers a deeper understanding of the electron transport behavior of molecules. Our research focuses on classifying different molecules with the help of Mechanically Controlled Break Junction (MCBJ) technique. Here we report electrical transport properties of fullerene molecules using a MCBJ setup. Fullerenes with their high stability and symmetry have become reference molecules for the development of measurement routines for molecular electronics applications. Our MCBJ setup enables us to evaporate C60 in situ and measure electrical characteristics under high vacuum conditions. Furthermore, low-temperature measurements down to 6 K are possible. Conductance histograms are recorded to measure the preferred conductance values of single C60 molecules. I-V curves, the differential conductance and inelastic electron tunneling spectra (IETS) are directly and simultaneously measured using lock-in measurement methods. IETS measurements are used to investigate electron-phonon Interactions. The experimental analysis of the charge transport by varying the electrode distance, the bias potential and the electrode metal at different conductance is presented.

TT 51.3 Wed 18:30 HSZ 304

Ab initio study of current-induced forces in nanojunctions — •Susanne Leitherer[1], Nick Papior[2], Jing-Tao Lü[3], and Mads Brandbyge[1] — [1]Department of Physics, Technical University of Denmark — [2]Department of Applied Mathematics and Computer Science, Technical University of Denmark — [3]School of Physics, Huazhong University of Science and Technology, Wuhan, China

In ballistic nanoscale conductors the high current density can lead to substantial changes in the atomic structure, as seen in experiments [1]. We calculate the current-induced forces on the atoms of different models of nanojunctions under a high applied bias voltage, employing first principles electronic structure and transport calculations. Our findings show how the forces on the atoms are related to the chemical bonds, as evidenced in scanning probe experiments exploring currents and forces between two C_{60} molecules [2], as well as the electrostatic potential landscape in the junctions [3]. To study further the dynamical motion of atoms in nanojunctions including current-induced forces, we perform molecular dynamics simulations based on a semi-classical Langevin approach in combination with DFT calculations [4]. This allows us to study the influence of Joule heating, i.e. inelastic scattering by phonons, as well as other contributions to current-induced forces that do not conserve the energy of the atomic motion.

[1] C. Schirm et al., Nat. Nanotechnol. 8, 645-648 (2013)
[2] J. Brand et al., Nano Lett. 19, 7845-7851 (2019)
[3] S. Leitherer et al.,Phys. Rev. B 100, 035415 (2019)
[4] J.T. Lü et al., Manuscript in preparation

TT 51.4 Wed 18:45 HSZ 304

Electrical transport through single polypeptides — •Diana Slawig[1], Nguyen Thi Ngoc Ha[2], Yossi Paltiel[3], Shira Yoshelis[3], and Christoph Tegenkamp[1,2] — [1]Leibniz Universität Hannover, Germany — [2]TU Chemnitz, Germany — [3]Hebrew University Jerusalem, Israel

The analysis of electrical transport through helical molecules gained a lot of interest within the last years, due to the unique spin filtering properties, named chiral induced spin selectivity (CISS) [1]. By utilizing this effect a proof of concept for a new type of chiral-based Si-compatible universal magnetic memory device was demonstrated [2]. Nevertheless, the electrical transport through helical peptides itself is not completely understood yet.

Our study focuses on transport through single lysine doped polyalanine (PA) molecules by means of mechanically controlled break junction. Molecular fragments containing different numbers of monomers were used to evaluate the length dependent transport behavior, leading to a strong indication for a tunneling dominated mechanism.

Based on the high number of observed stable conductance states in the statistical analysis, we propose a ratcheting model based on geometrical alignments of the molecules. This concept is closely related to the interdigitation effect observed by STM[3].

[1] R. Naaman et al., J. Phys. Chem. Lett., 3 (2012)
[2] O.Ben Dor et al., Nat. Commun. 4:2256 (2013)
[3] T. N.H. Nguyen et al., J. Phys. Chem. C 123, 612 (2019)

TT 52: Superconducting Electronics: SQUIDs, Qubits, Circuit QED, Quantum Coherence and Quantum Information Systems 2 (joint session TT/HL)

Time: Thursday 9:30–12:30 Location: HSZ 03

TT 52.1 Thu 9:30 HSZ 03

Waveguide Bandgap Engineering with an Array of Superconducting Qubits — •Jan David Brehm[1], Alexander N. Poddubny[2], Alexander Stehli[1], Tim Wolz[1], Hannes Rotzinger[1,3], and Alexey V. Ustinov[1,4,5] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Institut für Festkörperphysik, Karlsruher Institut für Technologie, Karlsruhe, Germany — [4]National University of Science and Technology MISIS, Moscow, Russia — [5]Russian Quantum Center, Skolkovo, Moscow, Russia

In one dimension the interaction of qubits with free space instead of a cavity gives rise to an effective qubit-qubit coupling which is of infinite range and can be tuned by varying the qubit separation. In this work, we experimentally study an array of eight superconducting transmon qubits with local frequency control, which are all coupled to the mode continuum of a superconducting waveguide. The spacing between adjacent qubits is substantially smaller than the wavelength corresponding to their excitation frequency, eliminating almost completely the coherent exchange type interaction between qubits. By consecutively tuning the qubits to a common resonance frequency we observe the formation of super- and subradiant states as well as the emergence of a bandgap. Furthermore, we study the nonlinear saturation of the collective modes with increasing photon number and electromagnetically induce a transparency window in the bandgap region of the ensemble.

TT 52.2 Thu 9:45 HSZ 03

Employing a real-time processor for experiments with superconducting qubits — •Richard Gebauer[1], Nick Karcher[1], Alexey V. Ustinov[2,3], Martin Weides[2,4], Marc Weber[1], and Oliver Sander[1] — [1]Institute for Data Processing and Electronics, KIT, Karlsruhe, Germany — [2]Physikalisches Institut, KIT, Karlsruhe, Germany — [3]Russian Quantum Center, National University of Science and Technology MISIS, Moscow, Russia — [4]School of Engineering, University of Glasgow, Glasgow, United Kingdom

The control of superconducting quantum bits (qubits) relies on the ability to read out their state with high precision and apply custom pulses on the nanosecond timescale. As the field progresses, experiment schemes tend to get more complicated once the number of pulses increases, complex parameter changes are necessary and further data processing is needed. Conventional setups consisting of arbitrary waveform generators and digitizers connected to a measurement computer are not ideally suited to cope with this increased complexity.

A faster and more flexible solution is FPGA-based electronics. It not only dramatically reduces costs and space requirements but also simplifies measurements and enables customized control schemes like quantum feedback. Combined with a real-time processor, complex experiment flows and online data processing render possible.

We will present our platform to control and readout superconducting qubits with a focus on the real-time processing subsystem. Furthermore, we will show multiple experimental applications where the real-time processor is utilized, like evaluating correlation functions.

TT 52.3 Thu 10:00 HSZ 03

High power dispersive qubit readout and state preparation without parametric amplifier — •Martin Spiecker[1], Daria Gusenkova[1], Richard Gebauer[2], Lukas Grünhaupt[1], Patrick Winkel[1], Francesco Valenti[1,2], Ivan Takmakov[1,2,3], Dennis Rieger[1], Alexey V. Ustinov[1,4], Wolfgang Wernsdorfer[1,3,5], Oliver Sander[2], and Ioan M. Pop[1,3] — [1]Physikalisches Institut, KIT, Germany — [2]Institute for Data Processing and Electronics, KIT, Germany — [3]Institute of Nanotechnology, KIT, Germany — [4]Russian Quantum Center, MISIS, Moscow, Russia — [5]Institute Neel, CNRS, Grenoble, France

High-fidelity qubit readout is an essential requirement for fault-tolerant quantum algorithms. In theory, within the dispersive readout scheme, the state discrimination can be improved significantly if the resonator's photon population increases [1]. However, in practice the optimal photon number does usually not exceed 2.5 photons [2], and parametric amplifiers are needed to achieve a substantial signal-to-noise ratio.
In order to investigate the limitations of the readout fidelity we used a fluxonium qubit with a granular aluminum superinductance [3] having the advantage of reduced nonlinearity in comparison to previously used Josephson junction arrays. We demonstrate qubit measurements without a parametric amplifier at readout powers corresponding up to 200 photons in the resonator.

[1] A. Blais et al., PRA 69(6), 062320 (2004)
[2] T. Walter et al., PRA 7.5, 054020 (2017)
[3] L. Grünhaupt and M. Spiecker et al., Nat. Mater. 18, 816-819 (2019)

TT 52.4 Thu 10:15 HSZ 03

Experimental violation of the standard quantum limit for parametric amplification of broadband signals — •K. Fedorov[1,2], M. Renger[1,2], S. Pogorzalek[1,2], C. Scheuer[1,2], Q. Chen[1,2], Y. Nojiri[1,2], M. Partanen[1], 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]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Phase-preserving amplification is a crucial part of many protocols in microwave quantum information processing, such as quantum teleportation, remote state preparation [1], or dispersive qubit readout. Josephson parametric amplifiers (JPAs) allow amplification close to the standard quantum limit (SQL), implying a fundamental bound of 50 % for the maximal quantum efficiency η for amplification of narrowband input signals. We demonstrate that the SQL does not hold for broadband input signals and experimentally find $\eta = 70\,\%$ with an amplification chain consisting of a JPA and a cryogenic HEMT amplifier. We show that η can reach 100 % and experimentally is limited by the Poissonian fluctuations in the JPA pump line.

We acknowledge support by Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (GrantNo.820505).

[1] S. Pogorzalek *et al.*, Nat. Commun. **10**, 2604 (2019).

TT 52.5 Thu 10:30 HSZ 03

Optimal control of a compact 3D quantum memory — Julia Lamprich[1,2], Stephan Trattnig[1,2], •Yuki Nojiri[1,2,3], Qiming Chen[1,2,3], Stephan Pogozarek[1,2], Michael Renger[1,2,3], Kirill Fedorov[1,2,3], Achim Marx[1,3], Matti Partanen[1,3], Frank Deppe[1,2,3], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Walther-Meißner-Strasse 8, D-85748 Garching, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany

Quantum memories are of high relevance in the context of quantum computing and communication. For building scalable architectures based on superconducting quantum circuits, 3D cavities are promising candidates for a quantum memory. Recently, a compact layout exploiting the multimode structure of a rectangular 3D cavity has been demonstrated [1]. In that work, the fidelity of the transfer process was also limited by state leakage. This can be overcome by pulse shaping using optimal control strategies [2]. Henceforth, we implement a search algorithm (CMA-ES) to find optimized pulses promising higher gate fidelities, and present first experimental results.

We acknowledge support by the Germany's Excellence Strategy EXC-2111-390814868, Elite Network of Bavaria through the program ExQM, and the European Union via the Quantum Flagship project QMiCS (Grant No. 820505).

[1] E. Xie et al., Appl. Phys. Lett. 112, 202601 (2018).
[2] Shai Machnes et al., Phys. Rev. Lett. 120, 150401 (2018)

TT 52.6 Thu 10:45 HSZ 03

Quasiclassical Green's Function Approach to Normal-Metal Quasiparticle Traps — •Raphael Schmit and Frank Wilhelm — Saarland University, Theoretical Physics Department

Superconducting qubits, such as the charge or the flux qubit, are thought to store the information needed for quantum information processing. However, unwanted interactions with the qubit's environment lead to decoherence of the qubit and thus information loss. In addition to these extrinsic sources for decoherence, there is also an intrinsic one: the coupling between the qubit and the non-equilibrium quasiparticle excitations in the superconductor the qubit is made of. Decoherence is due to quasiparticle tunneling through a Josephson junction, but there is also an inhomogeneous broadening caused by changes in the occupations of Andreev states in the junction. Both mechanisms are highly depending on the location of the quasiparticles: quasiparticles far away from junctions have much less contribution to decoherence than the ones close to it. While it is difficult to prevent the generation of quasiparticles, trapping them in less active regions of the device seems to provide a practicable way to improve the device performance.

We are aiming to establish a quantitative theory of normal-metal traps simply consisting of an island of normal metal which is in good metallic contact with the superconductor. To do so, we are applying a Green's function formalism - the Keldysh technique in the dirty limit with a quasiclassical approximation - to investigate the properties of non-equilibrium quasiparticles in mesoscopic devices.

TT 52.7 Thu 11:00 HSZ 03

Transmission spectra of an ultrastrongly coupled qubit-dissipative resonator system — •Luca Magazzù and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We calculate the transmission spectra of a flux qubit coupled to a dissipative resonator in the ultrastrong coupling regime. Such a qubit-oscillator system constitutes the building block of superconducting circuit QED platforms. The calculated transmission of a weak probe field quantifies the response of the qubit, in frequency domain, under the sole influence of the oscillator and of its dissipative environment, an Ohmic heat bath. We find the distinctive features of the qubit-resonator system, namely two-dip structures in the calculated transmission, modified by the presence of the dissipative environment. The relative magnitude, positions, and broadening of the dips are determined by the interplay among qubit-oscillator detuning, the strength of their coupling, and the interaction with the heat bath.
[1] L. Magazzù and M. Grifoni, J. Stat. Mech. 104002 (2019).

15 min. break.

TT 52.8 Thu 11:30 HSZ 03

Diagrammatic Resummation Theory Approach to Few-Photon Scattering and Dynamics in Waveguide QED — •Kiryl Piasotski and Mikhail Pletyukhov — RWTH Aachen University, Germany

In the present talk, the diagrammatic resummation theory approach to the problems of multi-photon scattering and dynamics in the single-qubit waveguide QED is presented. It is shown that within the rotating wave approximation, irrespectively of the number of radiation channels, dispersion of the modes they are supporting, and the nature of the radiation-qubit coupling, the determination of both scattering and dynamical observables in the subspace of the fixed excitation number, is reducible to a solution of the closed finite system of linear integral equations. Further, the above described theoretical machinery is showcased on the number of problems regarding the systems with delayed coherent quantum feedback, namely it is shown how the formalism could be applied to determine the coherence functions of radiation within the scattering setup, as well as the determination of certain dynamical characteristics of non-Markovian waveguide QED systems.

TT 52.9 Thu 11:45 HSZ 03

Josephson-Photonics Devices as a Source of Entangled Microwave Photons — •Björn Kubala[1], Ambroise Peugeot[2], Simon Dambach[1,3], Juha Leppäkangas[4], Marc Westig[2], Gerbold Menard[2], Yuri Mukharsky[2], Carles Altimiras[2], Patrice Roche[2], Philippe Joyez[2], Denis Vion[2], Daniel Esteve[2], Fabien Portier[2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Germany — [2]SPEC, CEA Paris-Saclay, France — [3]School of Physics and Astronomy, University of Nottingham, UK — [4]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

The realization and characterization of efficient sources of entangled microwave photons is of paramount importance for many future applications of quantum technology. Josephson-photonics devices are very promising candidates for this task since they allow one to create a broad range of different entangled states in a surprisingly simple and robust way. Such devices consist of a dc-voltage-biased Josephson junction which is placed in series to several microwave cavities. Steady states with multifaceted entanglement properties then appear in steady state resulting from the interplay of multiphoton creation processes associated with the inelastic tunneling of Cooper pairs and subsequent individual photon leakage from the cavities. In this talk, we present a detailed theoretical study of the bipartite entanglement between photon pairs in the output transmission lines. Numerical simulations, taking into account low-frequency fluctuations of the bias voltage and the finite bandwidth of microwave signal detectors, show excellent agreement with recent experimental data.

TT 52.10 Thu 12:00 HSZ 03

Theory of injection locking for the Josephson laser — •Ciprian Padurariu, Lukas Danner, Björn Kubala, and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, 89069 Ulm, Germany

An intriguing recent experiment [1] has observed features of lasing in the microwave emission of a cavity driven by inelastic Cooper pair tunneling across a dc-voltage biased Josephson junction. A successful theory was developed explaining the emission in the lasing regime [2], however, the theory of injection locking remained unexplained.
Here, we provide the theory for injection locking in Josephson photonic devices. Specifically, we provide an analytical derivation of the phenomenological Adler equation for a large class of Josephson devices. We extract detailed guidelines for designing circuits capable of locking the phase against noises and estimate the rate of thermal and quantum phase slips that limit the locking precision.
The work aims at providing the missing ingredient, phase-stabilized Josephson oscillations, required to demonstrate the quantum entanglement of the emitted microwave light.
[1] M.C. Cassidy et al., Science 355, 939 (2017).
[2] S. Simon and N. Cooper, Phys. Rev. Lett. **121**, 027004 (2018).

TT 52.11 Thu 12:15 HSZ 03

Electron transport and spin qubit manipulation with surface acoustic waves — •Mikel Olano[1] and Geza Giedke[1,2] — [1]Donostia International Physics Center, Donostia, Spain — [2]Ikerbasque Foundation for Science, Bilbao, Spain

Spin qubits in quantum dots are among the most promising systems for the implementation of quantum computation. While coherence times and gate operation times have become very competitive, the realization of long-range interactions to enable more flexible quantum gates remains a challenge.

Here we investigate theoretically an approach to tackle this problem using a moving electrons trapped in the potential of a surface acoustic wave, that serves as an intermediary between distant stationary quantum dots.

We analyse the coherent transport and transfer of spin qubits between stationary and moving dots and quantum gates between two interacting spin qubits. Applications for the generation of multipartite entanglement and joint measurement of several qubits are discussed. The talk will highlight the parameters to be taken into account if these processes are to be optimized. The impact of the main sources of decoherence and non-adiabatic behaviour due to the time-dependence of the potential are discussed.

TT 53: Topology: Majorana Physics

Time: Thursday 9:30–13:15 Location: HSZ 103

TT 53.1 Thu 9:30 HSZ 103

Finite-size effects in the in-gap bands of artificial spin chains on superconductors — •Lucas Schneider, Philip Beck, Levente Rózsa, Jens Wiebe, and Roland Wiesendanger — Department of Physics, Hamburg University, 20355 Hamburg, Germany

Magnetic chains on superconducting substrates are a promising system to realize topological superconductivity and Majorana bound states [1-5]. In this study, we use the tip of a scanning tunneling microscope to assemble magnetic chains atom-by-atom on the surface of an elemental superconductor and study the formation of multiple in-gap bands with increasing chain length. We observe different pronounced effects due to the finite length and an even or odd number of atoms in the chain. Furthermore, the symmetry of the underlying substrate offers multiple building directions with different inter-atomic spacings which enables to tune the electronic and magnetic interactions within the chain.

We acknowledge funding by the ERC via the Advanced Grant ADMIRE (No. 786020) and by the Cluster of Excellence 'Advanced Imaging of Matter' (EXC 2056 - project ID 390715994).

[1] Klinovaja *et al.*, PRL **111**, 186805 (2013)
[2] J. Li *et al.* PRB **90**, 235433 (2014)
[3] S. Nadj-Perge *et al.*, Science **346**, 6209 (2014)
[4] M. Ruby *et al.*, Nano Letters **17**, 4473, (2017)
[5] H. Kim *et al.*, Science Advances **4**, eaar5251 (2018).

TT 53.2 Thu 9:45 HSZ 103

High-Temperature Majorana Fermions in Magnet-Superconductor Hybrid Systems — Daniel Crawford[1], Eric Mascot[2], Dirk Morr[2], and •Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Parkville, VIC 3010, Australia — [2]University of Illinois at Chicago, Chicago, IL 60607, USA

Magnet-superconductor hybrid structures represent one of the most promising platforms to realize, control and manipulate Majorana modes using scanning tunneling methods. By depositing either chains or islands of magnetic atoms on the surface of a conventional superconductor such as Pb or Re, topological superconducting phases can emerge. They feature either localised Majorana bound states at the chain ends or dispersing chiral Majorana modes at the island's boundary. Yet many of these experiments have not reached the spectral resolution to clearly distinguish between topological Majorana and trivial Shiba peaks due to tiny gap sizes in experiments performed at sub-Kelvin temperatures. Here we consider superconducting substrates with unconventional spin-singlet pairing, including high-temperature d-wave and extended s-wave superconductors. We derive topological phase diagrams and compute edge states for cylinder and island geometries and discuss their properties. Also various time-reversal invariant topological superconducting phases of the Zhang-Kane-Mele type are found and discussed. Quite generally, we find that unconventional superconducting substrates work as well as the conventional s-wave substrates to realize topological superconducting phases.

TT 53.3 Thu 10:00 HSZ 103

Topological superconductivity of adatom chains as probe for unconventional pairing — •Andreas Kreisel[1], Timo Hyart[2], and Bernd Rosenow[1] — [1]Institut für Theoretische Physik, Universität Leipzig — [2]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences

Chains of magnetic atoms on the surface of s-wave superconductors, have been established as a laboratory for the study of Majorana bound states. In such systems, the breaking of time reversal due to magnetic moments makes the system a one-dimensional topological superconductor. However, in unconventional superconductors even nonmagnetic impurities can induce in-gap states since scattering of Cooper pairs changes their momentum but not their phase. Here, we propose a novel paradigm for creating topological superconductivity, which is based on an unconventional superconductor with a chain of nonmagnetic impurities on its surface. The system can be driven into the topological phase by tuning magnitude and direction of an external Zeeman field. We show that the topological energy gap can approach the minimum of the bulk energy gap. We develop a general mapping of films with impurity chains in multiband superconductors to one-dimensional lattice Hamiltonians. This allows us to illustrate the feasibility of our proposal in the case of the material Sr_2RuO_4 , and to demonstrate that the study of impurity chains can be employed as a diagnostic tool for the nature of the pairing symmetry. This enables to distinguish competing proposals for the pairing symmetry in Sr_2RuO_4.

TT 53.4 Thu 10:15 HSZ 103

Linear and non-linear transport in a finite Kitaev chain — •Nico Leumer[1], Bhaskaran Muralidharan[2], Magdalena Marganska[1], and Milena Grifoni[1] — [1]University of Regensburg — [2]Indian Institute of Technology Bombay

The Kitaev chain is an archetypal model for one dimensional topological superconductivity and known for the emergence of so-called Majorana fermions [1, 2]. These states yield a $2e^2/h$ signature in the conductance of a transport set up.

We study in depth both linear and non-linear transport across a finite Kitaev chain. The simplicity of the Kitaev chain allows us an exact and analytical treatment for the spectrum [3], its eigenstates as well as of the Green's function matrix elements necessary for the transport calculations. Setting up the transport formulation of the finite Kitaev chain via the non-equilibrium Green's function approach, we identify the transport signatures arising from Majorana zero modes and generic ultra low-lying excitations. We show that the coupling to the contacts changes the signatures as well as modulates the topological phase diagram of the Majorana zero modes, when compared with that of a pristine wire. Further, precise quantization of conductance is only found along contact-broadened Majorana lines; the latter sustain exact MZMs in the finite, isolated Kitaev chain. In exploring the non-linear transport, we note clearly the contributions from the Andreev, the direct transfer and the crossed Andreev processes to the currents.

[1] A. Y. Kitaev, Phys. Usp. 44, 131 (2001)
[2] R. Aguado, Riv. Nuovo Cimento 40, 16 (2017)
[3] N. Leumer et al., arXiv:1909.10971

TT 53.5 Thu 10:30 HSZ 103

Time scales for charge-transfer based operations on Majorana systems — •Rubén Seoane Souto[1,2], Karsten Flensberg[2], and Martin Leijnse[1,2] — [1]Division of Solid State Physics and NanoLund, Lund University, Box 118, S-22100 Lund, Sweden — [2]Center for Quantum Devices and Station Q Copenhagen, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

By now, there has been a lot of evidence of the existence of Majorana fermions at the ends of topological superconductors (TSs) [1]. However, a definitive proof of their topological origin will rely on the demonstration of their non-abelian statistics, which emerge after the exchange of two or more Majorana fermions. As an alternative, they can be also demonstrated using charge-transfer based operations, where the charge of a quantum dot (QD) is transferred to two TSs [2].

In this presentation I will analyze the efficiency of charge-transfer based operations between a QD and to two TSs [3], setting bounds to the manipulation time scales. The lower bound depends on the phase difference, due to a partial decoupling of the different parity sectors. In contrast, the upper bound is determined by poisoning processes due to the tunneling of quasiparticles to the MBSs. Using realistic parameters, we find that operations can be performed with a fidelity close to unity in the ms to μs timescales, demonstrating the absence of dephasing and accumulated dynamical phases.

[1] R. Lutchyn et al., Nat. Rev. Mat. 3, 52 (2019)
[2] K. Flensberg, Phys. Rev. Lett. 106, 090503 (2011)
[3] R. Seoane Souto, K. Flensberg and M. Leijnse, arXiv:1910.08420

TT 53.6 Thu 10:45 HSZ 103

Transport signatures of topological superconductivity in HgTe-based quantum wells — •Elena G. Novik[1,2], Björn Trauzettel[3], and Patrik Recher[4,5] — [1]Dresden High Magnetic Field Laboratory, HZDR, Dresden — [2]Institute of Theoretical Physics, Technische Universität Dresden — [3]Institute of Theoretical Physics and Astrophysics, University of Würzburg — [4]Institute for Mathematical Physics, TU Braunschweig — [5]Laboratory for Emerging Nanometrology Braunschweig

We investigate transport through a normal-superconductor junction composed of a quantum spin Hall insulator with helical edge channels and a chiral topological superconductor (TSC) made of the same material in contact to an s-wave bulk superconductor and subjected to a magnetic field. Using the extended two-dimensional Bernevig-Hughes-Zhang model (including axial spin symmetry breaking terms, induced s-wave superconductivity and a Zeeman field) in a ribbon geometry we show that the emergence of the TSC is represented by regions of conductance quantization at zero energy being either $4e^2/h$ in a trivial phase of the TSC or $2e^2/h$ being the indication of a non-trivial phase for the TSC. The latter phase can be traced back to Majorana bound states appearing at the NS interface in this ribbon geometry. These features occur only inside the two-dimensional topological non-trivial phase with non-zero Chern number when the sample width largely exceeds the extent of the chiral Majorana edge channels which is on the order of the superconducting coherence length.

TT 53.7 Thu 11:00 HSZ 103

Long-lived Polaronic Majorana Edge Correlation via Non-Markovianity — •Oliver Kästle[1], Ying Hu[2], and Alexander Carmele[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik von Halbleitern, Technische Universität Berlin, 10623 Berlin, Germany — [2]State Key Laboratory of Quantum Optics and Quantum Optics Devices, Institute of Laser Spectroscopy, Shanxi University, Taiyuan, Shanxi 030006, China

Majorana fermions of 1D wires are a hot topic, which is motivated by the interest to use topology as a way to make quantum systems robust against microscopic imperfections. However, it has been shown that quantum correlations between Majorana states will rapidly decay when the system is coupled to a Markovian bath, even when it preserves parity [1, 2]. Here we go beyond the Markovian approximation and study the dynamics of Majorana edge correlation in the presence of dissipation. Taking the example of an ideal Kitaev chain coupled to a phonon bath, we derive a second-order perturbative polaron master equation. We find that the inclusion of a memory kernel can lead to significant suppression of the decoherence of Majorana edge correlations, thanks to the time-dependent system correlations counteracting the dissipation effect in the weak coupling regime. Moreover, we find that the presence of a next-to-nearest-neighbour interaction can provide an additional mechanism for stabilizing the edge correlations.

[1] Ying Hu, Zi Cai, M. A. Baranov, and P. Zoller, Phys. Rev. B 92, 165118 (2015)
[2] A. Carmele, M. Heyl, C. Kraus, and M. Dalmonte, Phys. Rev. B 92, 195107 (2015).

15 min. break.

TT 53.8 Thu 11:30 HSZ 103

Interacting Majorana modes at surfaces of noncentrosymmetric superconductors — •Janna Elisabeth Rückert, Gergö Roósz, and Carsten Timm — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Noncentrosymmetric superconductors with line nodes are expected to possess topologically protected flat zero-energy bands of surface states, which can be described as Majorana modes. We investigate their fate if residual interactions beyond BCS theory are included. For a minimal square-lattice model with a plaquette interaction, we find string-like integrals of motion that form Clifford algebras and lead to exact degeneracies. By mapping the Majorana model onto two decoupled spin compass models we can further analyse the gap above the ground state. Moreover, we compare the topological properties of the interacting Majorana model to those of the toric-code model. The Majorana model has long-range entangled ground states that differ by $\mathbb{Z}_2$ fluxes through the system on a torus. We find that the ground states exhibit string condensation similar to the toric code but that the topological order is not robust.

TT 53.9 Thu 11:45 HSZ 103

Minimal models of interacting Majorana modes — •Gergo Roosz, Carsten Timm, and Janna Rückert — TU Dresden

In this talk we investigate flat-band Majorana systems with plaquette interactions. At first the possible experimental realizations are briefly summarized. Then a mapping to quantum compass models is given. With the help of this mapping certain ladder systems can be solved exactly, we discuss here these integrable ladders. With the help of the integrable ladder systems, numerical exact diagonalization of small two dimensional systems and the representation theory of Clifford algebras we obtain the ground state degeneracy.

TT 53.10 Thu 12:00 HSZ 103

Majorana-Kondo interplay in T-shaped double quantum dots — •Piotr Majek[1], Krzysztof P. Wójcik[2,3], and Ireneusz Weymann[1] — [1]Faculty of Physics, Adam Mickiewicz University, ul. Uniwersytetu Poznańskiego 2, 61-614 Poznań, Poland — [2]Physikalisches Institut, Universität Bonn, Nussallee 12, D-53115 Bonn, Germany — [3]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland

In this contribution, the electrical transport properties of a T-shaped double quantum dot side-coupled to a topological superconducting nanowire hosting Majorana zero-energy modes are considered theoretically by using the numerical renormalization group method. The corresponding spectral functions and linear response conductance are calculated as a function of model parameters and temperature. In the absence of coupling to Majorana wire, the double dot system exhibits the two-stage Kondo effect, where suppression of conductance at low temperatures is observed. It is shown that the coupling to Majorana wire gives rise to quantum interference, which suppresses the second stage of the Kondo screening in one of the spin channels. As a consequence, we find that the low-temperature conductance becomes equal to $e^2/2h$ in the case of long Majorana wires. On the other hand, for shorter wires, the overlap between Majorana quasiparticles develops, suppressing the quantum interference and restoring the two-stage Kondo effect. This work was supported by the National Science Centre in Poland through the Project No. DEC-2018/29/B/ST3/00937.

TT 53.11 Thu 12:15 HSZ 103

Majorana wires coupled to s-wave superconductors with vortices — •Alexander Nikolaenko[1,2] and Falko Pientka[2] — [1]Karazin Kharkiv National University, Kharkiv 61022, Ukraine — [2]Max Planck Institute for the Physics of Complex Systems,Nöthnitzer Str. 38, 01187 Dresden, Germany

One-dimensional systems proximity-coupled to a superconductor can be driven into a topological superconducting phase by an external magnetic field. Here, we investigate the effect of vortices created by the magnetic field in a type-II superconductor providing the proximity effect. We identify different ways in which the topological protection of Majorana modes can be compromised and discuss strategies to circumvent these detrimental effects. Our findings are also relevant to topological phases in proximitized quantum Hall edge states.

TT 53.12 Thu 12:30 HSZ 103

On-demand thermoelectric generation of equal-spin Cooper pairs — Felix Keidel[1], •Sun-Yong Hwang[2], Björn Trauzettel[1,3], Björn Sothmann[2], and Pablo Burset[4] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [4]Department of Applied Physics, Aalto University, 00076 Aalto, Finland

Superconducting spintronics is based on the creation of spin-triplet Cooper pairs in ferromagnet-superconductor (F-S) hybrid junctions. Manipulation of spin-polarized supercurrents typically requires the ability to carefully control magnetic materials. We here propose a quantum heat engine that generates equal-spin Cooper pairs and drives supercurrents on-demand without manipulating magnetic components. Our proposal is based on a S-F-S junction, connecting two leads at different temperatures, on top of the helical edge of a two-dimensional topological insulator. Remarkably, only crossed Andreev reflections contribute to the charge current while electron cotunneling is responsible for the heat flow to the cold lead. Such a purely nonlocal Andreev thermoelectric effect injects spin-polarized Cooper pairs at the superconductors producing a supercurrent that can be switched on/off by tuning their relative phase.

TT 53.13 Thu 12:45 HSZ 103

Quantum phases of a one-dimensional Majorana-Bose-Hubbard model — •Ananda Roy[1], Johannes Hauschild[1,2], and Frank Pollmann[1] — [1]Department of Physics, Technical University Munich — [2]Department of Physics, University of California, Berkeley

Majorana zero modes (MZM-s) occurring at the edges of a 1D, p-wave, spinless superconductor, in absence of fluctuations of the phase of the superconducting order parameter, are quintessential examples of topologically-protected zero-energy modes occurring at the edges of 1D symmetry-protected topological phases. In this work, we numerically investigate the fate of the topological phase in the presence of phase-fluctuations using the density matrix renormalization group (DMRG) technique. To that end, we consider a one-dimensional array of MZM-s on mesoscopic superconducting islands at zero temperature. Cooper-pair and MZM-assisted single-electron tunneling, together with finite charging energy of the mesoscopic islands, give rise to a rich phase-diagram of this model. We show that the system can be in either a Mott-insulating phase, a Luttinger liquid (LL) phase of Cooper-pairs or a second gapless phase. In contrast to the LL of Cooper-pairs, this second phase is characterized by nonlocal string correlation functions which decay algebraically due to gapless charge-e excitations. The three phases are separated from each other by phase-transitions of either Kosterlitz-Thouless or Ising type. Using a Jordan-Wigner transformation, we map the system to a generalized Bose-Hubbard model with two types of hopping and use DMRG to analyze the different phases and the phase-transitions.

TT 53.14 Thu 13:00 HSZ 103

(Super)symmetry in the Sachdev-Ye-Kitaev model — •Jan Behrends[1] and Benjamin Béri[1,2] — [1]T.C.M. Group, Cavendish Laboratory, University of Cambridge, J.J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom — [2]DAMTP, University of Cambridge, Wilberforce Road, Cambridge, CB3 0WA, United Kingdom

Supersymmetry is a powerful concept in quantum many-body physics. It helps to illuminate ground state properties of complex quantum systems and gives relations between correlation functions. In this work, we show that the Sachdev-Ye-Kitaev model, in its simplest form of Majorana fermions with random four-body interactions, is supersymmetric. In contrast to existing explicitly supersymmetric extensions of the model, the supersymmetry we find requires no relations between couplings. The type of supersymmetry and the structure of the supercharges are entirely set by the number of interacting Majorana modes, and are thus fundamentally linked to the model's Altland-Zirnbauer classification. The supersymmetry we uncover has a natural interpretation in terms of a one-dimensional topological phase supporting Sachdev-Ye-Kitaev boundary physics, and has consequences away from the ground state, including in q-body dynamical correlation functions. This talk will not only illuminate the role of supersymmetry, but also the underlying Altland-Zirnbauer classes that have been previously overlooked.

TT 54: Fe-based Superconductors

Time: Thursday 9:30–13:15 Location: HSZ 201

TT 54.1 Thu 9:30 HSZ 201

Many-body interaction in iron-based superconductors — •Jörg Fink[1,2,3], Emile Rienks[4], Jörn Bannies[2], Sabine Wurmehl[1], Saicharan Aswartham[1], Igor Morozov[1], Luis Craco[1], Helge Rosner[2], Claudia Felser[2], and Bernd Büchenr[1,3] — [1]IFW Dresden — [2]MPI Chemical Physics of Solids, Dresden — [3]TU Dresden — [4]HZB Berlin

In this talk we will report on the determination of the energy and momentum dependence of scattering rates in iron-based superconductors using angle-resolved photoemission spectroscopy. We receive information on the location of hot spots on the Fermi surface determining antiferromagnetism and superconductivity as well as on cold spots determining the normal state transport and optical properties. For the hole doped compounds, we obtain scattering rates well above the Planckian limit, indicating a highly incoherent normal state electronic structure. In this way we obtain a microscopic understanding of the electronic structure of these systems in the normal and in the superconducting state. The experimental results on ferropnictides are compared with DFT+DMFT calculations describing Hunds metal behavior. There are remarkable differences between theory and experiment. The reason for this is possibly that DFT+DMFT uses only local correlation effects and does not include non-local spin fluctuation excitations.

TT 54.2 Thu 9:45 HSZ 201

DMFT study of Hund's metals: the charge response of Fe-based superconductors — •Alexander Kowalski — Institut für Theoretische Physik und Astrophysik, Universität Würzburg

We investigate various multi-orbital Hubbard models for iron-based superconductors, from a five-orbital Wannier-based Hamiltonian of $BaFe_2As_2$ down to simpler three- and two-orbital descriptions. These systems have previously been analyzed using techniques such as slave-spin mean field [1], which have shown the existence of a Hund-driven strongly-correlated phase close in doping to the half-filled Mott transition. Our DMFT calculations using a continuous-time quantum Monte Carlo solver for one- and two-particle quantities [2] reveal the presence of regions of phase separation with diverging charge compressibility.

[1] L. de' Medici, Phys. Rev. Lett **118**, 167003 (2017)
[2] M. Wallerberger, A. Hausoel, P. Gunacker, A. Kowalski, N. Parragh, F. Goth, K. Held, G. Sangiovanni, Comput. Phys. Commun. **235**, 388 (2019)

TT 54.3 Thu 10:00 HSZ 201

Impurity-induced bound states in Fe-based superconductors with spin-orbit coupling — •Peayush Choubey and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

We investigate the effects of residual spin-orbit coupling (SOC), inherently present in Fe-based superconductors (FeSCs), and consequent admixture of singlet and triplet Cooper-pairing in the even parity channel in the superconducting state, on the in-gap bound states induced by point-like, magnetic and non-magnetic impurities. Using low-energy models, which capture all the symmetries of FeSCs and treat the atomic SOC consistently, we solve the impurity scattering problem in the T-matrix framework. We find that if $s_\pm$ pairing state has a significant triplet contribution at the electron pockets around $M = (\pi, \pi)$-point, the impurity-induced bound states are robust against the out-of-plane Zeeman field. The heavily suppressed Zeeman splitting of impurity states is a consequence of reduction in effective Landé g-factor caused by atomic SOC.

TT 54.4 Thu 10:15 HSZ 201

Tracking nematic fluctuations using the Nernst effect in iron based superconductors — •Christoph Wuttke[1], Federico Caglieris[1], Steffen Sykora[1], Frank Steckel[1], Xiaochen Hong[1], Seunghyun Kim[1], Rhea Kappenberger[1], Saicharan Aswartham[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 role of nematic fluctuations, shown to be present across the phase diagram of iron based superconductors, especially their correlation with possible quantum critical points and high temperature superconductivity, has been under constant debate. Here we show that the Nernst coefficient is sensitive to the nematic fluctuations in iron based superconductors. We detect a similar behavior of the Nernst effect and elastoresistivity measurements in Co doped LaFeAsO while a difference of these probes can be obtained in Rh doped $BaFe_2As_2$. In both materials the Nernst effect is tracking the superconducting dome upon doping, providing evidence for superconductivity supported by nematic fluctuations.

TT 54.5 Thu 10:30 HSZ 201

Elasto-Nernst effect: a sensitive probe for nematicity — •Federico Caglieris[1], Xiaochen Hong[1], Michael Wissmann[1], Christoph Wuttke[1], Steffen Sykora[1], Rhea Kappenberger[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Institut für Festkörperphysik, TU Dresden, 01069 Dresden — [3]Center for Transport and Devices, TU Dresden, 01069 Dresden, Germany

The discovery of a divergent elasto-resistivity in iron-based superconductors promoted the nematicity to the class of the electronic orders together with superconductivity and density-waves, supporting the intriguing idea of an intimate link among all electronic instabilities. In this work we investigate the nematic phenomenology in different families of iron-based superconductors using a novel technique, which combines a state-of-art setup for Nernst effect measurements with a piezoelectric device for the application of uniaxial strain. By studying the temperature-dependence of the strain-derivative of the Nernst coefficient, we discovered that a Curie-Weiss-like fashion governs also the elasto-Nernst effect, as a fingerprint of strong nematic fluctuations. However, despite the universal diverging behavior, we show that elasto-Nernst and elasto-resistivity are not equivalently representative of the nematic susceptibility, offering a new insight into the nematic puzzle. Moreover, the emerging scenario provides an evidence of a band-dependent nematicity.

TT 54.6 Thu 10:45 HSZ 201

^{75}As NMR under uniaxial pressure in $BaFe_2As_2$ — •Adam P. Dioguardi[1], Tobias Schorr[1], Clifford W. Hicks[2], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,3], and Hans-Joachim Grafe[1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Institut für Festkörperphysik, TU Dresden, 01062 Dresden, Germany

We have conducted systematic ^{75}As nuclear magnetic resonance (NMR) experiments in $BaFe_2As_2$ under controlled conditions of uniaxial pressure. We find that the electric field gradient (EFG), spin-lattice relaxation rate T_1^{-1}, spin-spin relaxation rate T_2^{-1} and Knight shift K at the As site are sensitive to applied uniaxial pressure. We find that uniaxial pressure increases, broadens, and separates the Néel temperature T_N and the tetragonal-to-orthorhombic structural transition T_S. Our spectral measurements in the magnetic state exhibit no evidence of a predicted spin reorientation for both positive and negative applied uniaxial pressure up to the point of sample failure.

TT 54.7 Thu 11:00 HSZ 201

Unconventional superconductivity and electronic structure of ultra-pure single crystal YFe_2Ge_2 — •Jiasheng Chen[1], Jordan Baglo[1,2], Keiron Murphy[1], Devashibhai Adroja[3], Pabitra Biswas[3], Jacintha Banda[4], Manuel Brando[4], and Malte Grosche[1] — [1]Cavendish Laboratory, Cambridge, UK — [2]Université de Sherbrooke, Canada — [3]ISIS Neutron and Muon Source Science, RAL, UK — [4]MPI CPfS, Dresden, Germany

The layered iron-based superconductor YFe_2Ge_2 exhibits an unusually high Sommerfeld coefficient of $\sim$ 100 mJ/molK^2 and a T$^{3/2}$ temperature dependence of electrical resistivity at low temperature [1-3], indicating strong electronic correlations. While superconductivity in YFe_2Ge_2 is widely observed below $T_c \sim$ 1.9 K in electric transport measurements, it is strongly suppressed by lattice disorder [1-3], hinting at an unconventional pairing mechanism.

Our new generation of single crystals reach residual resistivity ratios (RRR) in excess of 650. These crystals display a sharp superconducting heat capacity anomaly just below 1.2 K. For the first time, they enable detailed thermodynamic and spectroscopic studies of the normal and superconducting states of YFe_2Ge_2. These include low temperature heat capacity measurements, the resolution of key aspects of the electronic structure of YFe_2Ge_2 by quantum oscillation techniques and the determination of the penetration depth by muon spin rotation measurements.

[1] Y. Zou et al., PSS-RRL **8**, 928 (2014)
[2] J. Chen et al., PRL, **116**, 127001 (2016)
[3] J. Chen et al., PRB, **99**, 020501(R) (2019)

15 min. break.

TT 54.8 Thu 11:30 HSZ 201

Oxygen vacancies modulated superconductivity in monolayer FeSe on SrTiO3-δ — •Lili Wang — Tsinghua University, Beijing, China

The monolayer FeSe on SrTiO3-δ exhibits a twofold enlarged pairing gap compared with other electron-doped FeSe, which is postulated to originate from cooperative effects of interface charge transfer and electron-boson interaction that relate closely to surface oxygen vacancies in SrTiO3. We create gradient oxygen vacancies on the surface of SrTiO3-δ substrates by using direct current heating. Combining spatially resolved spectroscopy characterizations, we disclose gradient pairing gaps but negligible doping variation in monolayer FeSe on such substrates. As oxygen vacancy concentration gradually increases from anode to cathode region, the pairing gap increases from 12 to 17 meV, right beyond the values of electron-doped FeSe. This modulation provides a platform for spatially resolved investigations to unveil the interplay between electronic correlation and electron-phonon interaction and their cooperation to drive superconductivity.

TT 54.9 Thu 11:45 HSZ 201

Field-dependent Elastoresistance in FeSe — •Michael Wissmann[1], Federico Caglieris[1], Steffen Sykora[1], Saicharan Aswartham[1], Sabine Wurmehl[1], Bernd Büchner[1,2,3], and Christian Hess[1,3] — [1]IFW Dresden — [2]Institute for Solid State Physics, TU Dresden — [3]Center for Transport and Devices, TU Dresden

In iron-based superconductors, nematicity has been proposed to be closely related to the emergence of superconductivity. The introduction of uniaxial strain as a tuning parameter has been established as an important tool to probe nematic fluctuations at temperatures higher than the structural transition temperature T_S. This type of elastoresistance measurement has opened an exciting new route to understanding the interplay of nematicity, superconductivity and magnetism. However, the physical meaning of elastoresistance data for temperatures below T_S is rarely discussed. Here, we investigate the elastoresistance-behaviour in low temperatures under application of external magnetic fields inside the nematic phase of iron selenide (FeSe). FeSe is, under many aspects, an exceptional representative of the iron-based-superconductor-class. We observe a strong field-dependence as well as a second divergence towards the superconducting phase. Various scenarios for the origin of this novel observations will be discussed.

TT 54.10 Thu 12:00 HSZ 201

One-Electron-Pocket Model of FeSe: Quasiparticle Interference — •Matthias Eschrig[1,2], Luke C. Rhodes[2,3,4], Matthew D. Watson[4], and Timur K. Kim[4] — [1]Universität Greifswald, Germany — [2]Royal Holloway, University of London, UK — [3]University of St. Andrews, UK — [4]Diamond Light Source, Harwell Campus, UK

The one-electron-pocket model of FeSe was introduced to account for experimental observations in angle-resoved photoemission (ARPES) experiments. Quasiparticle interference (QPI) measurements of FeSe, obtained via scanning tunneling microscopy, have previously been interpreted as being consistent with a theoretical model where the Fermi surface consists of one hole pocket and two electron pockets and exhibits a large difference in the quasiparticle weight of the d_{xz} and d_{xy} orbitals. On the contrary, orbital sensitive measurements from ARPES have been interpreted as being consistent with a model with roughly equivalent quasiparticle weights for the d_{xz} and d_{yz} orbitals, but with only one hole pocket and one electron pocket at the Fermi surface present. Here, we show that the second, one-electron-pocket, model also explains QPI experiments. We find, that it is important to apply a selection rule for QPI, that only electronic states with vanishing component of the Fermi velocity perpendicular to the scanning surface contribute to the interference pattern. By using a three-dimensional tight-binding model of FeSe, fit to ARPES measurements, we directly reproduce the experimental QPI results, within a T-matrix formalism. This unifying result for QPI and ARPES on FeSe also highlights the importance of selection rules for QPI experiments via STM.

TT 54.11 Thu 12:15 HSZ 201

***Ab initio* investigation of dipole-dipole interactions in response to lattice distortions in FeSe** — •Felix Lochner[1], Ilya Eremin[2], Tilmann Hickel[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Deutschland

The electronic structure in unconventional superconductors holds a key to understand the momentum-dependent pairing interactions and the resulting superconducting gap function. In superconducting Fe-based chalcogenides, there have been controversial results regarding the importance of the k_z dependence of the electronic dispersion, including non-trivial topology and the gap structure and the pairing mechanisms of iron-based superconductivity. Here, we present a detailed investigation of the dipole-dipole response in FeSe, known as van-der-Waals (vdW) interaction, and its interplay with magnetic disorder and real space structural properties. Using density functional theory we show that they need to be taken into account upon investigation of the 3-dimensional effects, including non-trivial topology, of $FeSe_{1-x}Te_x$ and $FeSe_{1-x}S_x$ systems. In addition, the impact of paramagnetic disorder is considered within the spin-space average approach. Our calculations show, that the PM relaxed structure supports the picture of different competing ordered magnetic states in the nematic regime, yielding magnetic frustration.

TT 54.12 Thu 12:30 HSZ 201

MBE preparation and in-situ characterization of FeTe thin films — •Vanda M. Pereira[1], Chi-Nan Wu[1,2], Cheng-En Liu[1,3], Sheng-Chieh Liao[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,4], Cevriye Koz[1], Ulrich Schwarz[1], Hong-Ji Lin[4], Chien-Te Chen[4], Liu Hao Tjeng[1], and Simone G. Altendorf[1] — [1]MPI-CPfS, Dresden, Germany — [2]Dept. of Physics, NTHU, Hsinchu, Taiwan — [3]Dept. of Electrophysics, NCTU, Hsinchu, Taiwan — [4]NSRRC, Hsinchu, Taiwan

Within the family of Fe based superconductors, Fe chalcogenides have received particular attention due to their simple crystal structure. $Fe_{1+y}Te$, which is not superconducting, has been studied extensively in bulk form and, more recently, some efforts have been made regarding the synthesis of thin films, resorting to pulsed laser deposition and molecular beam epitaxy (MBE). Here we report the results of $Fe_{1+y}Te$ thin films grown by MBE under Te-limited growth conditions. We found that epitaxial layer-by-layer growth is possible for a wide range of excess Fe values, wider than expected from studies on the bulk material. Using XMCD at the Fe $L_{2,3}$ and Te $M_{4,5}$ edges, we observed that films with high excess Fe contain ferromagnetic clusters while films with lower excess Fe remain nonmagnetic. Moreover, x-ray absorption spectroscopy showed that it is possible to obtain films with very similar electronic structure as that of a high-quality bulk single crystal $Fe_{1.14}Te$. Our results suggest that MBE with Te-limited growth may provide an opportunity to synthesize FeTe films with smaller amounts of excess Fe as to come closer to a possible superconducting phase.

TT 54.13 Thu 12:45 HSZ 201

X-ray absorption spectroscopy measurements of $Fe_{1+x}Te$ — •Jan Fikáček[1], Jonas Warmuth[2], Fabian Arnold[3], Sunil Wilfred[4], Cinthia Piamonteze[5], Martin Bremholm[3], Ján Minár[4], Ján Lančok[1], Philip Hofmann[3], Jens Wiebe[2], and Jan Honolka[1] — [1]Institute of Physics of CAS, Prague, Czech Republic — [2]Hamburg University, Hamburg, Germany — [3]Aarhus University, Aarhus, Denmark — [4]University of West Bohemia, Plzeň, Czech Republic — [5]Paul Scherrer Institut, Villigen, Switzerland

Iron based chalcogenides (IBC) have a quasi two-dimensional crystal structure, which is the simplest one among Fe-based superconductors and makes IBC good candidates for both experimental and theoretical studies. FeSe is superconducting below T_c = 8 K [1] going above 100 K when an FeSe monolayer is grown on $SrTiO_3$ [2]. In contrast, the analog non-superconducting $Fe_{1+x}Te$ has an antiferromagnetic (AFM) ground state varying with the excess Fe concentration x.

Here, we report on results of X-ray absorption spectroscopy measurements of $Fe_{1+x}Te$ with x = 0.094 ordering antiferromagnetically below T_N = 62 K. X-ray magnetic circular dichroism up to 7 T scales linearly with the bulk magnetization. Both drop when $Fe_{1.094}Te$ enters the AFM state. In contrary, X-ray magnetic linear dichroism (XMLD) increases monotonically below T_N down to lowest temperatures. XMLD data are compared with results of our density functional theory calculations taking into account Fe excess up to x = 1.1.

[1] F. C. Hsu et al., PNAS 105, 14262 (2008).
[2] S. L. He et al, Nat. Mater. 12, 605 (2013).

TT 54.14 Thu 13:00 HSZ 201

Scanning tunneling microscopy and spectroscopy on $Fe_{1+y}Te$ (y=0.11, 0.12) — •Sahana Roessler, Cevriye Koz, Ulrich Schwarz, and Steffen Wirth — Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany

The antiferromagnetic compound $Fe_{1+y}Te$ with tetragonal structure at room temperature displays a complex phase diagram with several structural and magnetic phase transitions within the homogeneity range $0.06 \leq y \leq 0.15$ [1]. While $Fe_{1.11}Te$ undergoes a single-phase transition from a paramagnetic tetragonal to an antiferromagnetic monoclinic phase, $Fe_{1.12}Te$ exhibits a two-phase mixture of orthorhombic and monoclinic phases at temperatures below about 46 K. We compare the low-temperature microstructure [2] of these two compositions using scanning tunneling microscopy. The tunneling spectra on $Fe_{1.11}Te$ displayed a shoulder at a bias voltage of 7 mV, likely related to the energy scale of the antiferromagnetic spin-density-wave order. In contrast, in $Fe_{1.12}Te$, we occasionally observed a zero-bias conductance peak in the tunneling spectra, induced by magnetic impurity scattering originating from the segregated excess interstitial Fe on the surface.

[1] C. Koz et al., Phys. Rev. B, **88**, 094509 (2013)
[2] S. Rößler et al., Proc. Natl. Acad. Sci. **116**, 16697 (2019).

TT 55: Superconductivity: Tunnelling and Josephson Junctions

Time: Thursday 9:30–12:45 Location: HSZ 204

Invited Talk TT 55.1 Thu 9:30 HSZ 204

Probing Triplet Superconductivity by Scanning Tunneling Spectroscopy — Simon Diesch[1], Peter Machon[1], Michael Wolz[1], Christoph Sürgers[2], Detlef Beckmann[3], Wolfgang Belzig[1], and •Elke Scheer[1] — [1]Physics Department, University of Konstanz, Konstanz, Germany — [2]Physical Institute, KIT, Karlsruhe, Germany — [3]Institute for Nanotechnology, KIT, Karlsruhe, Germany

In this talk we address the proximity effect between a superconductor (S) and a normal metal (N) linked by a spin-active interface. With the help of a low-temperature scanning tunneling microscope we study the local density of states of trilayer systems consisting of Al (S), the ferromagnetic insulator EuS, and the noble metal Ag (N). In several recent studies it has been shown that EuS acts as ferromagnetic insulator with well-defined magnetic properties down to very low thickness [1]. We observe pronounced subgap structures that either reveal a zero-bias peak (ZBP) or an additional zero-bias splitting (ZBS) and that can be tuned by a magnetic field. We interpret our findings in the light of recent theories of odd-triplet contributions created by the spin-active interface [2,3]. In particular, we discuss that the ZBS is a hallmark for spin-polarized triplet pairs, able to carry long-ranged supercurrents into F, while the ZBP is a signature for short-ranged, mixed-spin triplet pairs.

[1] S. Diesch et al., Nature Commun. **9**, 5248 (2018)
[2] B. Li et al., Phys. Rev. Lett. **110**, 09700 (2013)
[3] A. Cottet et al., Phys. Rev. B **80**, 184511 (2009)

TT 55.2 Thu 10:00 HSZ 204

Josephson Tunneling through Magnetic and Non-Magnetic Impurities — •Christian Ast[1], Haonan Huang[1], Jacob Senkpiel[1], Robert Drost[1], Juan Carlos Cuevas[2], Alfredo Levy Yeyati[2], Ciprian Padurariu[3], Björn Kubala[3], Joachim Ankerhold[3], and Klaus Kern[1,4] — [1]MPI für Festkörperforschung, Stuttgart — [2]Universidad Autónoma de Madrid, Spain — [3]Universität Ulm — [4]EPFL, Lausanne, Switzerland

The Josephson effect describes the tunneling of Cooper pairs between two coupled superconductors. The critical current, which is the characteristic coupling parameter of a Josephson junction, carries valuable information about the coupled superconductors as well as the properties of the tunnel junction itself, such as the symmetry of the order parameters or the presence of magnetic impurities in the tunnel junction. We employ scanning tunneling microscopy (STM) to study the local properties of Josephson junctions in the presence of magnetic and non-magnetic impurities. We find that the critical current is reduced, depending on the coupling strength of the magnetic impurity to the superconducting substrate, which is extracted from the energy of the induced Yu-Shiba-Rusinov state. We further discuss the impact of non-magnetic impurities on the critical current.

TT 55.3 Thu 10:15 HSZ 204

Phase-dependent spin polarization of Cooper pairs in magnetic Josephson junctions — •Samme M. Dahir, Anatoly F. Volkov, and Ilya M. Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Superconductor-ferromagnet hybrid structures (SF) have attracted much interest in the past decades, due to a variety of interesting phenomena predicted and observed in these structures. One of them is the so-called inverse proximity effect. It is described by a spin polarization of Cooper pairs, which occurs not only in the ferromagnet (F), but also in the superconductor (S), yielding a finite magnetic moment M_S inside the superconductor. This effect has been predicted and experimentally studied. However, interpretation of the experimental data is mostly ambiguous. Here, we study theoretically the impact of the spin polarized Cooper pairs on the Josephson effect in an SFS junction. We show that the induced magnetic moment M_S does depend on the phase difference φ and, therefore, will oscillate in time with the Josephson frequency $2eV/\hbar$ if the current exceeds a critical value. Most importantly, the spin polarization in the superconductor causes a significant change in the Fraunhofer pattern, which can be easily accessed experimentally.

TT 55.4 Thu 10:30 HSZ 204

Coupling ferromagnetic insulators via quasiparticle states in a nodal superconductor — •Angelo Di Bernardo[1,2], Sachio Komori[2], Giorgio Livanas[3], Giorgio Divitini[2], Paola Gentile[3], Mario Cuoco[3], and Jason Robinson[2] — [1]Universität Konstanz, Department of Physics, Universitätsstraße 10, Konstanz, Germany — [2]Universitatstrasse 10 — [3]CNR-SPIN, c/o University of Salerno, I-84084 Fisciano, Salerno, Italy

The generation of parallel-aligned spin (spin-triplet) pairs of electrons at superconductor/ferromagnet (S/F) interfaces has triggered the field of superconducting spintronics –which aims at developing spintronic devices with high energy efficiency.

Even before the discovery of giant magneto resistance, which underlies spintronic spin valves, de Gennes predicted a FI/S/FI system (FI is a ferromagnetic insulator), where a variation in the critical temperature (ΔT_c) of S can be obtained by switching the FIs from parallel (P) to antiparallel (AP). In addition, if the S thickness (d_S) is smaller than its coherence length (ξ), S can favour an AP coupling of the FIs.

Recently, we have investigated a fully-oxide FI/S/FI system [1], where FI is the manganite $Pr_{0.8}Ca_{0.2}MnO_3$ and S is the nodal (d-wave) S $YBa_2Cu_3O_{7-\delta}$ (YBCO). Here, quasiparticle states at the Fermi surface of YBCO, induce a long-ranged exchange coupling between the FIs over a d_S up to 100 ξ, which is well-beyond de Gennes limit for a metallic FI/S/FI system. Such nodal exchange coupling reinforces an AP state at specific d_S and results in ΔT_c values up to 2 K.

[1] A. Di Bernardo et al., Nature Mater. **18**, 1194 (2019).

TT 55.5 Thu 10:45 HSZ 204

Skew Andreev reflection in superconducting junctions — •Andreas Costa[1], Alex Matos-Abiague[2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]Wayne State University Detroit, USA

Superconducting junctions offer unique possibilities to generate and control charge and spin supercurrents, particularly in combination with the antagonistic ferromagnetic phase. The interplay of superconductivity and ferromagnetism gets most fascinating in the presence of interfacial spin-orbit coupling (SOC), which invariably results from broken inversion symmetry. Our work [1] investigates the impact of SOC on the characteristic Andreev reflection (AR) processes at the interfaces of ferromagnet/superconductor junctions. We demonstrate that the resulting skew ARs spatially separate charge carriers and generate giant Hall currents in the ferromagnet, accompanied by sizable transverse supercurrent responses in the superconductor. Apart from that, the spin-active interface acts like a transverse electron spin filter and all predicted charge currents simultaneously come along with their spin current counterparts. We comment on various experimentally feasible ways to tune the currents, making them promising candidates for spintronics applications. In a next step, our results might become relevant for integrating Hall physics into Josephson junctions.

This work was supported by ENB IDK Topological Insulators, DFG SFB 1277 (B07), DARPA Grant DP18AP900007, and US ONR Grant N000141712793.

[1] Costa et al., Phys. Rev. B 100, 060507(R) (2019).

TT 55.6 Thu 11:00 HSZ 204

Photon-assisted resonant Andreev tunneling through Yu-Shiba-Rusinov states — •Olof Peters[1], Nils Bogdanoff[1], Sergio Acero Gonzalez[2], Larissa Melischek[2], Rika Simon[1], Gaël Reecht[1], Clemens B. Winkelmann[3], Felix von Oppen[2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [3]Univ. Grenoble Alpes, Institut Néel, 25 Avenue des Martyrs, 38042 Grenoble, France

The incoherent coupling of a photon field to the electrodes in a tunnel junction leads to photon-assisted tunneling expressed as symmetric sidebands. These bands can be very well described by the ac modulation of the energy levels in both electrodes [1].

We use scanning tunneling spectroscopy to investigate the Yu-Shiba-Rusinov (YSR) states of Mn adatoms inside the superconducting energy gap of Pb(111). At large tunneling resistance these YSR states show symmetric sidebands in an RF field of up to 40 GHz. At low resistance the tunneling process through the YSR state changes from single electron to resonant Andreev tunneling, which in contrast has asymmetric sidebands. By extending the theory of Tien and Gordon, we are able to explain and simulate this asymmetric splitting.

[1] P. K. Tien and J. P. Gordon, Phys. Rev. **129**, 647 (1963)

15 min. break.

TT 55.7 Thu 11:30 HSZ 204

Josephson and Andreev transport in a superconducting single electron transistor with a normal lead (SSN SET) — •Laura Sobral Rey[1,2], Susanne Sprenger[1], and Elke Scheer[1,2] — [1]Physics department, University of Konstanz, 78464, Konstanz, Germany — [2]QuESTech consortium

An island coupled via a tunnel barrier to two leads and a gate forms a single electron transistor (SET) that shows Coulomb blockade. All-superconducting SETs (SSS-SETs) have shown to enable multitude of possible charge transport processes which are not well understood, in particular in the strong-coupling regime [1]. To disentangle these processes, we study here the conceptually simpler SSN-SET, which has never been investigated experimentally before.

The SSN-SETs studied here consist of an S island coupled to an N lead via an oxide tunnel barrier, and to an S lead with a mechanically controlled break junction (MCBJ). Via the MCBJ, different coupling regimes can be tuned: from a tunnel contact when the MCBJ is broken to a point contact when it is closed. In that limit the MCBJ accommodates a small number of highly transmissive transport channels.

For weak coupling our experimental findings can be understood in terms of the orthodox theory [2]. For stronger couplings, we observe Andreev and Josephson transport, as well as a renormalization for the charging energy and dynamical coulomb blockade, which are also observed in the N state.

[1] T. Lorenz, J. Low Temp. Phys. 191, 301 (2017).
[2] R. J. Fitzgerald, Phys. Rev. B 57, R11073(R) (1997)

TT 55.8 Thu 11:45 HSZ 204

Microwave-assisted tunnelling and interference effects in superconducting junctions under fast driving signals — •Robert Drost[1], Peter Kot[1], Maximilian Uhl[1], Juan Carlos Cuevas[2], Joachim Ankerhold[3], and Christian Ast[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Institut für Komplexe Quantensysteme and IQST, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm, Germany

As scanning tunnelling microscopy is pushed towards fast local dynamics, a quantitative understanding of tunnel junctions under the influence of a fast AC driving signal is required, especially at the ultra-low temperatures relevant to spin dynamics and correlated electron states. We subject a superconductor-insulator-superconductor junction to a microwave signal from an antenna mounted in situ and examine the DC response of the contact to this driving signal. Basic quasi-particle tunnelling can be interpreted using a modified density of states in the electrodes. The situation is more complex when it comes to higher order effects such as multiple Andreev reflections. Microwave assisted tunnelling unravel these complex processes, providing deeper insights into tunnelling than are available in a pure DC measurement.

TT 55.9 Thu 12:00 HSZ 204

Supercurrent in topological insulator nanowire - superconductor Josephson junctions — •Michael Barth, Jacob Fuchs, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

Helical surface states of 3d topological insulator (TI) nanowires are expected to have very promising physical properties like forbidden backscattering [1]. Moreover it is predicted that a topological superconducting state which could possibly host Majorana fermions can be realized by bringing a normal s-wave superconductor in close proximity to a TI [2]. In our theoretical work we are studying such hybrid systems in a Josephson junction setup [3]. We numerically calculate the supercurrent in the system as a function of an applied external magnetic field parallel to the wire axis. Already in the normal state such a magnetic flux leads to Aharonov-Bohm oscillations of the conductance [4] but also in the superconducting state signatures of such oscillations can be observed as a consequence of spin-splitting in the superconducting TI.

[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)
[2] A. Cook and M. Franz, Phys. Rev. B **84**, 201105(R) (2011)
[3] B.D. Josephson, Phys. Lett. **1**, 251 (1962)
[[4] J. Ziegler et al., Phys. Rev. B **97**, 035157 (2018)

TT 55.10 Thu 12:15 HSZ 204

Transport signatures of the Higgs mode in a normal-superconductor junction — •Gaomin Tang[1], Wolfgang Belzig[2], Ulrich Zülicke[3], and Christoph Bruder[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [3]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, P.O. Box 600, Wellington 6140, New Zealand

The magnitude of the superconducting order parameter can be excited to oscillate under certain resonant conditions. We study the fingerprints of this so-called amplitude, or Higgs, mode in the transport properties of a voltage biased normal-superconductor tunnel junction when the superconducting contact is exposed to microwave radiation. As a key signature, the AC charge current at fixed voltage bias shows pronounced resonant behaviour when the microwave frequency coincides with the static part of the superconducting-gap amplitude. We also find an interesting nonmonotonic behavior of the AC charge current with increasing DC voltage bias.

TT 55.11 Thu 12:30 HSZ 204

Optimized proximity thermometer for ultra-sensitive detection — Bayan Karimi[1], •Danilo Nikolic[2], Tuomas Tuukkanen[1], Joonas T. Peltonen[1], Wolfgang Belzig[2], and Jukka P. Pekola[1] — [1]QuESTech and QTF Centre of Excellence, Department of Applied Physics, Aalto University School of Science, P.O. Box 13500, 00076 Aalto, Finland — [2]QuESTech and Fachbereich Physik, Universität Konstanz, D-78467, Germany

Due to its importance for understanding the quantum principles of nature as well as technological development, the possibility of measuring low temperatures has drawn attention over decades. We present a set of experiments to optimize the performance of the noninvasive thermometer based on proximity superconductivity. Current through a standard tunnel junction between an aluminum superconductor and a copper electrode is controlled by the strength of the proximity induced to this normal metal, which in turn is determined by the position of direct superconducting contact from the tunnel junction. Several devices with different distances were tested. We develop a theoretical model based on the Usadel equations and dynamic Coulomb blockade which reproduces the measured results and yields a tool to calibrate the thermometer and to optimize it further in future experiments. This project has received funding from the EU Horizon 2020 program (Marie Sklodowska-Curie action QuesTech 766025).

[1] B.Karimi, D.Nikolic, T.Tuukkanen, J.T.Peltonen, W.Belzig, and J.P.Pekola, arXiv:1911.02844 [cond-mat.mes-hall] (2019).

TT 56: Correlated Electrons: Quantum-Critical Phenomena

Time: Thursday 9:30–13:00 Location: HSZ 304

TT 56.1 Thu 9:30 HSZ 304

Quasiparticle critical slowing down in a heavy-fermion system — •S. Pal[1], C.-J. Yang[1], F. Zamani[2], K. Kliemt[3], C. Krellner[3], H. v. Löhneysen[4], J. Kroha[2], and M. Fiebig[1] — [1]ETH Zürich, Switzerland. — [2]Universität Bonn, Germany. — [3]Goethe-Universität Frankfurt, Germany. — [4]KIT Karlsruhe, Germany.

Rare-earth heavy-fermion systems such as $YbRh_2Si_2$ show a quantum phase transition between a fully Kondo-screened paramagnetic Fermi-liquid phase and an antiferromagnetically ordered phase. When excited by THz pulses, the Kondo state disintegrates and coherently recovers on timescales in the order of 2 ps, corresponding to the Kondo lattice temperature of $T_K^* = 25\,\mathrm{K}$. We use THz time-domain spectroscopy[1,2] to probe the coherent Kondo spectral weight of $YbRh_2Si_2$ in presence of an in-plane magnetic field. By tuning the magnetic field, we are able to map the logarithmic build-up of quasiparticle spectral weight around 25 K across the quantum phase transition. We find that near the critical magnetic field of $B_c = 67\,\mathrm{mT}$, first the Kondo weight rises logarithmically with decreasing temperature, reaching a maximum near the Kondo lattice temperature. It is then followed by a reduction until 10 K indicating Kondo breakdown. Upon decreasing the temperature further, we find that the THz response signal starts building up logarithmically until the lowest temperatures measured. A critical, two-band Fermi-liquid theory indicates that this signals quasiparticle critical slowing down for a fermionic field - an observation of which in our experiments is indeed intriguing.

[1] Nat. Phys. **14**, 1103 (2018)
[2] Phys. Rev. Lett. **122**, 096401 (2019).

TT 56.2 Thu 9:45 HSZ 304

Fermi surface topological transition in $Sr_3Ru_2O_7$ — •Dmitri Efremov[1], Alex Shtyk[2], Andreas Rost[3], Claudio Chamon[4], Andrew Mackenzie[6], and Joseph Betouras[5] — [1]IFW, Dresden — [2]Harvard University, Cambridge — [3]University of St Andrews,St Andrews — [4]Boston University, Boston — [5]Loughborough University, Loughborough — [6]Max Planck Institute for Chemical Physics of Solids, Dresden

A wide variety of complex phases in quantum materials are driven by electron-electron interactions, which are enhanced through density of states peaks. A well-known example occurs at van Hove singularities where the Fermi surface undergoes a topological transition. Here we discuss that higher order singularities, where multiple disconnected leaves of Fermi surface touch all at once, naturally can occur at points of high symmetry in the Brillouin zone. Such multicritical singularities can lead to stronger divergences in the density of states than canonical van Hove singularities. As a concrete example of the power of these Fermi surface topological transitions, we demonstrate how they can be used in the analysis of experimental data on $Sr_3Ru_2O_7$. Understanding the related mechanisms opens up new avenues in material design of complex quantum phases

TT 56.3 Thu 10:00 HSZ 304

Low temperature transverse susceptibility of $LiHoF_4$ — •Andreas Wendl, Felix Rucker, Christopher Duvinage, and Christian Pfleiderer — Physik Department TU München, James-Franck Straße 1, 85748 Garching

$LiHoF_4$ exhibits the experimental realisation of the simplest quantum spin model of a ferromagnetic quantum phase transition: the transverse field Ising model [1]. Application of a magnetic field perpendicular to the easy magnetic axis, suppresses long-range ferromagnetic order above a critical field, $B_c \approx 5.1\,\mathrm{T}$. We report measurements of the transverse ac susceptibility of a spherical single-crystal of $LiHoF_4$. For our study we used a bespoke miniature ac susceptometer optimised for measurements at milli-Kelvin temperatures under arbitrary directions of the applied magnetic field using a vector magnet. This allowed us to determine the phase diagram under tilted magnetic fields as well as the precise magnetic field dependence of the Curie temperature at low fields under strictly transverse field geometry. In addition, we tracked the thermal and quantum freezing of ferromagnetic domains.

[1] D. Bitko et al., Phys. Rev. Lett. **77**, 940 (1996)
[2] F. Rucker and C. Pfleiderer, Rev. Sci. Instrum. **90**, 073903 (2019).

TT 56.4 Thu 10:15 HSZ 304

Ferromagnetic magnons in $YbNi_4P_2$ — •Oliver Stockert[1], Kristin Kliemt[2], Zita Huesges[3], Stefan Lucas[1], Cornelius Krellner[2], Astrid Schneidewind[4], and Karin Schmalzl[5] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden — [2]Physikalisches Institut, Goethe-Universität, Frankfurt am Main — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin — [4]Forschungszentrum Jülich, Outstation MLZ, Garching — [5]Forschungszentrum Jülich, Outstation ILL, Grenoble

The heavy-fermion compound $YbNi_4P_2$ exhibits ferromagnetic order below the very low Curie temperature $T_C = 150\,\mathrm{mK}$. Upon substituting As for P the ordering temperature T_C in $YbNi_4(P_{1-x}As_x)_2$ can be continuously suppressed with the occurrence of a quantum critical point [1]. So far bulk measurements have been used to characterize the ferromagnetic order in $YbNi_4P_2$ [2]. In contrast, neutron diffraction failed in detecting any ferromagnetic signal. In order to better characterize the magnetism in $YbNi_4P_2$, we performed inelastic neutron scattering on a large $YbNi_4P_2$ single crystal [3] at the triple-axis spectrometers IN12 (ILL, Grenoble), PANDA (MLZ, Garching) and FLEXX (HZB, Berlin). We observe clear magnetic excitations in $YbNi_4P_2$ at low temperatures with a dispersion as expected for a ferromagnet. Our findings are a direct evidence of the ferromagnetic order in $YbNi_4P_2$.

[1] A. Steppke et al., Science 339 (2013) 933
[2] C. Krellner, C. Geibel, J. Phys. Conf. Ser. 391 (2012) 012032
[3] K. Kliemt, C.Krellner, J. Crystal Growth 449 (2016) 129.

TT 56.5 Thu 10:30 HSZ 304

Non-Fermi liquid behaviors in $Y_{1-x}Pr_xIr_2Zn_{20}$ studied by thermal expansion — •Andreas Wörl[1], Yu Yamane[2], Yoshifumi Tokiwa[1], Takahiro Onimaru[2], and Philipp Gegenwart[1] — [1]Experimental Physics 6, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany — [2]Graduate School of Advanced Sciences of Matter, Department of Quantum Matter, Hiroshima University, Japan

The overscreening of quadrupole moments by two-channels of conduction electrons, generally known as two-channel Kondo effect, causes non-Fermi liquid behavior. A prototype material to study this effect is the quadrupole Kondo lattice $PrIr_2Zn_{20}$ [1]. Y substituted $PrIr_2Zn_{20}$ single crystals exhibit non-Fermi liquid behaviors in specific heat [2], electrical resistivity [2] and elastic constants [3], which are compatible with the theoretical single-site two channel Kondo model. In this talk, we present results on the thermal expansion and magnetostriction of $Y_{1-x}Pr_xIr_2Zn_{20}$ single crystals which allow for a further characterization of this novel hybridization effect.

[1] T. Onimaru et al., Phys. Rev. B 94, 075134 (2016)
[2] Y. Yamane et al., Phys. Rev. Lett. 121, 077206 (2018)
[3] T. Yanagisawa et al., Phys. Rev. Lett. 123, 067201 (2019)

TT 56.6 Thu 10:45 HSZ 304

Deconfined critical point in a doped random quantum Heisenberg magnet — •Darshan Joshi, Chenyuan Li, and Subir Sachdev — Department of Physics, Harvard University, Cambridge MA 02138, USA

We study a t-J model with both t and J random and all-to-all. This model has been studied earlier [1], and can be mapped to an Anderson impurity coupled to self-consistent fermionic and bosonic baths. We employ renormalization group and large M (for models with SU(M) spin symmetry) analyses, and find evidence for a deconfined critical point at zero temperature and small doping. The critical spin correlations are similar to those in a random magnet [2]. A disordered Fermi liquid phase is expected at large doping, while a spin glass phase is expected at small doping. We note connections to the physics of the underdoped cuprates.

[1] O. Parcollet and A. Georges, Physical Review B 59, 5341 (1999).
[2] S. Sachdev and J. Ye, Physical Review Letters 70, 3339 (1993).

TT 56.7 Thu 11:00 HSZ 304

Nonordinary Edge Criticality of Two-Dimensional Quantum Critical Magnets — Lukas Weber[1], Francesco Parisen Toldin[2], and •Stefan Wessel[1] — [1]RWTH Aachen University, Germany — [2]Würzburg University, Germany

Based on large-scale quantum Monte Carlo simulations, we examine the correlations along the edges of two-dimensional semi-infinite quantum critical Heisenberg spin-1/2 and spin-1 systems. In particular, we consider coupled quantum spin-dimer systems at their bulk quantum critical points, including the columnar-dimer model and the plaquette-square lattice. The alignment of the edge spins strongly affects these correlations and the corresponding scaling exponents, with remarkably similar values obtained for various quantum spin-dimer systems. We furthermore observe subtle effects on the scaling behavior from perturbing the edge spins that exhibit the genuine quantum nature of these edge states.

15 min. break.

TT 56.8 Thu 11:30 HSZ 304

Emergent spin 1/2 chains at domain walls of Kekulé valence-bond solids — •Toshihiro Sato[1], Martin Hohenadler[1], Tarun Grover[2], John McGreevy[2], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Department of Physics, University of California at San Diego, USA

Dirac fermions with dynamically generated anticommuting Z_2 Kekulé valence-bond solid (KVBS) and SO(3) antiferromagnetic (AFM) mass terms allow for the generation of a topological θ-term in the low energy effective field theory. Such a topological term is at the origin of phase transitions beyond the Ginzburg-Landau paradigm: topological defects of one phase carry the charge of the other and proliferate at the transition. In the vicinity of criticality and in the KVBS phase, the θ-term implies that a domain wall of the Z_2 order parameter harbours a spin 1/2 Heisenberg chain. Using pinning fields to stabilize the domain wall, we show that our auxiliary field quantum Monte Carlo simulations indeed support the emergence of spin-1/2 chain at the Z_2 defect.

TT 56.9 Thu 11:45 HSZ 304

Quantum critical behavior of the Hubbard model on the honeycomb lattice — •Francesco Parisen Toldin and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We study the quantum critical behavior of the Hubbard model on the honeycomb lattice by means of large-scale projective Auxiliary-field quantum Monte Carlo simulations, which target the ground state of the model. At T=0 the model hosts a continuous phase transition between a Dirac semimetal and an antiferromagnetic Mott insulating phase, whose critical behavior belongs to the Gross-Neveu-Heisenberg universality class, also known as chiral Heisenberg. We investigate the universal properties of the phase transition by a finite-size scaling analysis of time-displaced critical correlation functions.

TT 56.10 Thu 12:00 HSZ 304

Nematic phase transitions of Dirac fermions — •Jonas Schwab[1], Lukas Janssen[2], Kai Sun[3], Zi Yang Meng[4], Igor Herbut[5], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [3]Physics Department, University of Michigan, Ann Arbor, MI 48109, USA — [4]Institute of Physics, Chinese Academy of Sciences, Beijing 100190,China — [5]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. We consider two models where the nematic transition reduces the initial C_{4V} (C_{2V}) symmetry to C_{2V} ($2V$). Auxiliary field quantum Monte Carlo simulations reveal that the C_{4V} (C_{2V}) symmetric model show a continuous (first order) transition. An analytical understanding of the transition is derived.

TT 56.11 Thu 12:15 HSZ 304

Doping a dynamically generated quantum spin Hall insulator — •Zhenjiu Wang[1], Toshihiro Sato[1], Yuhai Liu[2], Martin Hohenadler[1], Wenan Guo[2,3], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Beijing Computational ScienceResearch Center, Beijing 100193, China — [3]Department of Physics, Beijing Normal University, Beijing 100875, China

We consider a quantum spin Hall (QSH) insulator in which the spin-orbit coupling is dynamically generated by spontaneous symmetry breaking of the SU(2) spin symmetry. At the particle-hole symmetric point tuning the *band-width* leads to a direct and continuous quantum phase transition to an s-wave superconductor. This transition has an emergent Lorentz symmetry and is described by the theory of de-confined quantum criticality with emergent charged U(1) gauged spinons [1]. Here we will doped the QSH insulator by tuning the chemical potential. We observe a continuous quantum phase transition again to an s-wave superconductor. Such a phase transition has no emergent Lorentz invariance and fractionalized particles. In particular the dynamical exponent takes the value $z = 2$ and one observes pronounced long-wavelength Goldstone modes. The above stems from auxiliary field quantum Monte Carlo simulations of a designer model, that, by definition, is free of the negative sign problem.

[1] Yuhai Liu, Zhenjiu Wang, Toshihiro Sato, Martin Hohenadler, Chong Wang, Wenan Guo, and Fakher F. Assaad, Nature Communications 10 (2019), no. 1, 2658.

TT 56.12 Thu 12:30 HSZ 304

Soluble fermionic quantum critical point in two dimensions — •Shouryya Ray[1,2], Matthias Vojta[1,2], and Lukas Janssen[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

We study a quantum critical point in two spatial dimensions between a semimetallic phase characterized by a stable quadratic Fermi node, and an ordered phase in which the spectrum develops a dynamical band gap. The quantum critical behaviour can be computed exactly and we explicitly derive the scaling laws of various observables. While the correlation functions at criticality satisfy usual power laws with anomalous exponents $\eta_\phi = 2$ and $\eta_\psi = 0$, the correlation length and the order parameter exhibit essential singularities upon approaching the quantum critical point from the insulating side; phenomenological similarities to the classical Berezinskii-Kosterlitz-Thouless transition are elucidated. On the semimetallic side, the correlation length remains infinite, and leads to emergent scale invariance.

TT 56.13 Thu 12:45 HSZ 304

Gapless Coulomb State Emerging from a Self-Dual Topological Tensor-Network State — •Guo-Yi Zhu — Max-Planck-Institute for the Physics of Complex Systems

In the tensor network representation, a deformed Z2 topological ground state wave function is proposed and its norm can be exactly mapped to the two-dimensional solvable Ashkin-Teller model. Then the topological (toric code) phase with anyonic excitations corresponds to the partial order phase of the Ashkin- Teller model, and possible topological phase transitions are precisely determined. With the electric- magnetic self-duality, a novel gapless Coulomb state with quasi-long-range order is obtained via a quantum Kosterlitz-Thouless phase transition. The corresponding ground state is a condensate of pairs of logarithmically confined electric charges and magnetic fluxes, and the scaling behavior of various anyon correlations can be exactly derived, revealing the effective interaction between anyons and their condensation. Deformations away from the self-duality drive the Coulomb state into either the gapped Higgs phase or the confining phase.

TT 57: Skyrmions IV (joint session MA/TT)

Time: Thursday 9:30–11:15 Location: POT 6

TT 57.1 Thu 9:30 POT 6

Exploring the tunability of skyrmion lifetimes in 3D materials — •Markus Hoffmann, Gideon P. Müller, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Chiral magnetic skyrmions are of great scientific interests but also of potential relevance in information technology, data storage, processing, and neuromorphic computing. To compete with existing technology, those skyrmions have to fulfill stringent requirements: Long lifetimes at room temperature at small sizes. Therefore, a significant effort of the magnetism community lies on the analysis of the stability of such small skyrmions. One commonly used approach is the calculation of energy barriers by performing LLG and GNEB simulations as well as the determination of the lifetime prefactor by HTST [1]. Up to now, those were mainly performed for skyrmions in 2D systems, *i.e.* atomic layers. For technological applications, however, the third dimension can play a significant role. Particularly magnetic multilayers as well as exchange biased materials are in the focus of interest for technologically relevant materials. Yet, little is known about the stability of skyrmions in such materials. We therefore performed lifetime calculations within our Spirit code [2] and investigated the tunability of skyrmion lifetimes by effects such as exchange bias or interlayer coupling.

We acknowledge funding from the DARPA TEE program through grant MIPR (#HR0011831554) from DOI.

[1] P. F. Bessarab *et al.*, Phys. Rev. B **85** (18), 184409 (2012)
[2] Spirit spin simulation framework, spirit-code.github.io

TT 57.2 Thu 9:45 POT 6

Electrical Transport in FIB microstructures of $Mn_{1.4}PtSn$ — •M. Winter[1,2], S. Hamann[1,3], J. Gayles[3], P. Vir[3], M. Uhlarz[1], M. König[3], C. Felser[3], J. Wosnitza[1,2], and T. Helm[1,3] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

$Mn_{1.4}PtSn$ is a half-Heusler compound with tetragonal crystal structure. Only recently, Lorentz transmission electron microscopy measurements have shown that, so-called antiskyrmion phases can be stabilized by applying a magnetic field to the material. Futhermore, it is known that non-trivial magnetic structures such as skyrmions cause a topological contribution to the Hall effect. Therefore, investigations of the electrical transport properties of the material are highly desirable. By using a focused ion beam, we are able to produce samples with submicron feature size, close to the coherence length of the occurring magnetic structures, while maintaining the high quality of a single crystal. This opens the possibility to measure influences of the sample geometry, such as local effects and finite-size effects, on the topological Hall effect caused by the antiskyrmions in $Mn_{1.4}PtSn$.

TT 57.3 Thu 10:00 POT 6

Towards the 3D quantification of Skyrmions in thin helimagnets — •Sebastian Schneider[1,2], Daniel Wolf[1], Matthew J. Stolt[3], Song Jin[3], Marcus Schmidt[4], Darius Pohl[2,1], Bernd Rellinghaus[2,1], Bernd Büchner[1], Sebastian T. B. Goennenwein[2], Kornelius Nielsch[1], 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

The anticipated application of skyrmions as information carriers in magnetic thin film devices depends crucially on the stability and mobility of these solitons. Within the scope of this work the microscopic magnetic structure of skyrmions, which determines their transport properties, is investigated by means of magnetic measurement methods in transmission electron microscopy. To study the three-dimensional spin texture of Bloch skyrmions in thin helimagnets of FeGe and $Fe_{0.95}Co_{0.05}Ge$ focal series electron holography and off-axis electron holography is employed to determine quantitative maps of the projected in-plane magnetic induction. Although these magnetic induction maps carry the clear signature of Bloch skyrmions, their magnitude is much smaller than the values expected for homogeneous skyrmions extending throughout the thickness of the film. Such a reduction can amongst others be caused by a modulation of the underlying spin textures along the out-of-plane z direction. To further analyse these modulations first electron holographic tomography experiments on Bloch skyrmions in an FeGe needle are performed.

TT 57.4 Thu 10:15 POT 6

Skyrmions for reservoir computing — •Karin Everschor-Sitte — Institute of Physics, Johannes Gutenberg-University Mainz

The topological properties of magnetic skyrmions, their inherent compact particle-like nature and their complex and nonlinear dynamics make skyrmions interesting for spintronics applications and in particular unconventional computing schemes. [1] In this talk I will address the potential of magnetic skyrmions for reservoir computing, i.e. a computational scheme which allows to drastically simplify spatial-temporal recognition tasks. We have shown that random skyrmion fabrics provide a suitable physical implementation of the reservoir [2,3] and allow to classify patterns via their complex resistance responses either by tracing the signal over time or by a single spatially resolved measurement. [4]

[1] G. Finocchio et al., arXiv:1907.04601 [2] D. Prychynenko et al., Phys. Rev. Appl. **9**, 014034 (2018) [3] G. Bourianoff et al., AIP Adv. **8**, 055602 (2018) [4] D. Pinna et al., arXiv:1811.12623

TT 57.5 Thu 10:30 POT 6

Skyrmion size and shape within continuous magnetization model and atomistic spin model — •Anastasiia S. Varentsova[1,2] and Pavel F. Bessarab[1,2,3] — [1]ITMO University, St. Petersburg, Russia — [2]University of Iceland, Reykjavík, Iceland — [3]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

We explore the relationship between two approaches to the description of skyrmions in magnetic materials. One of the approaches involves characterization of magnetic states by a continuous magnetization field. Within the other approach, magnetic structures are represented by magnetic moments localized on vertices of a discrete lattice. By tracing contours of constant skyrmion size in the material parameter space, we demonstrate that the continuous magnetization model and the lattice model agree quite well for large skyrmions with smooth profiles, but predict different results for small skyrmions and skyrmions with bubble-like shape. We propose to link the two models by a material parameter transformation that does not rely on the assumption of small spatial variation of the magnetic structure on the scale of the lattice constant. As a result, good agreement between the continuous magnetization theory and the lattice model can be obtained for the whole skyrmion sector of the magnetic phase diagram.

This work was funded by the Russian Science Foundation (Grant No. 19-72-10138), the Icelandic Reseach Fund (Grant No. 184949-052) and Alexander von Humboldt Foundation.

TT 57.6 Thu 10:45 POT 6

Topologically Non-trivial Magnetic and Polar Patterns in Lacunar Spinels — •Markus Preissinger[1], Hans-albrecht Krug von Nidda[1], Axel Lubk[2], Sándor Bordács[3], Hiroshi Nakamura[4], Vladimir Tsurkan[1], and István Kézsmárki[1] — [1]Experimentalphysik V, Universität Augsburg — [2]Advanced Methods of Electron Microscopy, IFW Dresden — [3]Magneto-Optical Spectroscopy Group, Budapest University of Technology and Economics — [4]Department of Materials Science and Engineering, Kyoto University

The lacunar spinels $Ga(V/Mo)_4(S/Se)_8$ have been the first candidates, where the emergence of Néel-type skyrmions, induced by Dzyaloshinsky-Moriya interaction, has been reported. This group of materials undergo a Jahn-Teller transition at about 40 K losing inversion symmetry in the process. Upon further cooling the system enters a magnetically ordered state. The ground state is a cycloidal phase, while critical fields strongly depend on the direction in which the magnetic field is applied [1][2]. In an attempt to image skyrmions with Lorentz-transmission-electron microscopy (LTEM), we succeeded to find the cycloidal ground state in thin lamellae of $GaV_4(S/Se)_8$ (<100nm) at a hugely increased temperature simultaneously to the Jahn-Teller distortion. In thin lamellae of $GaMo_4S_8$ no magnetic texture but a regular pattern of polarised structural domains has been found, presumably indicating polar skyrmions.

[1] I. Kézsmárki, NMAT 2015, Vol14, pp 1116-1122;
[2] S. Bordács Sci. Rep. 2017, Vol 7, Article number 7548

TT 57.7 Thu 11:00 POT 6

Hopfions in magnetic crystals — Filipp N. Rybakov[1], •Nikolai S. Kiselev[2], Aleksandr B. Borisov[3], Lukas Döring[4], Christof Melcher[4], and Stefan Blügel[2] — [1]Department of Physics, KTH-Royal Institute of Technology, SE-10691 Stockholm, Sweden — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [3]Institute of Metal Physics of Ural Branch of Russian Academy of Sciences, Ekaterinburg 620990, Russia — [4]Department of Mathematics I & JARA FIT, RWTH Aachen University, 52056 Aachen, Germany

Hopfions are three-dimensional topological solitons, which can be thought of as skyrmion tubes with closed ends. In the pioneering work of Bogolyubsky [1], it was shown that in the micromagnetic model with higher-order derivatives of the order parameter, the hopfions might appear as statically stable solutions. Here we show that the general form of such a micromagnetic functional can be derived from classical spin-lattice Hamiltonians with competing Heisenberg exchange interactions. We present this advanced micromagnetic functional derived for lattices of cubic symmetry and provide a criterion for the existence of hopfions in the systems described by such a functional [2]. Following our approach, similar functionals can be derived for materials of any crystal symmetry. We discuss a variety of hopfion solutions, their static and dynamic properties, and provide concrete guidance for the search of magnetic crystals that allow the existence of hopfions.

[1] I. L. Bogolubsky, Phys. Lett. A **126**, 511 (1988).
[2] F. N. Rybakov, *et al.*, arXiv:1904.00250.

TT 58: Graphene I: Growth, Structure and Substrate Interaction (joint session O/TT)

Time: Thursday 10:30–12:00 Location: GER 37

TT 58.1 Thu 10:30 GER 37

Design principles for doping graphene for electrochemical CO2 reduction: Insights from Theory — •Sudarshan Vijay[1], Joseph Gauthier[2], Hendrik Heenen[1], Vanessa Bukas[1], Henrik Kristoffersen[1], and Karen Chan[1] — [1]CatTheory, Department of Physics, Technical University of Denmark — [2]SUNCAT Center for Interface Science and Catalysis, Department of Chemical Engineering

Graphene based 2D catalysts hold great promise for CO2 reduction to CO and CH4. Recent experimental investigations [1,2] show metal doped Iron-Nitrogen-Carbon (Fe-N-C) catalysts are able to reduce CO2 to CO at low overpotentials and with high selectivity. However, modelling these materials in an electrochemical environment poses several open challenges. In this work, we present a theoretical investigation on Fe-N-C catalysts which includes the effect of potential, interfacial pH, change in local spin states to properly elucidate the mechanism for CO2 reduction. We find that the electronic structure of Fe-N-C resembles graphene more than it does a metal, with significantly fewer states at the fermi level. Charge dependence of binding energies of key intermediates depend on the position of the highest energy d-orbital with respect to the fermi level. Using computed reaction energetics coupled with mean-field kinetic models, we are able to ascertain the mechanism for CO2 reduction and compare our results with experimental findings. We extend this analysis to other 2D material systems and propose rational design principles.

[1] Science 14 Jun 2019: Vol. 364, Issue 6445, pp. 1091-1094 [2] ACS Energy Lett. 2018, 3, 4, 812-817

TT 58.2 Thu 10:45 GER 37

Graphene/S/Ru(0001): a model system for studying intercalation — •Lars Buss[1,2], Jens Falta[2,3], Moritz Ewert[1], Polina Sheverdyaeva[4], Paolo Moras[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Institute for Solid State Physics, University of Bremen, Bremen, Germany — [3]MAPEX Center for Materials and Processes, University of Bremen, Bremen, Germany — [4]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy

The epitaxial growth of single-layer graphene on transition-metal substrates enables the growth of micrometer-sized islands with excellent crystalline quality, but the possibly strong binding to the substrate has proven detrimental to its materials properties. However, intercalation of foreign atoms lifts the interlayer coupling, restoring its unique electronic structure. We have investigated the intercalation of sulfur underneath graphene on Ru(0001) with low-energy electron microscopy (LEEM) and micro-diffraction (μLEED). We find that sulfur deposited from a molecular precursor at elevated temperatures intercalates through the edge of the island, eventually leading to wrinkles in the graphene. Intriguingly, the overlaying graphene limits the number of possible S/Ru(0001) reconstructions below, preventing the formation of less dense reconstructions like the $p(2\times2)$-S and $(\sqrt{3}\times\sqrt{3})$-S surface phases. Intensity-voltage LEEM and angle-resolved photoemission (ARPES) prove the free-standing character of the sulfur intercalated graphene, which is found to be p-doped by 380 meV.

TT 58.3 Thu 11:00 GER 37

Au intercalation under epitaxial graphene on Ru(0001): the role of graphene edges — •Sebastian Günther[1], Tevfik Onur Mentes[2], Robert Reichelt[1], Elisa Minussi[2], Benito Santos[2], Alessandro Baraldi[2], and Andrea Locatelli[2] — [1]TUM, Dept. Chemie, Lichtenbergstr.4, D-85748 Garching — [2]Sincrotrone Trieste, AREA Science Park I-34149 Trieste

Au intercalation at the graphene-Ru(0001) interface is investigated at elevated temperature by using low energy electron - and x-ray photoelectron emission microscopy (LEEM/XPEEM). Graphene (g) growth by ethylene decomposition at 1030 K on a Au pre-covered Ru surface pushes the Au adatoms towards the g-free surface area. When instead, evaporating Au on a partly g-covered surface, a modified Stranski-Krastanov growth on Ru with two atomic wetting layers followed by 3D islands is observed. At 970 K the growth follows a precise order: 1)The first wetting Au layer is grown exclusively on the g-free area of the Ru surface. 2)After completion of the Au/Ru layer, Au intercalation below g-flakes sets in. 3)Having completed the g/Au/Ru layer, second wetting Au layer growth ouside the g-covered area takes place. 4)After completion of the Au/Au/Ru layer, intercalation of the second Au layer underneath g sets in. At 970 K, Au is shown not to stick to g-covered surface regions. This crucial finding singles out the g-edges as the only intercalation channel. Chemical maps at different stages during Au growth point to a pronounced kinetic barrier at the g-edges preventing intercalation before the Au monolayer is completed outside the g-covered regions.

TT 58.4 Thu 11:15 GER 37

Covalent functionalization of epitaxial graphene on cubic-SiC(001) — •Dmitrii Potorochin[1,2,3], Olga Molodtsova[1,2], Victor Aristov[1,4], Alexander Chaika[4], Maxim Rabchinskii[5], Marina Baidakova[2,5], Nikolai Ulin[5], Pavel Brunkov[2,5], Dmitry Marchenko[6], and Serguei Molodtsov[2,3,7] — [1]DESY, Hamburg, Germany — [2]ITMO University, Saint Petersburg, Russian Federation — [3]TU Bergakademie Freiberg, Freiberg, Germany — [4]ISSP RAS, Chernogolovka, Russian Federation — [5]Ioffe Institute RAS, Saint Petersburg, Russian Federation — [6]Helmholtz-Zentrum Berlin, Berlin,Germany — [7]European XFEL, Schenefeld, Germany

Some properties of graphene, although being unique, can serve as a deterrent factor to its use in some fields of technology. For instance, the bandgap absence complicates the fabrication of graphene-based logic elements of electronics. Furthermore, the transparency in the visible spectral region imposes a restriction on the use of graphene as an active material for elements of photonics (photodetectors, photovoltaics, etc.). Covalent functionalization of graphene is a promising approach to overcome such limitations. In the current report, we present an investigation of the electronic structure and morphology of epitaxial graphene on cubic-SiC(001) covalently modified by organic dyes. Results of high-resolution X-ray photoelectron spectroscopy (HR-XPS), photoemission electron microscopy (PEEM), and scanning tunneling microscopy (STM) studies are given. This work was supported by RAS, RFBR (Grant Nos. 17-02-01139, 17-02-01291), and Minobrnauki of Russia (Project 3.3161.2017/4.6).

TT 58.5 Thu 11:30 GER 37

Controlled formation of nanobubbles in graphene — •Pin-Cheng Lin[1], Renan Villarreal[1], Harsh Bana[1], Ken Verguts[2,3], Steven Brems[3], Stephen de Gendt[2,3], Manuel Auge[4], Felix Junge[4], Hans Hofsäss[4], Hossein Ghorbanfekr[5], M Fallh[5], François Peeters[5], Mehdi Neek-Amal[5], Chris Van Haesendonck[1], and Lino da Costa Pereira[1] — [1]Quantum Solid State Physics, KU Leuven, 3001 Leuven, Belgium — [2]Departement Chemie, KU Leuven, 3001 Leuven, Belgium — [3]imec, 3001 Leuven, Belgium — [4]II. Institute of Physics, University of Göttingen, Göttingen 37077, Germany — [5]Department of Physics, University of Antwerp, 2020 Antwerp, Belgium

Strained nanobubbles have been used to engineer the electronic structure of graphene through the creation of pseudomagnetic fields (e.g. via strain imposed by a selected substrate or mechanical actuators), however, they provide limited controllability. Here we report on the controlled formation of noble gas (He, Ne, Ar) nanobubbles in graphene (on various substrates) using ultra-low energy (ULE) ion implantation. ULE ion implantation allows us to precisely tune the number of implanted ions and their kinetic energy, which in turn controls the bubble formation efficiency and bubble density. Our experimental approach is based on scanning tunneling microscopy/spectroscopy (STM/STS), synchrotron X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, among others, complemented by density functional theory (DFT) and molecular dynamics calculations (MD), which give insight into the bubble formation and stability mechanisms.

TT 58.6 Thu 11:45 GER 37

Simulating the scattering of a hydrogen atom from graphene using a high-dimensional neural network potential. — •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

Understanding the formation of covalent bonds due to atomic-scale motions and energy dissipation pathways involved is an ongoing challenge in the field of chemistry. Recent measurements of the translational energy loss distribution of hydrogen atoms scattered from graphene showed a bimodal pattern. The second generation reactive empirical bond order potential was fitted to ab initio electronic structure data obtained from embedded mean-field theory to generate a potential energy surface (PES). First-principles dynamics simulations using the provided PES were able to reproduce the bimodal feature of the energy loss spectrum and were in qualitative agreement with experimental results. But these investigations could not fully provide a detailed description of the scattering and sticking mechanisms. Therefore, we developed a full-dimensional neural network PES by fitting to the density functional theory data in order to further reduce the remaining errors by the fitting procedure of the PES underlying molecular dynamics simulations performed.

TT 59: Correlated Electrons: Quantum Impurities and Kondo Physics; Other Materials

Time: Thursday 15:00–18:30 Location: HSZ 03

TT 59.1 Thu 15:00 HSZ 03

Phase Diagram and Dynamics of an SU(N) Symmetric Kondo Lattice Model — •Marcin Raczkowski and Fakher Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the interplay between Kondo screening and the magnetic RKKY interaction in an SU(N) symmetric generalization of the two-dimensional half-filled Kondo lattice model (KLM) by quantum Monte Carlo simulations with N up to 8 [1]. While the long-range antiferromagnetic (AF) order in SU(N) quantum spin systems typically gives way to spin-singlet ground states with spontaneously broken lattice symmetry, we find that the SU(N) KLM in the totally antisymmetric self-adjoint representation is unique in that for each finite N its ground-state phase diagram hosts only two phases – AF order and the Kondo-screened phase. We believe that it is the enhanced range of the RKKY interaction that is the key to stabilize antiferromagnetism at large N. Given that the range of the RKKY interaction grows as a function of N, we generically expect that the relevant physics will become more mean-field-like. A resolved abrupt jump of the coherence temperature across the phase transition for $N > 2$ supports this line of arguing and sheds new light on the rapid loss of coherence at the magnetic phase transition in heavy-fermion systems.

[1] M. Raczkowski and F. F. Assaad, arXiv:1910.07540 (2019).

TT 59.2 Thu 15:15 HSZ 03

Magnetic doublon bound states in the Kondo Lattice Model — •Roman Rausch[1], Michael Potthoff[2], and Norio Kawakami[1] — [1]Kyoto University — [2]University of Hamburg

We present a novel pairing mechanism for electrons, mediated by magnons. These paired bound states are termed "magnetic doublons". Applying numerically exact techniques (exact diagonalization and the density-matrix renormalization group, DMRG) to the Kondo lattice model at strong exchange coupling J for different fillings and magnetic configurations, we demonstrate that magnetic doublon excitations exist as composite objects with extremely weak dispersion at excitation energies of the order of 3J/2 above the ground state. They are highly stable, support a novel "inverse" colossal magnetoresistance and potentially other effects like metastable superconductivity, or cooling via quantum distillation.

[1] R. Rausch, M. Potthoff, N. Kawakami, arXiv:1909.11896

TT 59.3 Thu 15:30 HSZ 03

Genuine RKKY-Kondo quantum phase transition — •Krzysztof P. Wójcik[1,2] and Johann Kroha[1] — [1]Physikalisches Institut, Universität Bonn, Germany — [2]Institute of Molecular Physics, Polish Academy of Sciences, Poznań, Poland

Since the seminal papers of Jones and Varma, the RKKY interaction (Y) between two Kondo impurities is conventionally modeled by a Heisenberg coupling term. It gives rise to a quantum phase transition (QPT) between the Kondo and the RKKY phases in the two-impurity Kondo model. Yet, the significance of this result is still controversial. Firstly, the QPT is extremely fragile to particle-hole (PH) asymmetry, changing the QPT to a crossover in its presence. This has lead to the common belief that it cannot be realized in a realistic 2-impurity system and has made its relevance for lattice models debatable. Moreover, in the model Y and the Kondo exchange J are considered independent, although Y is genuinely generated by J, and the Kondo temperature depends on Y, as has been shown experimentally [1] and theoretically [2]. Recently, it has been proven that the QPT can be restored for weaker PH symmetry by parameter fine-tuning [3]. We revisit the problem to show by numerical renormalization group calculations that in the geometry of [1], Y induced solely by J causes the QPT for a properly symmetric case. We also discuss potential consequences of our findings for the lattice model in the context of "Kondo destruction".

[1] J. Bork *et al.*, Nat. Phys. **7**, 901 (2011).
[2] A. Nejati, K. Ballmann, J. Kroha, PRL **118**, 117204 (2017).
[3] F. Eickhoff, B. Lechtenberg, F. Anders, PRB **98**, 115103 (2018).

TT 59.4 Thu 15:45 HSZ 03

Investigation of Yu-Shiba-Rusinov states of magnetic structures on the surface of β-Bi_2Pd superconductor — •Stefano Trivini, Jon Ortuzar, Javier Zaldivar, and Nacho Pascual — CICnanoGUNE, San Sebastiàn, Spain

Magnetic atoms deposited on superconductors induce a pair breaking effect that reflects in intragap states known as Yu-Shiba-Rusinov (YSR) states.[1]

Through their interaction with the substrate, the atoms can be magnetically coupled between each other. This magnetic interaction is reflected in the YSR sub gap structure.[2]

While the effect of magnetic coupling of atoms in extended wires on their Kondo interaction[2] or spin excitation[2] has been previously addressed, the behavior on their YSR is still being investigated.

Here, we do atomic manipulation of magnetic adatoms on β-Bi_2Pd by low temperature STM, building atomically perfect magnetic structures. The YSR states can be measured by means of STS with a β-Bi_2Pd superconducting tip with 100 ueV energy resolution.

TT 59.5 Thu 16:00 HSZ 03

Transport in interacting quantum dots: Analytical results from the path integral approach beyond the weak tunneling regime — •Luca Magazzù and Milena Grifoni — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We report on the progress in transport calculations with an analytical path integral technique applied to interacting quantum dots. Starting from the formally exact diagrammatic representation of the dot dynamics and current, a suitable parametrization of the paths of the dot variables allows to apply resummation schemes which address parameter regimes ranging from the noninteracting to the low temperature/strongly-interacting. The known analytical results are recovered in the appropriate limits.

TT 59.6 Thu 16:15 HSZ 03

Theory of scanning tunnelling spectroscopy of Co adatoms in a magnetic field: A Kondo problem of an extended impurity — •Bimla Danu[1], Fakher F. Assaad[1], and Frédéric Mila[2] — [1]Institut fur Theoretische Physik und Astrophysik, Universitat Wurzburg, Am Hubland, D-97074 Wurzburg, Germany — [2]Institute of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The ability to build and manipulate various Kondo nano-structures has been demonstrated in many recent experiments using scanning tunneling spectroscopy (STS). For example, recent STS experiments on chains of Co adatoms have revealed a series of level crossings as a function of magnetic field. Motivated by these experimental studies, we explore the magnetic field induced Kondo effect that takes place at symmetry protected level crossings in finite Co adatom chains. In particular, we provide a quantitative theory of STS signal based on auxiliary-field quantum Monte Carlo simulations, and, show that the physics at the vicinity of level crossings is a Kondo problem of an extended Impurity.

TT 59.7 Thu 16:30 HSZ 03

Nonlinear polaron dynamics — •Tomasz Wasak, Falko Pientka, and Francesco Piazza — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

A mobile impurity immersed into a degenerate Fermi system is a paradigmatic problem in many-body physics. In 2D, the impurity is dressed by particle-hole excitations and forms a new quasi-particle, called the polaron, with new dispersion relation and effective mass.

Recent observation of polaron signatures in 2D semiconductors renewed interest in this field. These systems, based on atomically thin transition metal dichalcogenides, offer promising applications in both linear and nonlinear optics, since the strongly bound excitons dominate the optical response. The presence of a bath of fermions leads to dressing of excitons resulting in the formation of exciton-polarons. These new excitations, when coupled to microcavity photons, can find applications in novel photonic devices, such as exciton-polariton lasers.

The description of the polaron physics in these systems was based on equilibrium quantum field theory or wave function techniques. However, due to finite lifetime of excitons, the system is non-equilibrium in nature, and a proper treatment is required that includes gain and loss into the theoretical description. We have developed a technique based on Keldysh non-equilibrium field-theoretical approach tailored for this open quantum system. We derived a quantum kinetic Boltzmann equation that consistently includes dissipation and drive, and allows to study the transitions between repulsive and attractive polaron branches, and non-equilibrium distributions.

15 min. break.

TT 59.8 Thu 17:00 HSZ 03

Unusual phase boundary of the magnetic-field-tuned valence transition in $CeOs_4Sb_{12}$ — •Kathrin Götze[1], Matthew Pearce[1], Paul Goddard[1], Marcelo Jaime[2], M. Brian Maple[3], Kalyan Sasmal[3], Tatsuya Yanagisawa[4], Alix McCollam[5], Thomas Khouri[5], Pei-Chun Ho[6], and John Singleton[2] — [1]University of Warwick, Coventry, UK — [2]National High Magnetic Field Laboratory, Los Alamos, USA — [3]University of California, San Diego, USA — [4]Hokkaido University, Sapporo, Japan — [5]High Field Magnet Laboratory (EMFL), Nijmegen, NL — [6]California State University, Fresno, USA

The H-T phase diagram of the filled skutterudite $CeOs_4Sb_{12}$ was mapped out in magnetic fields up to 60 T by resistivity, magnetostriction, and MHz conductivity. The semimetallic low-H, low-T L phase and the metallic high-H, high-T H phase are separated by a valence transition which – opposing the "elliptical" text-book behaviour for which $H^2 \propto T^2$ – exhibits a boundary with an almost wedge-like shape with a non-monotonic gradient that alternates between positive and negative. We ascribe the unusual behaviour of the phase boundary at low T to the presence of additional energy scales associated with a quantum critical point. Field-dependent, increasing effective masses derived from quantum oscillations close to the intersection of L, H and the ordered spin-density wave phase are interpreted as indicators of this quantum criticality. The high-T, low-H portion of the phase diagram may instead be associated with the proximity of $CeOs_4Sb_{12}$ to a topological semimetal phase induced by uniaxial stress.

TT 59.9 Thu 17:15 HSZ 03

Controlling electronic phases in an excitonic insulator by cryogenic scanning tunneling microscopy — •Qingyu He[1], Xinglu Que[1], Alexander Yaresko[1], Andreas Rost[1,3], Masahiko Isobe[1], Tomohiro Takayama[1], Lihui Zhou[1], and Hidenori Takagi[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Tokyo, Tokyo, Japan — [3]University of St. Andrews, St. Andrews, England

The excitonic insulator is a long conjectured correlated electron phase stabilized by weakly screened electron-hole interactions. Recent intensive studies have established Ta_2NiSe_5 as one of the most promising candidate materials. The precise control of a many-body electronic phase with an external handle is both challenging and interesting. In our study, we realized a full and controllable phase tuning of Ta_2NiSe_5 from the excitonic insulator ground state to a zero-gap semiconductor state by using a tip of scanning tunneling microscope. Such dramatic reconstruction of electronic states proves the many-body nature of the gap in Ta_2NiSe_5, and is consistent with excitonic insulator behavior.

TT 59.10 Thu 17:30 HSZ 03

Ab-initio study of the possible excitonic insulator Ta_2NiSe_5. Investigating the electronic properties of the structural transition and its excitonic features — •Lukas Windgaetter[1], Simone Latini[1], Hannes Huebener[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Center for Computational Quantum Physics (CCQ), Flatiron Institute, 162 Fifth Avenue, New York NY 10010, USA

The excitonic insulator is a theoretically predicted phase in which a condensate of bound electron hole pairs is the electronic groundstate of the crystal. Recently Ta_2NiSe_5 has been proposed as a promising candidate material with many experiments hinting towards the existence of such an excitonic insulating phase. However, it is still under debate whether the high temperature phase is semi-metallic or a small gap semiconductor and how the pure structural transition which accompanies the excitonic transition affects the materials properties. To settle these questions a thorough theoretical study using ab-initio methods is needed. We present DFT and GW calculations for the high-temperature orthorhombic phase as well as for the low temperature monoclinic phase of Ta_2NiSe_5. We show that our results suggest, that the high temperature phase starts from a semi-metallic groundstate which becomes a semiconductor in the low temperature phase after undergoing the structural phase transition. Furthermore we investigate the phonon spectrum and identify a soft phonon mode in the high temperature phase which drives the structural transition.

TT 59.11 Thu 17:45 HSZ 03

Zeeman spin-orbit coupling and magnetic quantum oscillations in an antiferromagnetic organic metal — Florian Kollmannsberger[1,2], Michael Kunz[1,2], Werner Biberacher[1], Pavel Grigoriev[3], Revaz Ramazashvili[4], Hideki Fujiwara[5], and •Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]L. D. Landau Institute for Theoretical Physics, Chernogolovka, Russia — [4]Laboratoire de Physique Théorique, Université de Toulouse, Toulouse, France — [5]Osaka Prefecture University, Osaka, Japan

We employ the layered organic antiferromagnetic (AF) superconductor κ-$(BETS)_2FeBr_4$ as an exemplary system for revealing theoretically predicted [1] Zeeman spin-orbit coupling (SOC). This novel type of SOC has been proposed as a generic feature of antiferromagnetic metals producing several unusual effects. In particular, it should lead to spin degeneracy of Landau levels, which can be probed by magnetic quantum oscillations [2]. To this end, we have carried out detailed studies of the magnetic quantum oscillations in the low-field, AF, as well as in the high-field, paramagnetic (PM) states of κ-$(BETS)_2FeBr_4$. We have found that the spin-splitting effect on the oscillation amplitude, observed in the PM state, completely disappears in the AF state [3]. We interpret this result as a direct signature of the Zeeman SOC.

[1] R. Ramazashvili, Phys. Rev. Lett. **101**, 137202 (2008).
[2] V.V. Kabanov et al., Phys. Rev. B **77**, 132403 (2008).
[3] R. Ramazashvili et al., arXiv:1908.01236 (2019).

TT 59.12 Thu 18:00 HSZ 03

LDA+DMFT view on electronic structure and magnetism of UGa_2 — •Banhi Chatterjee and Jindrich Kolorenc — Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic

Whether the uranium 5f electrons are closer to being localized or itinerant in the intermetallic compound UGa_2 is still debated. The experimental magnetic moments are large, approximately 3 μ_B, favoring the localized picture. LDA severely underestimates the moments. Although the moments are enhanced within LDA+U, they do not reach the experimental value for a reasonably large U [1]. We investigate if the picture can be improved within LDA+DMFT using exact diagonalization as the impurity solver. We can reproduce the recently measured x-ray absorption spectra at the uranium M edge better than LDA+U [1]. Distinctive spectral features are identified as fingerprints of the localized 5f electrons. We can further recover the experimental valence band photoemission spectra. We present two different formulations of the theory: In LDA+DMFT the polarization is induced only to the 5f states by means of a polarized self-energy, in LSDA+DMFT all states are allowed to polarize. It turns out that neither of the methods gives satisfactory magnetic moments without *ad hoc* manual intervention in tuning the spin polarized double counting.

[1] A. V. Kolomiets, M. Paukov, J. Valenta, A. V. Andreev, K. Kvashnina, F. Wilhelm, A. Rogalev, D. Drozdenko, P. Minarik, J. Kolorenc, B. Chatterjee, M. Richter, L. Havela (in preparation).

TT 59.13 Thu 18:15 HSZ 03

Metal-to-insulator transition in a Dirac semimetal: the case of $BaNi_xCo_{1-x}S_2$ — Benjamin Lenz and •Michele Casula — Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, 4 Place Jussieu, 75005 Paris, France

We study the mechanism behind the metal-to-insulator transition in the correlated $BaNi_xCo_{1-x}S_2$ series, by using advanced many-body first-principles methods, such as a combination of density functional theory and dynamical mean field theory (DFT+DMFT).
The $BaNi_xCo_{1-x}S_2$ family, first considered as a potential candidate for high-temperature superconductivity, has seen a renewed attention for its fascinating spin properties. $BaNiS_2$ is a Dirac semimetal, with 4 Dirac cones lying at the Fermi level, and with strong spin-orbit coupling, placing it close to a topological phase.
Rationalizing its phase diagram as a function of doping and temperature offers a unique opportunity to understand the interplay between topology and correlation in an experimentally accessible situation.

TT 60: Cryotechnique: Refrigeration and Thermometry

Time: Thursday 15:00–17:45 Location: HSZ 103

TT 60.1 Thu 15:00 HSZ 103

Characterization of mechanical vibrations and temperature oscillations on a low input power small scale 4 K pulse tube cryocooler — •Jack-Andre Schmidt[1,2], Bernd Schmidt[1,2], Jens Falter[1,2], Günter Thummes[1,2], and André Schirmeisen[1,2] — [1]Justus-Liebig-University Giessen — [2]TransMIT GmbH

Closed-cycle cryocoolers have become an important cooling concept tool for scientific research at low temperatures [1]. We here focus on Gifford-McMahon (GM) type pulse tube cryocoolers (PTC), which offer long measurement periods and low maintenance, but they exhibit undesired intrinsic effects due to the working principle.

The presentation will be about the study of these effects on a small scale 4 K PTC [2] driven by a helium compressor with adjustable input power between 0.9 and 2.3 kW [3]. The compressor makes it possible to characterize mechanical vibrations and temperature oscillations as a function of helium pressure level inside the cold head. Furthermore, the adjustment of the compressor has also influence on the cooling performance. On the basis of the attained results it is possible to propose new cooling procedures for future applications with pulse tube cryocoolers.

[1] R. Güsten, et al., Nature 568 (2019) 357-359
[2] B. Schmidt, et al., Cryogenics 88 (2017) 129-131
[3] C. Chialvo, et al., Cryocoolers 18 (2014)

TT 60.2 Thu 15:15 HSZ 103

Uniaxial strain cell for small-bore cryogenic systems — •Joonbum Park — Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

We present the development status of the miniaturized uniaxial strain cell for small-bore cryostats. This cell operates with two 18 mm piezoelectric stack actuators with a mechanical amplifier circuit and is capable of producing 1.0

TT 60.3 Thu 15:30 HSZ 103

Nanocalorimetry of Quantum Materials — •Mari C. Cole[1],

Craig V. Topping[1], Andreas Gauss[2], Maximilian Kühn[2], Thomas Reindl[2], Ulrike Waizmann[2], Jürgen Weis[2], and Andreas W. Rost[1] — [1]University of St Andrews, School of Physics and Astronomy, North Haugh, St Andrews, KY16 9SS — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

New strongly correlated quantum materials not yet available as large single crystals as well as designer heterostructures grown by thin film techniques are central to many condensed matter research programmes. Thermodynamic measurements can give clear information about excitations and phase transitions but both types of materials have total heat capacities too small to be studied directly by conventional specific heat experiments. The requirement for a thermometer to have low thermal mass, be field independent, and make a primary temperature measurement due to challenges in calibration lead us to develop a SiN membrane supported Coulomb Blockade Thermometer [1] using Nanofabrication techniques to fabricate $Al/Al_2O_3/Al$ tunnel junctions. Current target materials for our studies include micrometre sized crystals of spin liquid candidates as well as thin films of heavy fermion compounds. I will report on commissioning measurements using heavy fermion compounds such as $CeAuSb_2$.

[1] J. P. Kauppinen et al., *Rev. Sci. Instrum.*, **69**, 4166 (1998)

TT 60.4 Thu 15:45 HSZ 103

Cross Correlated Noise Thermometer for Milli-Kelvin Temperatures — •Christian Ständer, Sebastian Kempf, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University.

Within our search for easy-to-use and 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 silver is monitored simultaneously by two current sensing dc-SQUIDs. Operating both SQUIDs in voltage biased mode in a 2-stage 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 designed and fabricated SQUIDs with minimal coupling of input and feedback coil. We recently assembled a first small series of such thermometers to best reliability, reproducibility and user friendliness at beta-testing sites. In the complete investigated temperature range from 4 K down to 5 mK, the measured noisepower is linear in temperature. Statistical uncertainty below 0.1% is achieved within integration times of 45 s. The thermometers of the series agree within less than 0.1% in the complete temperature range.

TT 60.5 Thu 16:00 HSZ 103

A Microcalorimeter Based on Metallic Paramagnetic Temperature Sensors — •Matthew Herbst, Andreas Reifenberger, Clemens Velte, Sebastian Kempf, Loredana Gastaldo, Andreas Fleischmann, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg, Germany

We present a micro-fabricated platform designed to measure the heat capacity of mg-sized samples at temperatures between 10 mK and 500 mK. The set-up makes use of the relaxation method, where the thermal response following a well defined heat pulse is monitored in order to extract the specific heat. Thermometry is based on a paramagnetic Ag:Er temperature sensor, which is read out by a dc-SQUID via a superconducting flux transformer. This allows us to reach a relative temperature precision better than $30\,\mathrm{nK}/\sqrt{\mathrm{Hz}}$ and an addenda heat capacity of 400 pJ/K (at 50 mK). Besides the performance of the set-up, we also present the results of first measurements of holmium-doped noble metals. In conjunction with data obtained from other calorimetric set-ups, we are able to shed light on the complex dynamics of these materials, and precisely determine their specific heat at different temperatures and chemical compositions. The measurements also have direct application for projects such as the neutrino mass experiment ECHo, where the heat capacity of holmium alloys directly influences the energy resolution of the detector.

TT 60.6 Thu 16:15 HSZ 103

Chip-based calorimeter for micro- and nanostructures — •Julian Litzel, Sebastian Kölsch, Fabrizio Porrati, and Michael Huth — Institute of Physics, Goethe University, Max-von-Laue-Str. 1, Frankfurt am Main 60438, Germany

Recently, direct-write nanofabrication by focused electron or ion beam induced deposition (FEBID/FIBID) has gained significance in various areas of solid state physics and materials science [1]. Single or multi-component ferromagnetic, superconducting and granular electronic micro- and nanostructures can now be fabricated routinely at a lateral resolution that rivals advanced electron beam lithography but also allows the creation of complex three-dimensional nano-architectures. Due to the small size of these structures, standard techniques for heat capacity measurements cannot be applied.

We are developing a turn-chip based platform for heat-pulse calorimetry that uses a thin SiN_x membrane onto which the heater element and thermometer are deposited by applying direct-writing techniques. This membrane then serves as the platform for the material whose heat capacity is measured. We present the chip design and show first results.

[1] M. Huth, F. Porrati, O. V. Dobrovolskiy, Microelectronic Engineering, 185 - 186, 9 (2018)

15 min. break.

Invited Talk TT 60.7 Thu 16:45 HSZ 103

Heat and Work Fluctuations in a Quantum Heat Engine — Timo Kerremans, Peter Samuelsson, and •Patrick P. Potts — Physics Department and Nanolund, Lund University, Sweden

The fluctuations of thermodynamic observables shed insight into the non-classical nature of quantum thermal machines, paving the way for developing novel quantum technologies. I will present a detailed case study of heat and work fluctuations in the heat engine proposed in [Phys. Rev. B **93**, 041418(R)]. As a thermo-electric device, work fluctuations are directly linked to electrical current fluctuations, circumventing any ambiguity in defining work as a fluctuating quantity in the quantum regime. We find that while heat fluctuations can be described classically, the work fluctuations either require a quasi-probabilistic description, or an explicit description of the measurement process. The non-classicality of the work fluctuations implies that the first law of thermodynamics cannot be formulated for a single experimental run. This is in stark contrast to classical fluctuating systems, where only the second law may be violated for single runs.

TT 60.8 Thu 17:15 HSZ 103

Tunable refrigerator for non-linear quantum electric circuits — •Hao Hsu and Gianluigi Catelani — Forschungszentrum Jülich, Jülich, Germany

The emerging quantum technological devices call for fast and accurate initialization of the functional quantum states to a low-entropy state. To this end, we theoretically study a recently demonstrated quantum-circuit refrigerator [1][2] in the case of non-linear quantum electric circuits such as superconducting qubits. We find that for typical experimental parameters, the refrigerator is suitable for quickly cooling different qubit types close to their ground states. In fact, the maximum refrigeration rate of transmon and flux qubits is roughly an order of magnitude higher than that of usual linear resonators, providing additional flexibility in design criteria. The dynamic on/off ratio of the refrigeration rates assumes values above 10^4 with typical experimental parameters. Thus the refrigerator is a promising tool for quantum technology and for detailed studies of open quantum systems.

[1] K. Y. Tan et.al., Nat. Commun. 8 15189 (2017)
[2] M. Silveri et.al., Phys. Rev. B 96, 094524 (2017)

TT 60.9 Thu 17:30 HSZ 103

Enhanced Grüneisen Parameter in Supercooled Water — •Mariano de Souza[1], Gabriel Gomes[2], and Harry E. Stanley[3] — [1]São Paulo State University, IGCE - Department of Physics, Rio Claro - SP, 13506-900, Brazil — [2]University of São Paulo, Department of Astronomy, São Paulo, 05508-090, Brazil — [3]Boston University, Department of Physics, Boston, 02215, USA

We use the recently-proposed compressible-cell Ising-like model to estimate the ratio between thermal expansivity and specific heat (the Grüneisen parameter in supercooled water. Near the critical pressure and temperature, the Grüneisen parameter becomes significantly sensitive to thermal fluctuations of the order-parameter, a characteristic behaviour of pressure-induced critical points. Such enhancement of the Grüneisen parameter indicates that two energy scales are governing the system, namely the coexistence of high- and low-density liquids, which become indistinguishable at the critical point in the supercooled phase. The temperature dependence of the compressibility, sound velocity and pseudo-Grüneisen parameter are also reported. Our findings support the proposed liquid-liquid critical point in supercooled water in the No-Man's Land regime and indicates possible applications of this model to other systems [1]. In particular, an application of the model to the qualitative behaviour of the Ising-like nematic phase in Fe-based superconductors is also presented.

[1] G. Gomes, H.E. Stanley, M. de Souza, Scientific Reports 9, 12006 (2019).

TT 61: Ultrafast Dynamics of Light-Driven Systems (joint session TT/MA)

Time: Thursday 15:00–17:45 Location: HSZ 201

TT 61.1 Thu 15:00 HSZ 201

Out-of-equilibrium magnetism of Sr_2IrO_4 and La_2CuO_4 — •Ekaterina Paerschke[1], Yao Wang[2], and Cheng-Chien Chen[3] — [1]Institute of Science and Technology Austria, Am Campus 1, 3400 Klosterneuburg, Austria — [2]Department of Physics, Harvard University, Cambridge 02138, USA — [3]Department of Physics, University of Alabama at Birmingham, Birmingham, Alabama 35294, USA

Ultrafast pump-probe spectroscopy is an efficient tool to characterize and control strongly correlated materials due to its accessibility to both low-energy physics of the equilibrium phase and the novel excited states induced by the pump. Here, we investigate the ultrafast control of quantum magnetism in a half-filled Mott insulator, described by an extended Heisenberg model. This study reveals photo-manipulated magnetic properties for two archetypal Mott insulators: iridate Sr_2IrO_4 and cuprate La_2CuO_4. Understanding photo-manipulated spin fluctuations in cuprates and iridates can help to solve the long-standing question of superconductivity absence in the iridates, as spin fluctuations are believed to mediate superconductivity in transitional metal oxides. Starting from a broken-symmetry phase with a (π, π) ordering vector, we find that the various pump conditions can manipulate the competition with the subleading colinear AFM phase. Through the comparison of quantum quench simulations and Floquet analytical theory, we conclude that these manipulations are achieved through transient engineering of effective spin-exchange interactions.

TT 61.2 Thu 15:15 HSZ 201

Ultrafast spectroscopy of the Kitaev magnet $RuCl_3$ — •Raluca Aldea, Rolf B. Versteeg, Fumiya Sekiguchi, Anuja Sahasrabudhe, Kestutis Budzinauskas, Zhe Wang, and Paul H.M. van Loosdrecht — II. Physikalishes Institut, Universität zu Köln, Züplicher Str.77, Köln, Germany

Kitaev materials are a group of spin orbit assisted Mott insulators that bear strong bond-directional exchange interactions. This was discussed to result in a Kitaev liquid, implying that spins fractionalize in exotic Majorana fermion and Z_2 flux excitations. We use pump-probe spectroscopy in order to investigate the magnetization dynamics above and below the zigzag ordering temperature. We discuss the dynamics in terms of coupling between different degrees of freedom.

TT 61.3 Thu 15:30 HSZ 201

Ultrafast jamming transition in a charge-ordered system — •Yaroslav Gerasimenko[1,2], Jaka Vodeb[1], Jan Ravnik[1], Igor Vaskivskyi[1], Michele Diego[1], Viktor Kabanov[1], and Dragan Mihailoivic[1,2] — [1]Jozef Stefan Institute, Ljubljana, Slovenia — [2]CENN Nanocenter, Ljubljana, Slovenia

The combination of STM and in situ ultrafast excitation allows us to explore novel states of matter that can emerge from many-body interactions under highly non-equilibrium conditions. Most of such states are reminiscent of the nearby equilibrium ones. Here we show that a single femtosecond-scale optical pulse, applied to the prototypical transition metal dichalcogenide 1T-TaS2, can convert a perfect hexagonal charge order into a dramatically different metastable jammed state of strongly correlated electrons [1]. The mechanism for its formation is attributed to a dynamical localization of electrons through mutual interactions in absence of atomic disroder. We further build the phase diagaram of this transition as a function of fluence and temperature on multiple timescales. The time evolution of the localized charge pattern together with theoretical calculations [1, 2] confirm that charge order frustration is important for the state's unusual stability.

The work was supported by ARRS P1-0040 and ERC AdG "Trajectory".

[1] Ya. A. Gerasimenko et al., Nature Materials 18, 1078-1083 (2019)
[2] J. Vodeb et al., New J. Phys. 21, 083001 (2019)

TT 61.4 Thu 15:45 HSZ 201

Creating non-equilibrium orders in high-temperature superconductors — •Guido Homann[1], Jayson Cosme[1,2], and Ludwig Mathey[1,2] — [1]Zentrum für Optische Quantentechnologien und Institut für Laserphysik, Universität Hamburg, 22761 Hamburg, Germany — [2]The Hamburg Center for Ultrafast Imaging, 22761 Hamburg, Germany

We simulate far-out-of-equilibrium dynamics in cuprate superconductors, such as YBCO, employing a semiclassical approach. Our approach combines relativistic c-field theory with a $U(1)$ lattice gauge theory, resulting in a 3D lattice of intrinsic Josephson junctions. Our description includes dissipation and thermal fluctuations. It constitutes an extension of 1D sine-Gordon models, due to the inclusion of amplitude dynamics and of in-plane fluctuations. We implement a variety of driving protocols, which address the plasmonic or phononic degrees of freedom, and explore the resulting non-equilibrium scenarios. As a central example, we apply our method to transient phenomena induced in pump-probe protocols, and compare to observed phenomena. This work extends and builds on previous studies reported in [1,2], and has its main focus on the creation of metastable superconducting states.

[1] J. Okamoto, A. Cavalleri, L. Mathey, Phys. Rev. Lett. **117**, 227001 (2016).
[2] J. Okamoto, W. Hu, A. Cavalleri, L. Mathey, Phys. Rev. B **96**, 144505 (2017).

TT 61.5 Thu 16:00 HSZ 201

Detecting superconductivity out-of-equilibrium — •Sebastian Paeckel[1], Benedikt Fauseweh[2,3], Alexander Osterkorn[1], Thomas Kohler[4], Dirk Manske[3], and Salvatore R. Manama[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [4]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

Recent pump-probe experiments on underdoped cuprates and similar systems suggest the existence of a transient superconducting state above T_c. This poses the question how to reliably identify the emergence of long-range order, in particular superconductivity, out-of equilibrium. We investigate this point by studying a quantum quench in an extended Hubbard model and by computing various observables, which are used to identify (quasi-)long-range order in equilibrium. Our findings imply that, in contrast to current experimental studies, it does not suffice to study the time evolution of the optical conductivity to identify superconductivity. In turn, we suggest to utilize time-resolved ARPES experiments to probe for the formation of a condensate in the two-particle channel.

15 min. break.

TT 61.6 Thu 16:30 HSZ 201

Phase-sensitive analysis of Higgs oscillations in quenched superconductors with time- and angle-resolved photo emission spectroscopy — •Lukas Schwarz and Dirk Manske — Max Planck Institute for Solid State Research

Higgs oscillations in nonequilibrium superconductors provide a unique tool to obtain information about the underlying order parameter. Several quantities like the absolute value, existence of multiple gaps and the symmetry of the order parameter can be encoded in the Higgs oscillation frequency. Most works so far concentrate on experiments, where momentum averaged quantities like the optical conductivity or third-harmonic effects in the transmitted light field are investigated, which does not allow to access all possible information contained in the Higgs oscillations. Here, we study the time-resolved spectral function measured in angle-resolved photo emission spectroscopy after quenching the system using a general approach. We analyze the induced oscillations all over momentum space to study the creation process of collective Higgs oscillations and we extract phase information of the order parameter from the oscillations of the spectral function.

TT 61.7 Thu 16:45 HSZ 201

Controlling subdominant pairing symmetries in pumped unconventional superconductors — •Marvin A. Müller[1], Pavel A. Volkov[1,2], Indranil Paul[3], and Ilya Eremin[1,4] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany — [2]Department of Physics and Astronomy, Center for Materials Theory, Rutgers University, Piscataway, New Jersey 08854, USA — [3]Laboratoire Matériaux et Phénomènes Quantiques, Université de Paris, CNRS, F-75013 Paris, France — [4]Institute of Physics, Kazan Federal University, Kazan 420008, Russian Federation

We investigate the short-time dynamics in superconductors with multiple attractive pairing channels out of equilibrium. Studying a single-band square lattice model with a spin-spin interaction as an example, we find the signatures of collective excitations of the subdominant pairing symmetries (known as Bardasis-Schrieffer modes) as well as the order parameter amplitude (Higgs mode) in the short-time dynamics of the spectral gap and quasiparticle distribution after an excitation by a pump pulse. We show that the polarization and intensity of the pulse can be used to control the symmetry of the nonequilibrium state as well as frequencies and relative intensities of the contributions of different collective modes. We find particularly strong effects of the Bardasis-Schrieffer mode in the dynamics of the quasiparticle distribution function and propose possible signatures in trARPES experiments.

TT 61.8 Thu 17:00 HSZ 201

Revealing Hund's multiplets in Mott insulators under strong electric fields — •Nagamalleswararao Dasari[1], Jiajun Li[1], Philipp Werner[2], and Martin Eckstein[1] — [1]Department of Physics, University of Erlangen-Nuremberg, 91058 Erlangen, Germany — [2]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

We investigate the strong-field dynamics of a paramagnetic two-band Mott insulator using real-time dynamical mean-field theory. We demonstrate that strong electric fields can lead to a transient localization of electrons. This nonequilibrium quantum effect allows to reveal specific signatures of local correlations in the time-resolved photoemission spectrum. In particular, we demonstrate that the localization can be strong enough to produce atomic-like spin multiplets determined by the Hund's coupling J, and thus provide a way of measuring J inside the solid. Our simulation also fully incorporates non-linear field-induced tunnelling processes, which would lead to a dielectric breakdown in the steady state limit. A careful analysis of these processes however shows that they remain weak enough and do not prevent the measurement of the transiently localized spectra.

TT 61.9 Thu 17:15 HSZ 201

Ultrafast electronic correlations in ordered phases — •Riku Tuovinen[1], Denis Golež[2], Martin Eckstein[3], and Michael A. Sentef[4] — [1]QTF Centre of Excellence, Turku Centre for Quantum Physics, Department of Physics and Astronomy, University of Turku, 20014 Turku, Finland — [2]Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA — [3]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany — [4]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

We consider many-body correlations in an excitonic-insulator system acting as a prototypical ordered-phase material [1]. Out-of-equilibrium dynamics in such systems with a symmetry-broken ground state has been shown to be extremely sensitive to all the intricacies in the electronic structure [2]. For an accurate description of the important and interesting mechanisms we take into consideration strong external fields, many-body correlations, and transient effects at an equal footing by the nonequilibrium Green's function technique [3]. We drive the system out-of-equilibrium by a laser pulse, and we compare the resolved dynamics between the Kadanoff-Baym equations and the computationally less expensive generalized Kadanoff-Baym Ansatz [4].

[1] S. Mor et al. Phys. Rev. Lett. 119, 086401 (2017)
[2] R. Tuovinen et al. Phys. Status Solidi B 256, 1800469 (2018)
[3] G. Stefanucci and R. van Leeuwen, Nonequilibrium Many-Body Theory of Quantum Systems, CUP (2013)
[4] R. Tuovinen et al. in preparation

TT 61.10 Thu 17:30 HSZ 201

Ultrafast metal-to-insulator switching in a strongly correlated system — •Francesco Grandi and Martin Eckstein — Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany

Several experiments have shown the possibility to induce an ultrafast insulator-to-metal phase transition in correlated materials. Instead, it remains debated how to experimentally realize an ultrafast phase transition in the opposite direction, i.e. a metal-to-insulator phase change. Developing a protocol that can lead to such a transition is relevant for the realization of a Mottronic device able to operate at the ultrafast time scales. A possible candidate for the realization of this scenario is the oxygen-enriched $LaTiO_{3+x}$, a correlated metal close to the Mott insulator $LaTiO_3$.
Here, we consider an effective model that we believe captures the main physical properties of $LaTiO_{3+x}$. We describe the photo-doping of electrons into the valence bands of the material from the low-lying oxygens 2p-derived band using non-equilibrium Dynamical Mean-Field Theory. By applying a suitably designed chirped-pulse that leads to dipolar excitations, we analyze how fast we can induce the metal-to-insulator transition and how far the final state is from a thermal configuration.

TT 62: Correlated Electrons: Method Development 2

Time: Thursday 15:00–16:15 Location: HSZ 204

TT 62.1 Thu 15:00 HSZ 204

π-tons – Characteristics of vertex corrections to the optical conductivity in strongly correlated metals. — •Paul Worm, Clemens Watzenböck, Anna Kauch, and Karsten Held — Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The interaction of a solid with an electromagnetic field, or from a quantum point of view with photons, gives rise to new quasi-particles coined polaritons. For semi-conductors the exciton is the generic polariton, the characteristics of which are rather well understood. In strongly correlated systems the dominant polariton was shown to be different, namely a recent study using the parquet equations [1], which are not biased in favor or against certain channels or physics, observed in Hubbard-like systems new polaritons: π-tons. These π-tons manifest themselves in vertex corrections to the optical conductivity that are dominated by the contributions in the particle-hole transversal channel. They consist of two particle-hole pairs glued together by anitferromagnetic or charge density wave fluctuations.
In order to investigate the π-ton contributions in more detail and without the necessity of a cumbersome numeric analytic continuation we use a simplified real frequency formalism, which grants us complete control over the diagrams included. We reproduce the core features of the vertex corrections with simplified ladder diagrams in the particle-hole transversal channel [1]. This confirms these ladder diagrams are indeed the dominant vertex contributions.

[1] A.Kauch et al., arXiv:1902.09342

TT 62.2 Thu 15:15 HSZ 204

The role of the self-energy in the quantitative functional renormalization-group description of the two-dimensional Hubbard model — •Cornelia Hille[1], Fabian B. Kugler[2], Christian J. Eckhardt[3,4,5], Yuan-Yao He[6,7], Anna Kauch[3], Daniel Rohe[8], Carsten Honerkamp[4,5], Alessandro Toschi[3], and Sabine Andergassen[1] — [1]Universität Tübingen, Tübingen, Germany — [2]LMU München, Munich, Germany — [3]TU Vienna, Vienna, Austria — [4]RWTH Aachen University, Aachen, Germany — [5]JARA-FIT, Jülich Aachen, Germany — [6]Flatiron Institute, New York, USA — [7]College of William and Mary, Williamsburg, USA — [8]Forschungszentrum Jülich GmbH, Jülich, Germany

The recently introduced multiloop extension of the functional renormalization group (fRG), which sums up all parquet diagrams with their exact weights, allows us to perform the first quantitative analysis for the 2D Hubbard model and to compare the results to the parquet approximation and determinant quantum Monte Carlo. We show that for convergence of the Truncated Unity fRG (form-factor expansion of the fermionic momentum dependence) to the solution of the parquet approximation, the self-energy flow has to be reformulated in analogy to the Schwinger-Dyson equation. The presented methodological improvement provides the basis towards quantitative predictions for more general systems. On a qualitative level, this new formulation is also crucially important for the description of single-particle properties such as the pseudogap opening.

TT 62.3 Thu 15:30 HSZ 204

Consistent partial bosonization of the extended Hubbard model — •Viktor Harkov[1,2], Alexander I. Lichtenstein[1,2,3], and Evgeny A. Stepanov[1,3] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]European X-Ray Free-Electron Laser Facility, 22869 Schenefeld, Germany — [3]Theoretical Physics and Applied Mathematics Department, Ural Federal University, 620002 Ekaterinburg, Russia

A simple but efficient description of collective electronic excitations in realistic systems can be achieved performing a partial bosonization of collective fermionic fluctuations in leading channels of instability. In some approximations a simultaneous account for different bosonic channels gives rise to a famous Fierz ambiguity in decomposition of the local Coulomb interaction into considered channels, which drastically affects the final result of the method. We introduce a consistent partial bosonization of the fermionic problem that finally solves the famous Fierz ambiguity problem. We apply our method to extended Hubbard model and derive an effective theory that is formulated in terms of original fermionic degrees of freedom, new bosonic fields, and an effective fermion-boson interaction. We show that the fermion-fermion interaction can be safely excluded from the model, which results in a very simple approximation that significantly improves all existing partially bosonized theories. In addition, our approach allows an inclusion of magnetic fluctuations in the GW scheme in a consistent way.

[1] E. A. Stepanov, V. Harkov, and A. I. Lichtenstein, Phys.Rev. B 100, 205115 (2019).

TT 62.4 Thu 15:45 HSZ 204

Dimensional crossovers in the Hubbard model based on TUFRG — •Jannis Ehrlich[1,2], Jacob Beyer[1], and Carsten Honerkamp[1] — [1]Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Many correlated electron materials are layered systems, with varying degree of anisotropy or two-dimensionality. Resolving all three dimensions is desirable for a proper theoretical modelling but often faces computational limitations. In this talk we show that the truncated unity functional renormalization group (TUFRG) can be used to explore dimensional crossovers from one to three spatial dimensions in model systems. It employes a parquet-like channel decomposition of the effective interaction in combination with a form factor expansions of the wavevector dependence which allows us to reach relevant wavevector resolution at bearable numerical costs by exploiting the beneficial parallelizability of the recently developed TUfRG library. As example we explore the ground state phase diagram of the anisotropic three-dimensional Hubbard model, exposing the role of dimensionality for the strength of unconventional Cooper pairing.

TT 62.5 Thu 16:00 HSZ 204

Dual parquet scheme for the two-dimensional Hubbard model: modelling low-energy physics of high-T_c cuprates with high momentum resolution — Grigory Astretsov[1,2], •Georg Rohringer[1,3], and Alexey Rubtsov[1,2] — [1]Russian Quantum Center — [2]Lomonosov Moscow State University — [3]University of Hamburg

We present a new method to treat the two-dimensional (2D) Hubbard model for parameter regimes which are relevant for the physics of the high-T_c superconducting cuprates. Our approach consists in the following three-step procedure: (i) High energy correlations are treated exactly by dynamical mean field theory (DMFT). From the DMFT solution we (ii) construct an effective low-energy model which depends only on the lowest Matsubara frequencies. We (iii) apply the two-particle self-consistent parquet formalism which takes into account the competition between different low-energy bosonic modes. In this way, we were able to map out the phase diagram of the 2D Hubbard model as a function of temperature and doping. Consistently with the experimental evidence for hole-doped cuprates and previous dynamical cluster approximation calculations, we find an antiferromagnetic region at low doping and a superconducting dome at higher doping. Our results also support the role of the van Hove singularity as an important ingredient for the high value of T_c at optimal doping. At small doping, the destruction of antiferromagnetism is accompanied by an increase of charge fluctuations supporting the scenario of a phase separated state driven by quantum critical fluctuations.

TT 63: Quantum Magnets and Molecular Magnets (joint session TT/MA)

Time: Thursday 15:00–18:00 Location: HSZ 304

Invited Talk TT 63.1 Thu 15:00 HSZ 304

Linear magnets: a structure-property-relation for finding unquenched orbital moments — •Anton Jesche — EP VI, Center for Electronic Correlations and Magnetism, Augsburg University, 86135 Augsburg, Germany

The presence of orbital magnetic moments in rare-earth-elements is one of the major differences to transition metal compounds and is at the heart of magnetic anisotropy, stability, and functionality. A large crystal electric field effect acting on an unquenched orbital moment can lead to extremely large anisotropy and coercivity as experimentally verified for iron-doped lithium nitride [1]. In the dilute limit, those iron atoms can be considered as single-atom magnets and are ideal candidates to study the quantum dynamics of anisotropic spins [2]. This, together with the strong field dependence of the spin reversal, allows creating stable but switchable states that could act as a 'quantum bit' at elevated temperatures of 10 K. A recent Mössbauer study revealed dominant magnetic quantum tunneling at even higher temperatures [3]. The presence of orbital moments in iron-doped lithium nitride is not a coincidence and not a solitary case: based on the proposed structural motif of the 'linear chain', we have identified several other 'linear magnets' with similar physical properties: iron-doped Li_4SrN_2, $LiSr_2(CoN_2)$, $(Sr_6N)[FeN_2][CN_2]_2$, and K_2NiO_2.Implications and limitations of the linear coordination are discussed in relation to the electronic structure.

[1] M. Fix et al., PRB 97, 064419 (2018)
[2] M. Fix et al., PRL 120, 147202 (2018)
[3] S. A. Bräuninger et al., arXiv:1909.12774

TT 63.2 Thu 15:30 HSZ 304

The power of typicality applied to magnetic molecules and low-dimensional quantum spin systems — •Jürgen Schnack — Universität Bielefeld, Fakultät für Physik

Molecular or low-dimensional quantum spin systems often prevent an exact calculation of their magnetic properties due to a prohibitively large size of the related Hilbert spaces. Typicality-based approaches such as the finite-temperature Lanczos method allow to investigate rather large systems with unprecedented accuracy. This way quantum critical as well as magnetocaloric properties of large cyclic clusters could be elucidated [1]. For the kagome lattice antiferromagnet it became possible to model a lattice of size N=42 (!) quasi exactly. This enabled us to study in particular that the low-lying density of singlet states moves up in energy contrary to common believe [2]. In addition, we could demonstrate for lattices up to 72 sites that magnon crystallization occurs slightly below the saturation field, an effect driven by the existance of flat energy bands [3].

[1] A. Baniodeh et al., npj Quantum Materials 3,10 (2018)
[2] J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B 98, 094423 (2018)
[3] J. Schnack, J. Schulenburg, A. Honecker, J. Richter, arXiv:1910.10448

TT 63.3 Thu 15:45 HSZ 304

Resonant photon absorption in $GdPc_2$ molecular magnet — •Gheorghe Taran[1], Eufemio Moreno-Pineda[2], Edgar Bonet[3], and Wolfgang Wernsdorfer[1,2,3] — [1]Physikalisches Institute, KIT, Karlsruhe — [2]Institute of Nanotechnology (INT), Karlsruhe — [3]Néel Institute, CNRS, Grenoble, France

Single ion molecular magnets (SIMMs) champion a magnetic center (*e.g.* a 3d or 4f ion) whose properties are modulated by the coordinated organic ligands. Their relative simple structure makes the task of correlating structural characteristics to physical properties considerably easier and thus, opens the doors for chemical tailoring for technological applications that range from refrigeration to storage and processing of quantum information.

In this study, we investigate the resonant photon absorption in diluted single crystals of $GdPc_2$ SIMM using micro-SQUID technique at subkelvin temperatures. Combining the advantages of EPR (*e.g.* the ability to explore the anisotropy character of the magnetic interactions) and those of micro-SQUID techniques (*e.g.* time-resolved dynamics on a micro-second scale) we construct the map of resonant transitions in the [1:40] GHz frequency range. The transitions are analyzed in the framework of a single spin Hamiltonian describing the ground state, $S = 7/2$, of the $GdPc_2$ complex and the predictions are compared to the ones made by ab-initio calculations. The unprecedented resolution of the resonant frequency-field maps allows a critical evaluation of the state of the art ab-initio methods for ligand field estimations and sets the base for future investigations into the coherent dynamics.

TT 63.4 Thu 16:00 HSZ 304

Quantum magnetism in Boleite - an Archimedean Solid with strong magnetic frustration — Stefan Lebernegg[1,2], Jürgen Schnack[3], Oleg Janson[4], Johannes Richter[5], Jörg Sichelschmidt[2], Tobias Förster[6], Alexander Tsirlin[7], and •Helge Rosner[2] — [1]Technical University of Munich, 80335, Munich, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [3]Bielefeld University, Faculty of Physics, Universitätsstr. 25, D-33615 Bielefeld, Germany — [4]IFW Dresden Helmholtzstraße 20 01069 Dresden Germany — [5]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden Germany — [6]Dresden High Magnetic Field Laboratory — [7]Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combined theoretical and experimental effort, applying electronic structure calculations and numerical simulations as well as chemical analysis, X-ray diffraction and magnetic measurements had to be joined by mineralogical expertise to unveil the quantum magnetism of the mineral Boleite. This mineral is a strongly frustrated quantum magnet with 24 spin 1/2 Cu sites arranged on the vortices of a truncated cube, one of the famous Archimedean solids. We find that the system with its typical 1/3 magnetization plateau can be well understood by two leading interactions and their "randomness" describing a certain distribution of these exchange interactions.

TT 63.5 Thu 16:15 HSZ 304

Multi band modelling of exchange couplings in edge-sharing Cu-O chains — •Dijana Milosavljevic[1], Oleg Janson[2], Jan Tomczak[3], and Helge Rosner[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [3]Technical University of Vienna, Austria

One of the structural features that has a crucial role in the determination of the exchange coupling constant in chain containing compound is the Cu-O-Cu bond angle. However the angle is not the only factor. Equally important influence on the exchange coupling has the presence of the side groups coupled to the O-ligands. To demonstrate this we show two representatives of edge sharing chain cuprates with similar Cu-O-Cu bond angles but drastically different exchanges. From detailed DFT studies and subsequently derived multi band tight binding models we find that the crucial parameter is the difference in onsite energies of ligand O $2p_x$ and O $2p_y$ orbitals parallel and perpendicular to the Cu-O chain. Using this parameter, a microscopic explanation for the drastically different magnetic exchanges can be established. To illustrate the crucial influence of side groups we provide examples of H-containing compounds where a rotation of H even leads to a sign change of the superexchange interaction from strongly ferromagnetic to strongly antiferromagnetic.

15 min. break.

TT 63.6 Thu 16:45 HSZ 304

Field tunability of BKT correlations in the square-lattice Heisenberg antiferromagnet CuPOF — •D. Opherden[1,2], C. P. Landee[3], F. Bärtl[1,2], M. Uhlarz[1], Y. Skourski[1], A. N. Ponomaryov[1], S. A. Zvyagin[1], 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 realization of the 2D square-lattice $S = \frac{1}{2}$ Heisenberg antiferromagnet with well-separated Cu(pz) layers and a moderate intraplane coupling $J/k_B = 6.8$ K. We present a focus study of the low-T phase transition to long-range order, performed via ^1H and ^{31}P nuclear magnetic resonance and bulk magnetometry. A weak intrinsic easy-plane anisotropy, revealed by magnetization data, yields a temperature-driven crossover of the spin-exchange anisotropy from isotropic Heisenberg to anisotropic XY-type behavior. The application of a magnetic field normal to the easy-plane yields a field-driven increase of the magnetic anisotropy with the occurrence of Berezinskii-Kosterlitz-Thouless correlations, revealed by results of the ^{31}P spin-lattice relaxation rate close to the transition temperature to long-range order. A detailed analysis of the temperature-dependent order parameter demonstrates the possibility for a continuous tuning of the spin-exchange anisotropy in CuPOF, from almost ideal isotropic Heisenberg to nearly XY-type exchange at elevated fields.

TT 63.7 Thu 17:00 HSZ 304

Y-, La- and Lu-Agardite, preparation, crystal structure, vibrational and low-dimensional magnetic properties — •Aleksandr M. Golubev[1], Eva Brücher[1], Armin Schulz[1], Reinhard K. Kremer[1], Robert Glaum[2], and Myung-Hwan Whangbo[3] — [1]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany — [2]Institut für Anorganische Chemie, Universität Bonn, 53121 Bonn, Germany — [3]Department of Chemistry North Carolina State University Raleigh, North Carolina 27695-8204, USA

We have prepared polycrystalline samples of Y, La- and Lu-agardite with composition $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n $\approx$ 3) and characterized their structural and vibrational properties as well as the magnetic behavior of the Cu^{2+} entities. The arsenates $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n $\approx$ 3) are isostructural with the mineral mixite and crystallize with a hexagonal structure which contains ribbons of edge-sharing $[CuO_5]$ square-pyramids extending along the hexagonal axis. They interconnect via $(AsO_4)^{3-}$ groups to form hexagonal tubes of about 10 Å inner diameter. Such zeolite-like tubes host water molecules, which can be reversibly removed at moderate temperature ($\approx$ 100 °C). Like in mixite the Cu^{2+} cations in $RECu_6(OH)_6(AsO_4)_3 \cdot n\ H_2O$ (RE = Y, La, Lu; n $\approx$ 3) exhibit low-dimensional antiferromagnetic properties the character of which is subject to changes in the Cu-O-Cu bonding distances and bonding angles due to the lanthanide contraction. DFT calculations indicate that the strongest spin exchange pathways couple the Cu^{2+} S=1/2 magnetic moments predominantly within the hexagonal tubes.

TT 63.8 Thu 17:15 HSZ 304

Quantum phase transitions of Ising ferromagnets in tilted transverse fields — •Heike Eisenlohr and Matthias Vojta — Institut für theoretische Physik, Technische Universität Dresden, Germany

Transverse-field Ising magnets constitute a paradigmatic example for quantum phase transitions, with experimental realisations in e.g. $LiHoF_4$ and $CoNb_2O_6$. Here we theoretically analyze the fate of the field-driven zero-temperature transition upon tilting the field away from the direction perpendicular to the easy axis. While the transition turns into a crossover if the ordered phase is single-domain, a sharp transition remains in the multi-domain case relevant for a ferromagnet. We characterize this transition in detail, also discussing effects of domain-wall motion. Upon including nuclear spin degrees of freedom, we are able to link our results to experiments on $LiHoF_4$.

TT 63.9 Thu 17:30 HSZ 304

Chemical design strategies and field-induced phases in antiferromagnetically coupled organic spin-dimer systems — •Bernd Wolf[1], Lars Postulka[1], Paul Eibisch[1], Ulrich Tutsch[1], Martin Baumgarten[2], and Michael Lang[1] — [1]Physics Institute, Goethe-University, SFB/TR49, D-60438 Frankfurt (M) — [2]Max-Planck-Institute for Polymer Research, SFB/TR49, D-55128 Mainz

Coupled antiferromagnetic spin-dimer systems based on the stable organic radical units nitronyl-nitroxide (NN) and imino-nitroxide (IN) are recognized as suitable candidates for exploring critical phenomena under well-controlled conditions. For these systems the *intra-* and *inter*-dimer magnetic exchange interactions can be modified in specific ways. Depending on the geometry of the *inter*-dimer couplings, various scenarios can be observed. We discuss the magneto-structural correlations of selected materials based on tolan molecules linked together with NN- and IN-units. Furthermore, using low-temperature ac susceptibility and specific heat measurements we characterize the field-induced magnetic phases of these materials and discuss their critical behavior. In addition, we present a new approach for designing intermolecular magnetic exchange interactions based on planar π-bridges of benzo[1,2 -*b*:4,5 -*b'*] dithiophene derivatives which connect the stable NN and IN radical units. Our results demonstrate that π-stacking of the planar bridges allows a good control of the *inter*-molecular magnetic exchange.

TT 63.10 Thu 17:45 HSZ 304

Field-induced magnetic phase in quasi-one-dimensional $YbAlO_3$ — •Stanislav Nikitin[1,2], Liusuo Wu[3], Aleksandr Sukhanov[1,2], Nikolay Pavlovskiy[4], Jianhui Xu[5], Manuel Brando[1], Leonid Vasylechko[6], and Andrey Podlesnyak[7] — [1]Max Planck Institute CPfS, Dresden, Germany — [2]Technical University Dresden, Germany — [3]Southern University of Science and Technology, Shenzhen, China — [4]Kirensky Institute of Physics, Krasnoyarsk, Russia — [5]Helmholtz-Zentrum Berlin, Berlin, Germany — [6]Lviv Polytechnic National University, Lviv, Ukraine — [7]Oak Ridge National Laboratory, TN , USA

The antiferromagnetic Heisenberg S = 1/2 chain in magnetic field is one of the simplest model, which exhibits quantum critical behavior. In finite magnetic field below the QPT, a weak interchain interaction can stabilize an incommensurate spin-density wave phase, which propagation vector can be continuously tuned by magnetic field.

$YbAlO_3$ is a quasi-1D spin chain compound, where Yb moments form spin chain along the *c*-axis. In this work we studied excitation spectrum and magnetic structure of this materials by means of neutron scattering in magnetic field. We found that the excitation spectra are well described by simple Heisenberg model in magnetic field. However, in contrast to the simple spin-density wave ordering with propagation vector $\mathbf{q} = 2k_F$ as predicted by the Heisenberg model, the magnetic structure shows more complex behavior and drastically changes at $M/3$ plateau. We discuss a possible theory explanation for this behavior.

TT 64: Poster: Active Matter and Microswimmers (joint session DY/TT)

Time: Thursday 15:00–18:00 Location: P1A

TT 64.1 Thu 15:00 P1A

Colloidal rods with visual perception: a simple cone of sight model. — •Anton Lüders, Philipp Stengele, and Peter Nielaba — Universität Konstanz, Konstanz, Deutschland

We introduce a simple model system of two-dimensional colloidal spherocylinders which become self-propelled under visual stimuli triggered by their neighboring particles. Via conventional Brownian dynamics simulations, the clustering phenomena and the collective motion in systems of multiple colloidal rods with visual perception are analyzed. In our model system, every particle is linked to a predefined cone of sight. A specific particle moves according to active Brownian motion if there is another particle's center inside the corresponding cone of sight but fluctuates according to normal passive Brownian motion otherwise. By analyzing the clustering phenomena of large systems we find a regime dominated by a clustering mechanism characteristic for the rods with visual perception in the range of small number densities. This regime leads to an unusual enhancement of the mean cluster size by reducing the number density of the system. Furthermore, it is studied how a small number of grouped spherocylinders with visual perception spread inside an infinite system. We find that the dynamics of rods inside this system is based on metastable states of passive Brownian motion and small flocks of activated particles. The dynamics of the particles inside the infinite system is further compared to more complex model systems of colloidal spherocylinders with visual perception.

TT 64.2 Thu 15:00 P1A

Inertial effects in collective microswimmer hydrodynamics — •Jan Cammann and Michael Wilczek — Max Planck Institute for Dynamics and Self-Organization, Göttingen

Microswimmers, such as bacteria, sperm cells, and motile algae, are typically found in regimes where the relevant length and velocity scales allow their hydrodynamic interactions to be studied in the limit of low Reynolds numbers. This simplifies the Navier-Stokes to the Stokes equations. In this approximation, inertial effects are completely neglected. For individual swimmers, this approximation is known to work well, whereas for the collective motion of a large number of swimmers the situation is less clear. For dense suspensions, the hydrodynamic flows produced by the individuals may interfere constructively, making inertial effects relevant. To elucidate this, we perform direct numerical simulations of swimmers immersed in a fluid described by either the Navier-Stokes or the Stokes equations. By directly comparing the dynamical properties, we probe the limits of this approximation for the collective hydrodynamics.

TT 64.3 Thu 15:00 P1A

Target search of active agents in complex environments. — •Luigi Zanovello[1,2], Michele Caraglio[1], Pietro Faccioli[2], and Thomas Franosch[1] — [1]Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 21A, A-6020 Innsbruck, Austria — [2]Statistical and Biological Physics Group, Dipartimento di Fisica, Università degli studi di Trento, Via Sommarive 14, 38123 Trento, Italy

Often living microorganisms, i.e. bacteria, move in complex landscapes in search of some target, i.e. nutrients, and use self propulsion to optimize their search.

Transport properties of single active Brownian particles in disordered environments are here investigated by computer simulations. Typically, in such random environments many paths exist connecting a starting region to the target. Furthermore, reaching the target likely involves the overcome of many barriers, which introduces a separation of time scales and makes the target search a rare event. Thus, with naive brute force molecular dynamics, characterizing the transition paths ensemble can be very demanding, if not unfeasible.

To cope with these issues, we design enhanced sampling techniques for active Brownian particles, which are inspired from methods used for the determination of rate constants in chemical reactions and protein folding. In particular, we design an active particle's version of transition path sampling and self-consistent path sampling. As a case study, the transition paths properties of active particles are compared with those of passive ones in simple potential landscapes with few local minima.

TT 64.4 Thu 15:00 P1A

Shearing an Active Glass — •Rituparno Mandal[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Göttingen, Germany — [2]King's College London, London, United Kingdom

Recent experiments and simulations have revealed glassy features of cytoplasm, tissues and dense assemblies of self propelled colloids. This prompts the fundamental question of whether non-equilibrium (active) amorphous materials are essentially equivalent to their passive counterparts, or whether they can present qualitatively different behaviour. To tackle this challenge we investigate the yielding and mechanical behaviour of a model active glass former, a Kob-Andersen glass in two dimensions where each particle is driven by a constant propulsion force whose direction varies diffusively over time. Using extensive Molecular Dynamics simulations, we focus in particular on the effects of the intermittent dynamics in the regime of highly persistent activity and reveal a novel type of shear induced orientational ordering in the system.

TT 64.5 Thu 15:00 P1A

Collective behaviour of self-propelled elliptical particles — •Ashreya Jayaram, Andreas Fischer, and Thomas Speck — Institute of Physics, Johannes Gutenberg-University Mainz, Germany

Ensembles of anisotropic self-propelled particles exhibit a rich variety of emergent phases. A combination of short-ranged excluded volume interactions, which induce inter-particle forces and torques, and self-propulsion determines the resulting macroscopic structure. Starting from a point in parameter-space which displays motility-induced phase separation (MIPS) for isotropic particles, we systematically increase the aspect ratio of the constituent ellipses. On doing so, first, MIPS breaks down paving way to a spatially homogeneous state comprising polar domains. Secondly, at sufficiently large aspect ratios, particles aggregate into polar bands. We rationalize these observations from simulations by extracting two effective parameters, *viz.*, the force imbalance coefficient and the coupling to the local polarization, that enter the mean-field description of the system.

TT 64.6 Thu 15:00 P1A

Chimera states and waves in cilia arrays — •Albert von Kenne, Markus Bär, and Thomas Niedermayer — Physikalisch-Technische Budesanstallt (PTB), Berlin 10587

The study of coupled oscillators revealed a multitude of collective dynamics including synchronous motion, asynchronous motion, wave-like motion and a peculiar synchronization pattern known as chimera state. Here, a population of identical oscillators branches into coexisting subpopulations that are synchronized and desynchronized, respectively. Particularly, the constituents of living matter often exhibit cyclic processes with a tendency to synchronize. For example motile cilia and flagella – hair-like projections of eukaryotic cells that push fluid in motion to cause transport phenomena. We study numerically a generalized version of a simple phase oscillator model for the coupling of cilia. The model is linked to wave formation [1] and encompasses the features relevant for the emergence of chimera states [2]. We investigate chimera states and waves in cilia arrays and discuss its properties with respect to transport generation and switching of motility states.

[1] Niedermayer et. al., Chaos: 18(3) 2008; [2] Niedermayer et. al., DPG Spring Meeting 2017: Contributed talk DY 52.1

TT 64.7 Thu 15:00 P1A

Nanoscale Temperature Imaging using Liquid Crystal Phase Transitions — •Martin Fränzl and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Universität Leipzig, Germany

With the growing number of applications of thermoplasmonics in a variety of different fields there is a need to for a simple and reliable temperature measurement of optically heated metal nanostructure. We present a method to study such temperature distributions at the nanoscale utilizing the 5CB liquid crystal nematic-isotropic phase transition. The technique is based on a conventional optical microscopy and capable of imaging isothermal contours around heated nanostructures as well as to retrieve the absolute temperature increment. The setup is easy to implement with any conventional optical microscope requiring no external modifications of additional components. We demonstrate our technique for various plasmonic nanostructures such as gold nanoparticles, Janus particles and continuous gold films. The spatial resolution of this technique is diffraction limited and temperature variations smaller than 0.1 K can be detected.

TT 64.8 Thu 15:00 P1A

Random Caustics in active random walks in random environments — •King Hang Mok[1,2] and Ragnar Fleischmann[1] — [1]Max-Planck-Institut für Dynamik und Selbstorganisation, Göttingen, Germany — [2]Institut für Dynamik komplexer Systeme, Georg-August-Universität Göttingen

The trail patterns of Argentine ants can show striking resemblance to the branched flow patterns of waves in correlated random environments. Branched flow is a general phenomenon that is widely observable in nature, such as in the electron flow in semiconductors, tsunami waves in the ocean or the propagation of light and sound through turbulent media. An important mechanism in branched flows is the formation of random caustics, singularities in the ray density corresponding to the wave flow.

We study the density fluctuations of active random walks biased by correlated random environments, resembling the motion of Argentine ants in Gaussian random fields of pheromones. We analyse in which parameter regimes reminiscences of the caustics of the deterministic dynamics in quenched disorder can be observed in the random walk.

TT 64.9 Thu 15:00 P1A

Can a passive colloid in an active bath be modeled as an active Brownian particle? — •Jeanine Shea[1], Friederike Schmid[1], and Gerhard Jung[2] — [1]Johannes Gutenberg University — [2]University of Innsbruck

Passive colloids in baths of active particles exhibit vastly different behavior than passive colloids in thermal baths. In particular, Wu and Libchaber [1] found experimentally that a passive colloid immersed in an active bath exhibits superdiffusive behavior on short time scales and normal diffusive behavior in the long-time limit. This behavior is analogous to that of an active particle, which is characterized by this transition between superdiffusive and diffusive behavior. Although Wu and Libchaber were able to relate this crossover time to experimental observables such as the length scale of collective motion, they did not explicitly relate the parameters of the system of active particles, such as the density, the rotational diffusion coefficient, or the force of active particles, to this characteristic crossover time. We investigate the detailed mechanisms that lead to the "activity" of the passive colloid and aim to explicitly map the dynamics of a passive colloid in an active bath to the model of an Active Brownian Particle.

[1] Wu, X.-L., and A. Libchaber, 2000, "Particle diffusion in a quasi-two-dimensional bacterial bath," Phys. Rev. Lett. 84, 3017-3020.

TT 65: Poster Session Topological Topics

Time: Thursday 15:00–19:00 Location: P2/EG

TT 65.1 Thu 15:00 P2/EG

Quasiparticle interference and spin texture in thin film topological insulator — •Alireza Akbari[1,2,3,4] and Peter Thalmeier[3] — [1]Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang 790-784, Korea — [2]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Department of Physics, POSTECH, Pohang, Korea

The protected surface states of topological insulators (TI) form gapless Dirac cones corresponding non-degenerate eigenstates with helical spin polarization. The presence of a warping term deforms the isotropic cone of the most simple model into snowflake Fermi surfaces as in Bi_2Se_3 and Bi_2Te_3. Their features have been identified in STM quasiparticle interference (QPI) experiments on isolated surfaces. Here we investigate the QPI spectrum for the TI thin film geometry with a finite tunneling between the surface states. This leads to a dramatic change of spectrum due to gapping and a change in pseudo spin texture that should leave distinct signatures in the QPI pattern. We consider both normal and magnetic exchange scattering from the surface impurities and obtain the scattering t-matrix in Born approximation as well as the general closed solution. We show the expected systematic variation of QPI 'snowflake' features by varying film thickness and study in particular the influence on back scattering processes. We show that a closing of the gap at special thickness due nonmonotonic tunneling matrix element should be visible in QPI.

TT 65.2 Thu 15:00 P2/EG

Signature of Unconventional Topological Superconductivity in Magnetic Penetration Depth — •Mehdi Biderang[1] and Alireza Akbari[1,2] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang, Korea

We propose a theoretical microscopic formulation of magnetic penetration depth for unconventional superconductors, considering both London (with local effects) and Pippard (with nonlocal effects) types. We examine our calculations for a variety of systems, including Sr_2RuO_4 as an example of multi-orbital superconductors, heavy fermion systems such as noncentrosymmetric superconductor $CePt_3Si$ with potential topological phase, a chiral superconductor UPt_3 with nontrivial Fermi arc surface state, and $CeCoIn_5$ with trivial topology. We find that for the London type superconductors the penetration depth varies linearly in temperature, for topologically nontrivial systems and it can demonstrate a signature of nodes in the gap function. However, the non-local response results in significant deviations from the linear behavior into a power-law temperature dependence.

TT 65.3 Thu 15:00 P2/EG

The Meservey-Tedrow technique applied to surface states of topological insulators — •Matthias Götte and Thomas Dahm — Universität Bielefeld, Bielefeld, Germany

The spin polarization of topological surface states is commonly measured by spin and angle resolved photoemission spectroscopy (SARPES), however with some ambiguities. As the spin polarization can be an important quantity for the efficiency of topological insulator materials in spintronic applications, we theoretically investigate an alternative technique.

The so called Meservey-Tedrow technique is based on spin dependent tunneling from a superconducting electrode and is an established technique for measuring the polarization of ferromagnets. Here, we show that it can be adapted to topological insulators to determine the in-plane component of the surface state spin polarization as well as the spin-flip scattering rate of surface electrons.

TT 65.4 Thu 15:00 P2/EG

Ferromagnetic topological insulators used as magnetic field sensors — •Matthias Borcherding and Thomas Dahm — Universität Bielefeld, Bielefeld, Germany

We investigate numerically the possibility of using ferromagnetic topological insulators to measure small changes in magnetic fields. For that, we calculate the intrinsic part of both the anomalous Hall and the spin Hall conductivity. Both the anomalous Hall effect and topological insulators are connected to the Berry curvature. We use a model for a three dimensional topological insulator and an effective two dimensional model. The latter is obtained from the first by applying a symmetric confining potential. We demonstrate conditions under which the sensitivity of such sensors becomes strongly increased.

TT 65.5 Thu 15:00 P2/EG

Electrical transport properties of Vanadium doped $Bi_2Te_{2.4}Se_{0.6}$ — Christian Riha[1], Birkan Düzel[1], Karl Graser[1], Olivio Chiatti[1], Oliver Rader[2], Jaime Sánchez-Barriga[2], Oleg Tereshchenko[3], and •Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Helmholtz-Zentrum-Berlin für Materialien und Energie, 12489 Berlin, Germany — [3]Physics Department, Novosibirsk State University, 630090 Novosibirsk, Russia

Magnetic doping of topological insulators is predicted to break the time reversal symmetry of the edge states and to cause the opening of a gap in the Dirac cone. This enables the observation of a transition from weak anti-localization to weak localization, as well as the occurrence of the anomalous quantum Hall effect. In this work, we investigate the transport properties of Vanadium doped $Bi_2Te_{2.4}Se_{0.6}$ and measure the low-field magnetoresistance at temperatures down to $T = 0.3$ K. All the samples show weak anti-localization and a hysteresis at low temperatures, which depends on the sweep-rate of the applied magnetic field.

TT 65.6 Thu 15:00 P2/EG

Magnetotransport phenomena of the quaternary topological insulator $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ — •Erik Zimmermann, Michael Schleenvoigt, Jonas Kölzer, Daniel Rosenbach, Gregor Mussler, Peter Schüffelgen, Hans Lüth, Detlev Grützmacher, and Thomas Schäpers — Forschungszentrum Jülich GmbH

Three-dimensional topological insulators form a new material class which may enable topological quantum computing using robust Majorana states. The interest in ternary and quaternary topological insulators recently increases as the magnetotransport of binary topological insulators is dominated by contributions from the bulk due to intrinsic doping. By varying the stoichiometry, we aim to place the Fermi level into the band gap within the bulk and close to the Dirac point at the surface in order to enhance the contributions from the surface states. We present cryogenic magnetotransport measurements performed on a selective-area grown $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ nano-Hallbar, revealing pronounced universal conductance fluctuations caused by the surface states. Furthermore, a unique temperature dependence reinforces that the universal conductance fluctuations originate from two-dimensional transport.

TT 65.7 Thu 15:00 P2/EG

Mobility spectrum analysis on the topological insulator $BiSbTeSe_2$ — •Jimin Wang[1], Alexander Kurzendorfer[1], Lin Chen[1], Zhiwei Wang[2], Yoichi Ando[2], Yang Xu[3], Ireneusz Miotkowski[3], Yong P. Chen[3], and Dieter Weiss[1] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany — [3]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47907, USA

We conducted mobility spectrum analysis on high quality 3D topological insulator $BiSbTeSe_2$ to extract mobility μ, and carrier density n. Top and bottom gates were applied to tune the carrier density independently on top and bottom surfaces. At 1.5 K, when the conduction is almost entirely dominated by the Dirac surface states, we always find two dominant conduction channels (top and bottom surfaces), with $\mu = 1000 - 3000\,\mathrm{cm}^2/\mathrm{Vs}$, and n on the order of $10^{12}\,\mathrm{cm}^{-2}$. However, at sufficiently high temperature ($T = 85\,\mathrm{K}$), when the bulk contributes, a third channel opens ($\mu \sim 200\,\mathrm{cm}^2/\mathrm{Vs}$, and $n \sim 10^{12}\,\mathrm{cm}^{-2}$). Our analysis shows the feasibility of the method, which is also promising for similar material systems.

TT 65.8 Thu 15:00 P2/EG

Electron spin resonance spectroscopy measurement of a magnetic topological insulator material $MnBi_4Te_7$ — •Kavita Mehlawat[1,3], Alexey Alfonsov[1,3], Anna Isaeva[1,2,3], Bernd Buechner[1,2,3], and Vladislav Kataev[1,3] — [1]Institute for Solid State and Materials Research, Leibniz IFW Dresden, Dresden, Germany — [2]Faculty of Physics, Technische Universitaet Dresden, Dresden, Germany — [3]Wuerzburg-Dresden Cluster of Excellence ct.qmat

The van der Waals compound $MnBi_4Te_7$ belongs to the family of $(Bi_2Te_3)_n(MnBi_2Te_4)$, (n = 0, 1, 2) heterostructures and is the first example of a compound which features both, the intrinsic net magnetization and band inversion. Static magnetic susceptibility (χ) and magnetization (M) measurements as a function of the applied field (H) on $MnBi_4Te_7$ show an antiferromagnetic state at $T_N = 13$ K and a ferromagnetic-like hysteresis occurring upon cooling below 5 K [1]. We performed electron spin resonance (ESR) spectroscopy measurements to explore the dynamic magnetic properties of $MnBi_4Te_7$. From high-frequency ESR measurements, we obtain evidence that $MnBi_4Te_7$ is an easy-axis type ferromagnet and ferromagnetic spin correlations persist up to T = 30 K on the time scale of an ESR experiment (10^{-10} - 10^{-11} s).

[1] Raphael C. Vidal et. al, arXiv:1906.08394

TT 65.9 Thu 15:00 P2/EG

Controlling a band gap at the K-points in graphene — •Frederik Bartelmann, Daniela Pfannkuche, Marta Prada, and Alexander Chudnovskiy — Universität Hamburg

In a tight-binding description without spin orbit interaction (SOI), the valence and conduction band of graphene touch at the K-points of the Brillouin zone [1]. SOI creates a band gap proportional to the contribution of atomic d-orbitals to the band states [2-4]. This contribution can be influenced via electric interactions, and consequently can the size of the gap. The effect of time-periodic electric fields on a tight-binding model of graphene is studied numerically by Floquet formalism and analytically by perturbation theory, to determine a method of controlling the band gap.

[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, Rev. Mod. Phys. 81, 109, 2009
[2] S. Konschuh, M. Gmitra, and J. Fabian, Phys. Rev. B, 2010
[3] J. Sichau, M. Prada, T. Anlauf, T. J. Lyon, B. Bosnjak, L. Tiemann, and R. H. Blick, Phys. Rev. Lett. 122, 046403, 2019
[4] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801, 2005

TT 65.10 Thu 15:00 P2/EG

Magnetoelectric screening at the interface of a topological insulator and a ferromagnetic insulator — •Marius Scholten[1], Ilya Eremin[2], Jeroen van den Brink[1,3], and Flavio S. Nogueira[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [3]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

It is well known that a ferromagnetic insulator (FMI) proximate to the surface of a topological insulator (TI) gaps the Dirac fermions when the out-of-plane component of the magnetization at the interface is non-vanishing. Consequently, a Chern-Simons (CS) term is generated by fluctuations of the Dirac fermions at the TI surface. This CS term consists of a magnetoelectric (ME) coupling and an additional Berry phase for the interface magnetization. For nonzero chemical potential, integrating out the Dirac fermions also generates a Dzyaloshinskii-Moriya interaction (DMI) which stabilizes skyrmions at the TI-FMI interface. In this work we discuss the consequences of the interplay between the CS and DMI terms in the effective action for the electrical screening. We discuss how the ME coupling to the magnetization modifies the dielectric function as a function of temperature and how this may lead to anti-screening effects at the interface. The dependence of the dielectric constant on temperature follows from the behavior of the interfacial magnetic susceptibility, which due to the DMI term also features a momentum space instability at the Curie temperature.

TT 65.11 Thu 15:00 P2/EG

Dynamical density and spin response of Fermi arcs and their consequences for Weyl semimetals — •Sayandip Ghosh[1] and Carsten Timm[2] — [1]Istituto Italiano di Tecnologia, Graphene Labs, Via Morego 30, 16163 Genova, Italy — [2]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Weyl semimetals exhibit exotic Fermi-arc surface states, which strongly affect their electromagnetic properties. We derive analytical expressions for all components of the composite density-spin response tensor for the surfaces states of a minimal Weyl-semimetal model. Based on the results, we discuss the electromagnetic susceptibilities, the current response, and other physical effects arising from the density-spin response. We find a magnetoelectric effect caused solely by the Fermi arcs. We also discuss the effect of electron-electron interactions within the random phase approximation and investigate the dispersion of plasmon excitations formed by Fermi-arc states. Our work is useful for understanding the electromagnetic and optical properties of the Fermi arcs.

TT 65.12 Thu 15:00 P2/EG

Negative Longitudinal Magnetoconductance at Weak Fields in Weyl Semimetals — •Andy Knoll, Carsten Timm, and Tobias Meng — Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany

Weyl semimetals are topological materials that provide a condensed-matter realization of the chiral anomaly. A positive longitudinal magnetoconductance quadratic in magnetic field has been promoted as a diagnostic for this anomaly. By solving the Boltzmann equation analytically, we show that the magnetoconductance can become negative in the experimentally relevant semiclassical regime of weak magnetic fields. This effect is due to the simultaneous presence of the Berry phase and the orbital magnetic moment of carriers and occurs for sufficiently strong intervalley scattering.

TT 65.13 Thu 15:00 P2/EG

de Haas–van Alphen measurements of CoSi — •B.V. Schwarze[1,2], J. Hornung[1,2], K. Manna[3], T. Förster[1], 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 Chemische Physik fester Stoffe, Dresden, Germany

It is known from angle-resolved photoemission spectroscopy (ARPES) that CoSi hosts unconventional chiral fermions. It exhibits a topological threefold band-touching node with a Chern number of +2 at the Γ point and a topological fourfold band-touching node with a Chern number of -2 at the R point. These nodes are protected by crystal symmetries and connected by giant surface Fermi arcs. They generate spin-1 fermions and charge-2 double Weyl fermions, respectively. We performed de Haas-van Alphen (dHvA) measurements up to 18 T and down to 40 mK. The angular dependence of the fundamental dHvA frequencies as well as their effective masses are in good agreement with our density-functional-theory calculations, confirming the topologically non-trivial band structure. We also observed multiple magnetic-breakdown frequencies, providing further information on the topological phase shift.

TT 65.14 Thu 15:00 P2/EG

Investigation of quantum oscillations in the topological chiral semimetal CoSi — •Nico Huber, Grace Causer, Georg Benka, Lukas Worch, Laura Stapf, Andreas Bauer, Marc Wilde, and Christian Pfleiderer — Technical University of Munich, 85748 Garching, Germany

Chiral semimetals are predicted to host massless topological fermions that are distinct from Dirac and Weyl fermions. Ab initio density functional theory (DFT) suggests the existence of such fermions in the transition-metal silicide CoSi.[1] In turn, electron orbits with a chiral charge around the R point in the Brillouin zone were deduced from quantum oscillations in the thermoelectrical properties of this material.[2] We report the results of Shubnikov-de Haas and de Haas-van Alphen measurements of CoSi down to milli-Kelvin temperatures. Our data confirm the oscillation frequencies reported in Ref. [2]. In addition, we performed angle-resolved measurements to determine the influence of the crystallographic orientation on these oscillations. We compare our results with comprehensive DFT calculations.

[1] Peizhe Tang, Quan Zhou, and Shou-Cheng Zhang, Phys. Rev. Lett. **119**, 206402 (2017)
[2] Xu et al., Phys. Rev. B **100**, 045104 (2019)

TT 65.15 Thu 15:00 P2/EG

Mirror anomaly induced anomalous Hall effect in $ZrTe_5$ — •Yongjian Wang, Alexey Taskin, and Yoichi Ando — Institute of Physics II, University of Cologne, D-50937 Cologne, Germany

Dirac semimetals with band crossings (i.e., Dirac nodes) protected by combined inversion symmetry, time reversal symmetry and additional crystal symmetry attract lots of interest due to their interesting topological properties [1,2]. Besides chiral anomaly, a new topological phenomenon, mirror anomaly induced anomalous Hall effect was recently theoretically predicted in Dirac semimetals [3]. In a Dirac semimetal, when the Dirac nodes are at a time reversal invariant momentum, the anomalous Hall conductivity is predicted to exhibit a step-like change when the field is rotated.

$ZrTe_5$ is a Dirac semimetal with only one Dirac point at the Γ point when the temperature is close to the resistivity peak temperature T_P [4], which provides a good platform for observing the mirror-anomaly-induced anomalous Hall effect. We have grown $ZrTe_5$ single crystals with very low T_P and observed a clear anomalous Hall effect in these samples. We report the magnetic-field-orientation dependence of the anomalous Hall conductivity and discuss whether it is consistent with the theoretical prediction.

[1] S. M. Young, et al., Phys. Rev. Lett. 108.14: 140405 (2012)
[2] Z. J. Wang, et al., Phys. Rev. B 88.12: 125427 (2013).
[3] A. A. Burkov, Phys. Rev lett. 120.1: 016603 (2018).
[4] B. Xu, et al., Phys. Rev. lett. 121.18: 187401 (2018).

TT 65.16 Thu 15:00 P2/EG

Phase diagrams of topological superconductors — •Jannis Neuhaus-Steinmetz, Elena Vedmedenko, Thore Posske und Levente Rózsa — Department of Physics, University of Hamburg, Hamburg, Germany

Non-collinear spin structures interacting with s-wave superconductors are promising candidates for topological superconductivity and Majorana physics. We study the interplay between non-collinear magnetic states and superconductivity theoretically by means of tight-binding calculations in combination with Monte Carlo simulations within the Heisenberg model. We derive the parameters of the Heisenberg Hamiltonian by fitting the energy dispersion originating from tight-binding calculations. The resulting magnetic ground states and phase diagrams will be discussed.

TT 65.17 Thu 15:00 P2/EG

Majorana zero modes in skyrmion-vortex pairs — •Jonas Nothhelfer[1,2], Kjetil Hals[3], Matteo Rizzi[4,5], and Karin Everschor-Sitte[1] — [1]Institut für Physik, JGU Mainz — [2]MPGC Mainz — [3]University of Agder, Grimstad, Norway — [4]Institute of Complex Systems, Forschungszentrum Jülich — [5]Institute for Theoretical Physics, Universität zu Köln

Ferromagnet-superconductor heterostructures allow for composite topological excitations such as skyrmion-vortex pairs [1], which can support the occurrence of localized Majorana bound states [2,3]. The non-abelian exchange statistics of Majorana modes makes them promising candidates for topological quantum computation. Our goal is to controllably braid Majorana modes via manipulating the skyrmions in such ferromagnet-superconductor composite topological excitations. To this end, we model a magnetic skyrmion imprinted in the ferromagnet and a vortex in the superconductor. We solve the eigensystem of the superconductor in the Bogoliubov-de Gennes formalism self-consistently for the superconducting gap under the influence of the magnetic field generated by the magnetic thin film and spin-orbit coupling. As predicted by [1] we reproduce that composite topological excitations can emerge as pairs of superconducting vortices bound to magnetic skyrmions. Exploiting the finite binding energy, we

expect that the Majorana zero modes can be efficiently braided via the skyrmions using spintronic techniques.
[1] Kjetil Hals et al., PRL 117, 017001 (2016)
[2] Jonas Nothhelfer, Master Thesis
[3] Stefan Rex et al., PRB 100, 064504 (2019)

TT 65.18 Thu 15:00 P2/EG

Signatures of the Majorana spin and nonlocality in the electrical transport through a Majorana - quantum dot hybrid system — •Alexander Schuray[1], Manuel Rammler[1], and Patrik Recher[1,2] — [1]Institute for Mathematical Physics, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

We investigate the electronic transport properties of a Majorana bound state (MBS) system in which more than one MBS is coupled to a spinful normal conducting lead on one side and a quantum dot on the other side. We use the full counting statistics to show that the only process contributing to the current is Andreev reflection in up to two channels that can be attributed to the two spin channels in the lead. The coupled quantum dot leads to the emergence of Fano resonances and the symmetry properties of these give insight about the coupling strength to both MBSs. We support our findings using a numerical tight binding model of a spin orbit coupled nanowire in proximity to a superconductor with an applied Zeeman field and treat the quantum dot using a self consistent mean field theory for the Coulomb interaction on the quantum dot.

TT 65.19 Thu 15:00 P2/EG

Probing Majorana bound states with an optical quantum dot — •Lena Bittermann[1], Daniel Frombach[1], Christophe De Beule[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, Braunschweig, Germany

Majorana bound states (MBSs) arise at the ends of a semiconducting nanowire in proximity to a superconductor when a sufficiently strong magnetic field is applied. Ever since signatures of MBSs were discovered, there has been a lot of research exploring their properties. Nevertheless, their spin structure [1] has only recently attracted attention. By coupling a quantum dot to one of the ends of the wire [2], the spin and nonlocal properties can be investigated [3,4].

Here, we propose a setup where we use an optical quantum dot tunnel-coupled to the end of a Majorana nanowire and to a hole reservoir forming a pn-junction as a spectroscopic tool. First, we solve the low-energy model for the wire coupled to the quantum dot and calculate the corresponding transition rates for the creation of photons via optical recombination. Furthermore, we use a master equation formalism to obtain the steady-state occupation probabilities. By analyzing the resulting photon emission intensities, we can draw conclusions on the spin polarization and nonlocality of the MBSs.
[1] D. Sticlet, C. Bena and P. Simon, PRL 108, 096802 (2012)
[2] M. T. Deng et al., Science 354, 1557 (2016)
[3] A. Schuray, L. Weithofer and P. Recher, PRB 96, 085417 (2017)
[4] E. Prada, R. Aguado and P. San-Jose, PRB 96, 085418 (2017)

TT 65.20 Thu 15:00 P2/EG

Floquet-Majoranas in a Cooper Pair Box — •Anne Matthies and Achim Rosch — Universität zu Köln, Institut für Theoretische Physik

A topological superconductor in one dimension can host Majorana zero modes at its edge. By driving the system periodically, so-called π modes (also named Floquet-Majoranas) can arise. These are topologically protected modes with an energy at the quasi-energy π/T where T is the period of the drive. We consider the role of π modes in the presence of long-ranged Coulomb interactions. We study a Cooper pair box made of two Josephson coupled superconducting topological quantum wires. Time-dependent gate voltages periodically drive the system. We investigate how to obtain and control π modes and study their stability in the presence of interactions.

TT 65.21 Thu 15:00 P2/EG

Decoherence of Majorana edge modes under quasi-adiabatic drives — •Zihao Gao, Yuval Vinkler-Aviv, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany

In this project we study how Majorana edge modes behave under slow, quasi-adiabatic movement in the presence of disorder, interactions and thermal fluctuations.

In a 1D Kitaev chain, zero-energy Majorana bound states are formed at the edges of the topological region. Such Majorana edge modes are robust due to protection by an energy gap and their spatial separation. Therefore they can effectively encode a qubit. By controlling the chemical potential we have the ability to adiabatically move these Majorana edge modes. During this process, we analyze the Majorana qubit's fidelity loss induced by disorder, interactions and thermal fluctuations. Furthermore, we numerically calculate the time-evolution of a Majorana qubit in such a setup in order to measure the decoherence from different sources.

TT 65.22 Thu 15:00 P2/EG

Disorder effects on the spectral gap of topological insulator based Majorana zero modes — •Alexander Ziesen and Fabian Hassler — RWTH Aachen University, Aachen, Germany

We consider a 3D topological insulator (TI) proximitized by an s-wave superconductor with a vortex. It is known that the vortex traps a single unpaired Majorana zero mode (MZM). We numerically investigate the disorder dependence of the in-gap states. In particular, we concentrate on onsite potential disorder effects on the spectral gap for a chemical potential both being close and far away from the Dirac point. A large gap is desirable for this MZM to potentially be used for quantum information applications. We also show that one can efficiently simulate the 2D surface transport of a 3D TI using a three dimensional tight binding model and that we can restrict ourselves to purely surface disorder to correctly model the vortex setup.

TT 65.23 Thu 15:00 P2/EG

Transport and scanning tunneling microscopy study on $EuMnBi_2$ — •Xinglu Que[1], Jan Bruin[1], Mohammad Pakdaman[1], Claus Mühle[1], Jürgen Nuss[1], Qingyu He[1], Lihui Zhou[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

The quantum Hall effect (QHE) has been a compelling topic in physics in which the interplay of correlation and topology plays a key role. Though it is usually exclusive to two-dimensional electron systems, multilayered form of QHE has been reported in 3D materials with the layered pnictide $EuMnBi_2$ being a notable example. In this system antiferromagnetically ordered Eu ions decouple the Bi square net layers which host Dirac fermions, exhibiting rich magnetic textures. By controlling the magnetic phase distinct electronic structures are accessible.

We report our investigation on $EuMnBi_2$ utilizing transport measurement and scanning tunneling microscope (STM). Quantized Hall signals in both electrical and thermal conductance are clearly observed, with charge and entropy carriers characterized by Wiedemann-Franz law in this QHE system. STM results reveal atomically resolved surface after low temperature cleavage, and local spectroscopy finds features derived from Bi which is in good agreement with band structure calculations.

TT 65.24 Thu 15:00 P2/EG

Conductance through a quantum-Hall-superconductor junction from a tunneling perspective — •Fernando Dominguez Tijero[1] and Ewelina Maria Hanckiewicz[2] — [1]Institute for Mathematical Physics, TU Braunschweig, D-38106 Braunschweig, Germany — [2]Institute for Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat,University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Motivated by the increasing number of transport experiments between a quantum-Hall (QH) bar and a superconducting (S) contact [1-5], we have investigated the current and noise between these two different subsystems using a tunneling approximation. This perturbative approach allows to understand the transport mechanism in a clearer way than previous numerical results based on an extended BTK formalism [6]. In addition, it allows to derive analytical results for the conductance and makes it possible to extend the study to other scenarios, such as QH-S-QH or fractional QH-S.
[1] P. Rickhaus et al. Nanoletters 12 1942 (2012)
[2] F. Amet et al. Science 352 966 (2016)
3] G.-H. Lee, et al.Nat. Phys. 13 693 (2017)
[4] M. R. Sahu et al. Phys. Rev. Lett. 121 086809 (2018)
[5] A. Seredinski et al. Science Adv. (2019)
[6] Hope et al. Phys Rev. Lett. 84 1804 (2000)

TT 65.25 Thu 15:00 P2/EG

0-π transitions in Josephson junctions out of 3D topological insulator nanowires with parallel magnetic field — •Jacob Fuchs, Michael Barth, Raphael Kozlovsky, Cosimo Gorini, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

Josephson junctions out of 3D topological insulators (TIs) are investigated and Andreev bound states and supercurrents are calculated. Upon adding a (orbital) parallel magnetic field, bands with opposite angular momenta are split (similar to a Zeemann field splitting of the spin states). Because the field is also present in the superconducting part of the wire, Andreev reflection is modified. This leads to an energy shift of the Andreev bound states which, in turn, induces interesting 0-π transitions.

TT 65.26 Thu 15:00 P2/EG

Tunneling spectroscopy of $Tl_2Mo_6Se_6$ nanowires — •Mengmeng Bai, Yongjian Wang, and Yoichi Ando — Physics Institute II, University of Cologne, 50937 Cologne, Germany

Quasi-one-dimensional $Tl_2Mo_6Se_6$ is predicted to be a topological superconductor [1]. It is known that a pair of Majorana fermions will be induced at the end of a one-dimensional topological superconductor nanowire. Here we report our tunneling spectroscopy experiments on superconducting $Tl_2Mo_6Se_6$ nanowires. The $Tl_2Mo_6Se_6$ nanowires were exfoliated from the fiberlike single crystals. After that, they were fabricated into devices and then measured at temperatures down to 10 mK. A thin layer of Al_2O_3 is grown as a tunnel barrier for tunneling spectroscopy study. The preliminary tunneling spectroscopy results show rich structures both in and out of the superconducting gap.

[1] S.-M. Huang, C.-H. Hsu, S.-Y. Xu, C.-C. Lee, S.-Y. Shiau, H. Lin, and A. Bansil, Phys. Rev. B 97, 014510 (2018).

TT 65.27 Thu 15:00 P2/EG

Three-dimensional quantum Hall effect and thermopower in $ZrTe_5$ — •Toni Ehmcke and Tobias Meng — Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany

Motivated by recent, unpublished experiments, we model electric and thermoelectric transport coefficients in $ZrTe_5$, a promising candidate material to realize the three-dimensional analogue of the quantum Hall effect due to its weakly coupled layer structure. Using a low-energy continuum model, we apply linear response theory to investigate the magnetic-field dependence of the longitudinal and Hall conductivities as well as the thermoelectric Seebeck and Nernst coefficients. We compare the results for different experimentally relevant situations and find good agreement with the experimental data.

TT 65.28 Thu 15:00 P2/EG

Topological charge pumping under realistic conditions — •Eric Bertok[1], Andrew Hayward[1,2], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Göttingen — [2]Arnold-Sommerfeld Center for Theoretical Physics, Munich

Recent experiments with ultra-cold atomic gases have realized topological charge pumps [1,2]. Non-adiabatic effects due to finite pumping speeds have already been studied via a Floquet analysis in the periodic system [3], but the combined effect of an external harmonic trap, a finite particle number, and these non-adiabatic effects due to a finite pump speed has not been considered. In our work, the interplay between these realistic aspects are explored and an interpretation of the mechanisms for topological charge pumping in a trapped system is developed. The full time-dependent Schroedinger equation is solved by exact diagonalization for the non-interacting system, and the dependence of the quantized particle transport on the pumping frequency and the trap strength is identified. Breakdowns from exact quantization due to excitations to the higher band are observed and are found to be highly dependent on the pumping frequency, with deviations for slow pumping and special pumping frequencies appearing at intermediate pumping times at which the pumping breaks down entirely.

This work was supported by the DFG (Deutsche Forschungsgemeinschaft) via Research Unit FOR2414.

[1] Lohse et al. *Nature Phys* **12**, 350-354 (2016)
[2] Nakajima et al. *Nature Phys* **12**, 296-300 (2016)
[3] Privitera et al. *Phys. Rev. Lett.* **120**, 106601 (2018)

TT 65.29 Thu 15:00 P2/EG

Effects of the classical analog of the spin Berry curvature in adiabatic spin dynamics — •Simon Michel and Michael Potthoff — I. Institute of Theoretical Physics, Department of Physics, Universität Hamburg

We study the real-time dynamics of interacting many-body models consisting of slow and fast degrees of freedom in the adiabatic (Born-Oppenheimer-like) limit where certain topological terms can emerge in the effective equations of motion. In particular, we consider systems of slow classical spins coupled to fast spin or electron degrees of freedom. Using a Lagrangian approach, the fast variables are eliminated via suitable constraints such that one is left with an effective slow spin dynamics. This can be highly anomalous as is known, e.g., for a single classical spin coupled to a fast conduction-electron system, where the spin Berry curvature can lead to a strongly renormalized precession frequency [1].

Here, we study one or more slow classical spins coupled to a fast classical spin system using analytical as well as numerical techniques. For a single slow spin, we recover the anomalous precession [1] found earlier, even quantitatively. However, in the effective equation of motion the (quantum) Berry curvature is replaced by a (classical) topological charge density, similar to a skyrmion density but for skymions living on a product of Bloch spheres rather than in Euclidean space. For two and more slow spins, the geometrical spin torques resulting from the topological charge density give rise to unconventional effective RKKY-type couplings and dynamics.

TT 65.30 Thu 15:00 P2/EG

Magnetic properties of spin chain materials $Cs_2Co(Cl/Br)_4$ — •Thomas Leich[1], Daniel Brüning[1], Ladislav Bohatý[2], Petra Bohatý[2], Oliver Breunig[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universitat zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Cs_2CoCl_4 has been identified as an effective spin-1/2 chain material with strong XY anisotropy [1]. Due to inter-chain coupling it shows long-range magnetic order below 0.23 K with complex phase diagrams up to magnetic fields of 2.5 T [2]. Here we present a study of the isostructural substitution series $Cs_2CoCl_{4-x}Br_x$. Cs_2CoBr_4 shows some similar phases, but they are more stable and extend to tempeatures up to 1.35 K and magnetic fields up to 4 T. Measuring specific heat, magnetocaloric effect, thermal expansion and magnetization at temperatures down to 250 mK, the magnetic order of the different phases is characterized, as the material shows strong magnetic field dependence of magnetization, entropy and magnetostriction coefficient. We present phase diagrams for different field directions and discuss the origin of the phases. The 1D spin-chain physics is partly covered by the 3D magnetic order, and an increased single-ion anisotropy of about 20 K is determined, compared to 13.9 K in Cs_2CoCl_4.

Funded by DFG via Project No. 277146847- CRC 1238

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[2] O. Breunig et al., PRB 91, 024423 (2015)

TT 65.31 Thu 15:00 P2/EG

Interacting magnons in the easy-axis square-lattice XXZ model — •Matthias Walther[1], Götz S. Uhrig[2], and Kai P. Schmidt[1] — [1]Institut für Theoretische Physik, FAU Erlangen-Nürnberg, 91058 Erlangen, Germany — [2]Lehrstuhl für Theoretische Physik I, Technische Universität Dortmund, 44221 Dortmund, Germany

The easy-axis square-lattice XXZ-model interpolates between the Ising model and the isotropic Heisenberg model. The system displays always long-ranged Néel order. However, the elementary excitations, except for the SU(2) symmetric Heisenberg point, correspond to gapped magnons and the spectrum is known to possess multi-magnon bound states. We follow the the excitation spectrum from the Heisenberg to the Ising model in order to find possible connections between , e.g., the amplitude Higgs resonance and the long-lived two-magnon bound states known from the Ising limit. Technically, this is achieved by the method of non-perturbative continuous similarity transformations in momentum space, which has been proven to capture the physics quantitatively in the Heisenberg limit.

TT 65.32 Thu 15:00 P2/EG

Linked cluster expansions for non-Hermitian quantum spin systems — •Lea Lenke and Kai Phillip Schmidt — Chair for Theoretical Physics I, FAU Erlangen-Nürnberg, Germany

In quantum mechanics, the standard axiom of Hermitian Hamiltonians can be replaced by the axiom of PT-symmetric Hamiltonians without automatically loosing the realness of the energy spectrum. The properties of PT-symmetric quantum mechanics is investigated by applying the formalism of linked cluster expansions to the exactly solvable Ising chain in a complex transverse magnetic field. In a next step the gained experience will be used to study topological phase transitions in Kitaev's toric code in a magnetic field.

TT 66: Poster Session Transport

Time: Thursday 15:00–19:00 Location: P2/EG

TT 66.1 Thu 15:00 P2/EG

Simulating the nonequilibrium transport through quantum dots coupled to Holstein phonons using matrix-product states methods — •David Jansen and Fabian Heidrich-Meisner — Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Molecular nano structures play an increasingly important role in everyday technology and the field has experienced enhanced experimental and theoretical interest [1]. To better understand the influence of electron-phonon interactions on such structures we investigate a system consisting of two metallic leads connected by a quantum dot with vibrational degrees of freedom. We use matrix-product states based techniques that are designed for an efficient treatment of phonons [2] to calculate transport properties of the system when a bias voltage is applied. We first show that our results agree with those of a functional RG calculation [3]. By diagonalizing the reduced density matrix of the quantum dot we are also able to identify the optimal modes of the system. We show that taking advantage of these modes has computational benefits for our system and we analyze how these optimal modes and their structure are changed by the voltage.

This research is supported by the Deutsche Forschungsgemeinschaft via SFB 1073 (project B09).

[1] M. Galperin et al., J. Phys.: Condens. Matter 19, 103201 (2007)
[2] C. Brockt et al., Phys. Rev. B 92, 241106(R) (2015)
[3] A. Khedri et al., Phys. Rev. B 98, 195138 (2018)

TT 66.2 Thu 15:00 P2/EG

Kondo impurities in two dimensional Dirac semimetals — •Michael Turaev and Johann Kroha — Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany

In this work we study the effects of Kondo as well as static spin impurities on the surface of a three dimensional topological Kondo insulator, which is a Dirac semimetal. Recently there have been scanning tunneling spectroscopy measurements (STM) [1] of the surface state of Gd-substituted SmB_6. Gd has a half filled 4f shell, constituting to a static spin, and a single electron in the 5d shell that can be described as a Kondo impurity. The static spin impurity opens up a local gap and suppresses the local density of states whereas the Kondo impurity can lead to a Kondo peak in the density of states. A realistic theoretical description of the STM experiments requires both of these effects to be taken into account. We use T-matrix and non crossing approximation techniques to analyze a position dependent local density of states that is measured in [1].

[1] L. Jiao et al., Sci. Adv. 4, eaau4886 (2018)

TT 66.3 Thu 15:00 P2/EG

Applications of a general duality relation in fermionic open systems — •Jens Schulenborg[1], Valentin Bruch[2], Maarten Wegewijs[2,3], and Janine Splettstoesser[4] — [1]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Denmark — [2]Institute for Theory of Statistical Physics, RWTH Aachen, Germany & JARA-FIT — [3]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [4]Department of Microtechnology and Nanoscience, Chalmers University of Technology, Göteborg, Sweden

Complex Hamiltonians of closed quantum systems are successfully simplified with symmetries, topology or mappings to more easily understandable systems. The ubiquity of *open systems* thus makes an analogous treatment of their effective Liouvillian highly desirable. However, dissipation and memory due to the coupled environment can substantially reduce the number of symmetry relations to draw from.

For a large class of fermionic systems with bilinear system-bath couplings, one such relation derives merely from Pauli exclusion and the principle of total fermion-parity conservation: the *fermionic duality*[1]. This duality yields insights into the dynamics of the system by mapping it to a dual model with inverted energies. Focussing on weakly coupled, Markovian environments, this poster gives an overview of recent and potential future applications of fermionic duality. We address in particular non-equilibrium, stationary and time-dependent charge- and energy transport through nanoscale devices characterized by multiple orbitals with strong many-body interactions.

[1] J. Schulenborg et al.: Phys. Rev. B **93**, 081411 (2016)

TT 66.4 Thu 15:00 P2/EG

Current induced switching in atomic copper junctions — •Patrick Haiber, Martin Prestel, David Weber, and Elke Scheer — Universität Konstanz, Konstanz, Deutschland

Electromigration is intensively studied in micron-size conductors as it is a major cause of failure in integrated circuits. Though, not much is known about the phenomenon when downscaling the sample size to the atomic size.

Here, we study current-induced switching of atomic-size contacts of Cu, a metal that is used as backend in integrated circuits. We present the fabrication of thin-film mechanically controlled break-junctions, using electron beam lithography on a phosphor bronze substrate and thin-flm (80 nm) evaporation. The transport experiments are performed at low temperature under cryogenic vacuum. The conductance histogram obtained from hundreds of conductance vs. distance traces shows a pronounced maximum at $G = 1\ G_0$ as expected for monovalent metals [1] revealing the high sample quality.

The electromigration experiments are performed for contacts with conductance between 1 G_0 and 7 G_0 by applying an alternating bias current [2]. With this process, bistable as well as monostable conductance switching is observed. We discuss the statistical behavior of the switching phenomena as well as the dependence of the switching process on the ramping speed of the alternating current.

[1] Agraït et al., 2003, Phys. Rep. 377, 81-279
[2] Schirm et al., 2013, Nature Nanotech. 8, 645-648

TT 66.5 Thu 15:00 P2/EG

Noise and transport measurements in atomic contacts of rare-earth and transition metals — •Marcel Strohmeier, Martin Prestel, and Elke Scheer — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

We study the formation of atomic-scale magnetic ordering in rare-earth and transition metals. For Gd, a well-known Heisenberg ferromagnet with localized 4f electrons, theoretical studies predict a spin-polarized (SP) transport behavior in reduced dimensions [1]. Otherwise there are paramagnetic materials like Pd or Ir, where an emerging magnetic ordering in small dimension is expected due to the Stoner instability [2, 3]. Nonmonotonic magnetotransport has been reported for atomic contacts of Pt [4], Pd [5], and Ir [6]. Here, we extend the investigations by measurements of the shot noise. Shot noise allows insights into the channel configuration [7] and is sensitive to SP [8]. We study atomic contacts of Gd, Ir, Pd, Pt, and Co using the mechanically controllable break junction (MCBJ) technique at low temperatures. While no evidence for SP is observed for Pt and Pd, we find clear deviation from the usual shot-noise behavior for Gd and Ir.

[1] Olivera et al., PRB 95, 075409 (2017)
[2] Delin et al., PRL 92, 057201 (2004)
[3] Delin et al., PRB 68, 144434 (2003)
[4] Strigl et al., Nat. Comm. 6, 6172 (2015)
[5] Strigl et al., PRB 94, 144431 (2016)
[6] Prestel et al., PRB, accepted
[7] Kumar et al., PRL 108, 146602 (2012)
[8] Burtzlaff et al., PRL 114, 016602 (2015)

TT 66.6 Thu 15:00 P2/EG

A theoretical study of the interplay of electron and phonon transport in nanosystems — •Jakob Bätge and Michael Thoss — Institute of Physics, University of Freiburg, Freiburg, Germany

In view of the tremendous recent progress in experimental techniques to study charge and heat transport in nanostructures based on single atoms or molecules [1,2], theoretical research on basic transport prop-

erties of nanosystems is of significant interest.
Here, we investigate the mutual influence of electronic and phononic transport driven by voltage and temperature gradients through basic model systems from a theoretical perspective. For this purpose, we use the hierarchical quantum master equation approach [3], which generalizes perturbative master equation methods by including higher-order contributions as well as non-Markovian memory and allows for the systematic convergence of the results.

[1] L. Cui *et al.*, Science **355**, 1192 (2017).
[2] M. Popp *et al.*, Appl. Phys. Lett. **115**, 083108 (2019).
[3] C. Schinabeck *et al.*, Phys. Rev. B **94**, 201407(R) (2016).

TT 66.7 Thu 15:00 P2/EG

Spin-orbit coupling drives entangled dynamics in a single molecule junction — •Moritz Frankerl and Andrea Donarini — Institut für Theoretische Physik, Universität Regensburg, 93035 Regensburg, Germany

Experiments based on THz-STM have shown how to obtain both space and time resolution of single molecule vibrations on their intrinsic length and time scales [1]. We report here the theoretical investigations on electronic dynamics of a copper-phthalocynanine in a THz-STM set-up. The quasi-degenerate anionic states of the molecule allow for a coupled spin and pseudo-spin description [2]. The spin-orbit interaction on the metallic centre is responsible, in combination with the ligand, for an intrinsic molecular spin-anisotropy .The latter is modulated, in the junction, by the coupling to the ferromagnetic tip which moreover, generates exchange fields on the molecule [3,4]. We study the resulting entangled spin and orbital dynamics directly in the time domain within a generalized master equation approach.

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[2] B. Siegert et al., Beilstein J. Nanotechnol. 6, 2452 (2015)
[3] M. Braun et al., Phys. Rev. B 70, 195345 (2004)
[4] A. Donarini et al. Nano Lett. 9, 2897 (2009)

TT 66.8 Thu 15:00 P2/EG

Electronic Transport through PEEB between Au(111) facets: A High-throughput Study — •Lokamani Lokamani[1,2], Florian Günther[3], Jeffrey Kelling[2], Torsten Sendler[1], Filip Kilibarda[1], Jannic Wolf[4], Thomas Huhn[4], Peter Zahn[1], Artur Erbe[1,5], and Sibylle Gemming[1,6] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Department of Information Services and Computing, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, Brazil — [4]Department of Chemistry, Universität Konstanz, Germany — [5]Department of Physics, Universität Konstanz, Germany — [6]Institute of Physics, Technische Universität Chemnitz, Germany

Electrical current transport through single molecules promises new possibilities for down-scaling electronic circuits. The family of p-phenylene-ethynylene derivatives provides excellent candidates for molecular electronics. Here, we present a study on the geometrical and electronic structure of 4-bis(phenylethynyl)-2,5-bis(ethoxy)benzene (PEEB) between Au-electrodes, as it is realized in mechanical break-junction experiments. We identify energetically most favorable configurations of PEEB derivatives between pyramidal Au(111) facets and investigate the electronic transport properties with semi-infinite leads using the DFTB+ code. We discuss the electronic transport properties of single PEEB molecules with anchoring groups -SH, -NH_2 and -CN depending on the anchoring positions on the Au(111) facets.

TT 66.9 Thu 15:00 P2/EG

Characterization and classification of molecular IV data — •Filip Kilibarda[1], Alexander Strobel[1], Michael Mortensen[2], Kurt Gothelf[2], Thomas Huhn[3], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Centre for DNA Nanotechnology, Aarhus , Denmark — [3]University of Konstanz, Konstanz, Germany

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 a liquid solution and under ambient conditions, and the other one in a cryogenic environment, under vacuum. As a testbed for these measurements, we use salen and C60 molecules respectively. We show how this data fits to the basic Single Level Model and what are the possible pitfalls of this approach. As an alternative, we offer modified versions of the SLM and compare them at predicting the transport properties of the molecules. Furthermore, due to the inherently stochastic processes of molecular binding to the nanoscopic junction, we propose an efficient approach based on the Machine Learning to further cluster the data into subsets. By using auto-encoders and decision trees with minimal amounts of supervised learning we can cluster large quantities of data. This allows us to evaluate different binding positions and events, with most appropriate models, and extract the underlying data.

TT 66.10 Thu 15:00 P2/EG

Hydrodynamic Bounds to the Entropy Production in 1D Systems — •Dennis Hardt, Philipp Weiss, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

A typical strategy of realizing an adiabatic change of state is to vary system parameters/quench very slowly in time τ. In the ideal case of adiabatic state preparation $\tau \to \infty$ the entropy production vanishes. This approach is hampered by hydrodynamic long-time tails, i.e. hydrodynamic fluctuations relax *algebraically slowly.* This behavior transfers to various observables. Therefore, a power-law decay of the entropy production $\sim \tau^{-\alpha}$ is expected for slow quenches.

We investigate the non-equilibrium dynamics of a classical diatomic gas with point like particles in 1D to study the entropy production as a function of τ. In order to model the long time behavior of such a system, we simulate a large number of scattering events ($\sim 10^9$) in a population of $\sim 10^5$ particles, over a relaxation timescale 10^5 times larger than the average scattering time.

The resulting curve of the entropy production shows a long-time tail $\sim \tau^{-1/2}$ matching to theoretical predictions from linear fluctuating hydrodynamics.

TT 66.11 Thu 15:00 P2/EG

Phase slip signatures in fully proximitized carbon nanotubes embedded in van der Waals stacks — •Christian Bäuml, Lorenz Bauriedl, Michaela Eichinger, Nicola Paradiso, and Christoph Strunk — University of Regensburg, Regensburg, Germany

Recently, Marganska et al. suggested that Majorana fermions (MFs) can occur in carbon nanotubes (CNTs) proximitized by superconductor (SC) in large fields perpendicular to the CNT axis [1].

In this work, we demonstrate the first building blocks of the proposed device. As a SC we chose a bilayer $NbSe_2$ crystal, an Ising SC capable to sustain large in-plane magnetic fields. A 7 μm-wide bilayer flake is stamped on top of a 9 μm-long CNT, laterally contacted via Au edge-contacts [2,3]. $NbSe_2$ and edge Au contacts turn out to be extremely transparent. Consequently, we observe a large supercurrent induced even in the 2 μm-long portion of CNT not directly proximitized by $NbSe_2$, with a 2-terminal conductance exceeding 120 e^2/h. Moreover, the conductance through the CNT shows sharp magnetic field-dependent dips, which we attribute to phase slippage events within the 1D superconducting system, a 1D analogue of what observed recently in 2D systems as $NbSe_2$ [4].

[1] M. Marganska et al., Phys. Rev. B 97, 075141 (2018)
[2] L. Wang et al., Science 614, 342 (2013)
[3] J.-W. Huang et al., Nano letters 15, 10 (2015)
[4] N. Paradiso et al., 2D Mater. 6, 025039 (2019)

TT 66.12 Thu 15:00 P2/EG

Electronic Tranport in Graphene Nanoribbons with Edge Disorder — •Tom Rodemund[1,2], Fabian Teichert[2], and Jörg Schuster[1,3] — [1]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany — [2]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany

Graphene possesses many interesting properties like high charge carrier mobilities and concentration. This makes it particularly suited for electronic applications. However, while using Graphene in form of nanoribbons (GNRs) edge disorder cannot be avoided. We study the influence of edge roughness on electron conductance using a density-functional-based tight-binding model to calculate the conductance of rough GNRs. We analyze large ensembles of GNRs with random edges and varying chirality in order to gain insight into the electronic structure.

A GNR represents a quasi-one-dimensional system with disorder and is thus expected to have strongly localized states. This leads to an exponential dependence of the conductance on the length of the ribbon with a characteristic localization length. We express the localization length as a function of roughness, width and chirality of the system.

TT 66.13 Thu 15:00 P2/EG

Adsorped or intercalated nickel atoms in graphene based materials: stability and electronic properties — •Daniel Dick[1,2,3], Florian Fuchs[2,3,4], and Jörg Schuster[2,3,4] — [1]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [2]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany — [3]Forschungsfabrik Mikroelektronik, Berlin, Germany — [4]Center for Microtechnologies, Technische Universität Chemnitz, Chemnitz, Germany

Graphene based materials such as graphene fibers or thin films offer promising electrical properties, which can be further improved by adsorption or by intercalation of dopants. A variety of electron donating species can be considered to fabricate intercalation compounds, many of which have not been studied yet.

We investigate structure, stability and electronic structure of nickel doped graphene, bilayer graphene and graphite using density functional theory. Different positions of the nickel atom are compared. We demonstrate that the energetically optimal position of the nickel atom depends on the nickel concentration. While the nickel atom is in the middle of a hexagon in graphene, it is located at an off-center position in graphite. Furthermore, the stability of the nickel intercalant decreases with increasing nickel concentration. The nickel atom introduces additional bands in the band structure. These bands are located near the Fermi level, leading to improved conductance.

TT 66.14 Thu 15:00 P2/EG

Angle-dependent magnetoresistance in ballistic semi-metals — •Felix Spathelf[1,2], Benoît Fauqué[2], and Kamran Behnia[1] — [1]Laboratoire de Physique et d'Étude des Matériaux (CNRS), ESPCI Paris, Université PSL, Paris, France — [2]JEIP, USR 3573 CNRS, Collège de France, Université PSL, Paris, France

We performed electric transport measurements on bismuth and tungsten single crystals of several shapes, orientations and qualities in mangetic fields up to 13.8 T and at temperatures down to 2 K. In order to study the angular dependence of the magnetoresistance, we applied a current parallel to a high symmetry axis and rotated the magnetic field in the plane perpendicular to it. Due to the Fermi surface topology, the Lorentz force depends on the angle between the crystal axes and the applied magnetic field. Therefore, the magnetoresistance is angle-dependent.

We observed that at low temperatures the magnetoresistance loses also the symmetry of the underlying crystal. This happens in both bismuth, which has a very small Fermi surface, and tungsten, whose Fermi surface is much larger. The observed behaviour is thought to be connected to the shape of the sample [1], but at least in the case of bismuth, the sample shape cannot explain completely this effect [2].

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[2] Z. Zhu et al., Nature Phys. 8, 89-94 (2012)

TT 66.15 Thu 15:00 P2/EG

Detecting superconductivity out-of-equilibrium in extended Hubbard and t-J models — Sebastian Paeckel[1], Benedikt Fauseweh[2,3], •Alexander Osterkorn[1], Thomas Köhler[4,1], Dirk Manske[2], and Salvatore R. Manmana[1] — [1]Institut für Theoretische Physik, U. Göttingen, D-37077 Göttingen — [2]MPI für Festkörperforschung, D-70569 Stuttgart — [3]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [4]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

Recent pump-probe experiments, e.g., on underdoped cuprates suggest the existence of a transient superconducting state above T_c. This poses the question how to reliably identify the emergence of long-range order, in particular superconductivity, out-of-equilibrium. We investigate this by studying a quantum quench in an extended Hubbard model and a variant of the t-J model using matrix product state time-evolution schemes. We compute various observables, which are used to identify (quasi-)long-range order in equilibrium. Our findings imply that it does not suffice to study the time-evolution of the optical conductivity to unambiguously identify superconductivity. In turn, we suggest to utilize time-resolved pair-ARPES experiments to probe for the formation of a condensate in the two-particle channel.

We acknowledge financial support by SFB 1073 (projects B03, B07) and Research Unit FOR 1807 (project P7) of the DFG, by the Max-Planck-UBC-U Tokyo Center for Quantum Materials, and by ERC Starting Grant No. 758935.

TT 66.16 Thu 15:00 P2/EG

Thermal and nonthermal responses of the low temperature charge order in $IrTe_2$ to femtosecond laser pulses — •Gregor Jecl[1], Venera Nesretdinova[2], Yaroslav Gerasimenko[1], Claude Monney[3], Fabian von Rohr[4], and Dragan Mihailovic[1,2] — [1]Department for Complex Matter, Jozef Stefan Institute, Slovenia — [2]Center of Excellence on Nanoscience and Nanotechnology, Slovenia — [3]Département de Physique and Fribourg Center for Nanomaterials, Université de Fribourg, Switzerland — [4]Department of Chemistry, University of Zürich, Switzerland

$IrTe_2$ is a layered material which exhibits a structural transition at T_{C1} = 275 K to a low temperature (LT1) phase which is accompanied by the appearance of stripe order. A second transition (LT2 phase) at T_{C2} = 180 K changes the dominant periodicity of the stripes. Superconductivity can be introduced below 3.1 K by doping or in undoped samples at surface patch domains of hexagonal symmetry. We have investigated the dynamics of all three phases on sub-picosecond timescales by means of ultrafast optical spectroscopy in a temperature range between 8 and 295 K. Additionally, by imaging the surface after photoexcitation in STM, we have investigated the degree to which the stripe order can be controlled by ultrafast optical pules on long timescales. At helium temperatures and under high fluence photoexcitation we observe a non-thermal photoinduced response of the transient reflectivity. Additionally, exposure to high fluence pulse trains results in the stabilisation of the LT1 phase at low temperatures and to changes in the orientation of the stripe phase.

TT 66.17 Thu 15:00 P2/EG

Microwave cavity-free hole burning spectroscopy of Er^{3+}:Y_2SiO_5 at sub-Kelvin temperatures — •Nadezhda Kukharchyk[1], Anton Mladenov[1], Natalya Pankratova[2], Dmitriy Sholokhov[1], Alexey A. Kalachev[3], Sebastian Probst[4], Vladimir Manucharyan[2], and Pavel A. Bushev[1,5] — [1]Experimentalphysik, Universität des Saarlandes, D-66123 Saarbrücken, Germany — [2]Department of Physics, Joint Quantum Institute and Center for Nanophysics and Advanced Materials, University of Maryland, College Park, MD 20742, USA — [3]RFC Kazan Scientific Center of RAS, 420029 Kazan, Russian Federation — [4]Quantronics group, SPEC, CEA, CNRS, Universite Paris-Saclay, CEA Saclay 91191 Gif-sur-Yvette Cedex, France — [5]JARA-Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, 52428 Jülich, Germany

Spectral hole burning technique is well-deployed in optical inhomogeneously broaden medium for realization of slow light and optical memory based on atomic frequency combs. First implementation of this technique into the microwave regime has been recently demonstrated with NV-centers coupled to a cavity [1]. Here, we develop this idea by applying spectral hole burning technique to Erbium spin ensemble in a cavity-free regime. We investigate Erbium-doped Y_2SiO_5 crystal coupled to a superconducting transmission line. Here, we show the influence of the magnetic field and temperature on the dynamics of the attained spectral hole and discuss processes governing it.

[1] Putz, S., Angerer, A., Krimer, D. et al. Nature Photon **11**, 36-39 (2017)

TT 66.18 Thu 15:00 P2/EG

Damping of the Anderson-Bogolyubov mode in Fermi mixtures by spin and mass imbalance — •Piotr Zdybel and Pawel Jakubczyk — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

We study the temporally nonlocal contributions to the gradient expansion of the pair fluctuation propagator for spin- and mass-imbalanced Fermi mixtures. These terms are related to damping processes of sound-like (Anderson-Bogolyubov) collective modes and are relevant for the structure of the complex pole of the pair fluctuation propagator. We derive conditions under which damping occurs even at zero temperature for large enough mismatch of the Fermi surfaces. We compare our analytical results with numerically computed damping rates of the Anderson-Bogolyubov mode.

[1] P. Zdybel and P. Jakubczyk, Phys. Rev. A 100, 053622 (2019)

TT 67: Cold Atomic Gases and Superfluids

Time: Thursday 16:30–18:30 Location: HSZ 204

TT 67.1 Thu 16:30 HSZ 204

Real time dynamics of impurity and disorder scattering with interacting Fermion wave packets — •Sebastian Eggert, Kevin Jägering, Imke Schneider, Benajmin Nagler, and Artur Widera — Physik and OPTIMAS, Technische Universität Kaiserslautern

Recent advances for ultra-cold gases allow the controlled scattering by disorder and localized impurities using moving interacting Fermion wave packets in a trap after a quick displacement in position. We analyze the damping and scattering behavior from large scale numerical t-DMRG simulations in 1D as a function of interaction, displacement and disorder strength in a regime where a comparison with our experiments is possible. Attractive interactions make the wave-packets more susceptible for both single impurities and disorder scattering, which leads to a significant larger damping and quicker breakdown of the oscillations. Repulsive interactions have a much smaller effect, but overall a reduction of scattering can be observed. The corresponding experiments for 3D scattering show maximum stability and minimal damping near the unitary point.

TT 67.2 Thu 16:45 HSZ 204

Damping of the Anderson-Bogolyubov mode in Fermi mixtures by spin and mass imbalance — •Piotr Zdybel — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Warsaw, Poland

During the speech, we will present the results of a study about the temporally nonlocal contributions to the gradient expansion of the pair fluctuation propagator for spin- and mass-imbalanced Fermi mixtures. These terms are related to damping processes of sound-like (Anderson-Bogolyubov) collective modes and are relevant for the structure of the complex pole of the pair fluctuation propagator. We derive conditions under which damping occurs even at zero temperature for large enough mismatch of the Fermi surfaces. We compare our analytical results with numerically computed damping rates of the Anderson-Bogolyubov mode.

[1] P. Zdybel and P. Jakubczyk, Phys. Rev. A 100, 053622 (2019)

TT 67.3 Thu 17:00 HSZ 204

Detecting topology in interacting fermionic wires via postquench observables — Andreas Haller[1], Pietro Massignan[2,3], and •Matteo Rizzi[4,5] — [1]Institute of Physics, Johannes Gutenberg University, D-55099 Mainz, Germany — [2]Departament de Fìsica, Universitat Politècnica de Catalunya, Campus Nord B4-B5, 08034 Barcelona, Spain — [3]ICFO – Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [4]Forschungszentrum Jülich, Institute of Quantum Control, Peter Grünberg Institut (PGI-8), 52425 Jülich, Germany — [5]Institute for Theoretical Physics, University of Cologne, D-50937 Köln, Germany

We exploit a simple observable called "mean chiral displacement" (MCD) for interacting fermionic wires and study numerically the interacting Su-Schrieffer-Heeger (SSH) chain by means of matrix product state calculations. In particular, we propose to study the time-evolution of a simple local quench which relates the MCD to the many-body topological invariant of the Hamiltonian for weakly-correlated interacting models. We study both a short-range correlated and a long-correlated model exhibiting topological/trivial insulators and a (trivial) symmetry breaking phase, and we link the behavior of the MCD to all three phases. We provide an experimental blueprint to obtain the long-range correlated model hosting all three phases.

TT 67.4 Thu 17:15 HSZ 204

Reduced-density-matrix functional theory for the N-boson Hubbard model: Universal functionals, v-representability and quantum depletion as emerging phenomenon — •Jakob Wolff[1], Carlos Benavides-Riveros[1], Christian Schilling[2,3], and Miguel Alexandre Lopes Marques[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle (Saale), Germany — [2]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, 80333 München, Germany — [3]Wolfson College, University of Oxford, Oxford OX2 6UD, United Kingdom

The Hohenberg-Kohn theorem and its generalization to non-local external potentials initiated the development of density and one-matrix functional theory. While such methods were applied so far only to fermionic quantum systems, the realization of ultracold gases urges the development of analogous bosonic functionals. In the form of the Hubbard dimer model for arbitrary number of bosons, we study the building block of one-dimensional optical lattices. Close to the Bose-Einstein condensation (BEC), we determine the one-matrix functional analytically. Remarkably, its gradient is found and proven to diverge repulsively in the regime of almost complete BEC. This possibly provides in particular a more fundamental explanation than the concept of quantum depletion for the absence of BEC of full degree in nature. Moreover, we obtain an analytic description of the set of v-representable one-body matrices for all N.

TT 67.5 Thu 17:30 HSZ 204

Finite-temperature effects and quench dynamics in interacting bosonic flux-ladders — •Maximilian Buser[1], Fabian Heidrich-Meisner[2], and Ulrich Schollwöck[1] — [1]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics (ASC), Munich Center for Quantum Science and Technology (MCQST), Fakultät für Physik, Ludwig-Maximilians-Universität München, 80333 München, Germany — [2]Institute for Theoretical Physics, Georg-August-Universität Göttingen, 37077 Göttingen, Germany

Flux-ladders constitute the minimal setup enabling a systematic understanding of the rich physics of interacting particles in strong magnetic fields and in lattices. These systems were also realized in a series of experiments and therefore, they have attracted great interest. We study ground-state phases, quench dynamics, and the effect of finite temperatures in interacting bosonic flux-ladders using matrix-product-state techniques. The focus is on experimentally accessible observables such as the chiral current and the leg-population imbalance; typical particle-current patterns and momentum-distribution functions are exemplified. We demonstrate that quantum quenches from suitably chosen initial states can be used to probe the equilibrium properties in the transient dynamics.

TT 67.6 Thu 17:45 HSZ 204

Topological Thouless pumps in commensurate and incommensurate optical lattices — •Pasquale Marra[1,2] and Muneto Nitta[2] — [1]Graduate School of Mathematical Sciences, The University of Tokyo — [2]Department of Physics, Keio University

Topological quantum pumps can be experimentally realized in cold atoms in optical lattices, by the superposition of two lattices with different, but commensurate spatial periods. These systems exhibit a topologically non-trivial phase where the topological invariant coincides with the quantized charge pumped at each pumping cycle. This quantization is analogous to the quantum Hall effect. Moreover, the charge transferred at well-defined fractions of the pumping period can be quantized as integer fractions of the Chern number. This fractional quantization is topological in nature and it is a direct consequence of the symmetries of the system, and does not rely on the presence of interactions. Here, we describe how to extend these findings to the case of quasiperiodic quantum pumps, which can be obtained by the superposition of two different lattices with incommensurate spatial periods. These quasiperiodic systems have no translational symmetry: It is therefore not possible to define the topological invariant as an integral of the Berry curvature in the momentum space. We will discuss here how to extend the definition of Chern number to the quasiperiodic case, and describe the transport signatures of the corresponding nontrivial topological phases.

TT 67.7 Thu 18:00 HSZ 204

Numerical generation of snapshots for fermionic quantum gas microscopy — •Stephan Humeniuk[1] and Yuan Wan[1,2] — [1]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [2]University of Chinese Academy of Sciences, Beijing 100049, China

Fermionic quantum gas microscope experiments with single-site single-atom resolution have enabled the detection of snapshots of the many-body wavefunction in occupation number space, which has opened the way for analysis techniques that go beyong standard correlation functions. Employing a nested, direct sampling approach for fermion pseudo density matrices as they arise naturally in determinantal quantum Monte Carlo simulations, a stream of Fock space configurations on large systems can be generated numerically. This approach is useful for carefully benchmarking and emulating equilibrium quantum gas microscope experiments.

TT 67.8 Thu 18:15 HSZ 204

Surface chiral excitations in time-reversal broken crystals — •Claudio Benzoni — TUM, Munich, Germany

We have studied an elastic model analogous to the isotropic body but in which the dynamics is non-Newtonian. In the long-wavelength regime this gapless model exhibits non-linear dispersing Rayleigh excitations that propagate in a chiral fashion. We found out that the chirality of the surface waves is determined by an interplay between the elasticity and the term that violates time-reversal symmetry and not only by the sign of the latter. Three regimes have been identified. Realizations of this model can be in two-dimensional Wigner crystals and in gyroscopic metamaterials.

TT 68: Annual General Meeting

Time: Thursday 18:30–20:00 Location: HSZ 03

Duration: 90 min.

TT 69: Nano- and Optomechanics (joint session TT/HL/CPP)

Time: Friday 9:30–10:30 Location: HSZ 03

Invited Talk TT 69.1 Fri 9:30 HSZ 03

Microwave Optomechanics with Superconducting Quantum Interference Cavities — •Daniel Bothner, Ines C. Rodrigues, and Gary A. Steele — Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600GA Delft, The Netherlands

Within the recent decade, cavity optomechanics has achieved tremendous breakthroughs regarding the detection and control of macroscopic mechanical oscillators with electromagnetic radiation. Among the most groundbreaking results are displacement sensing beyond the standard quantum limit, quantum ground-state sideband cooling and the generation of non-classical states of motion in massive mechanical objects. With most current approaches for optomechanical systems, however, the nonlinear single-photon regime seems still far out of reach.

Here, I will introduce a recently realized, novel approach for coupling microwave fields in a superconducting circuit to mechanical motion: flux-mediated microwave optomechanics. In this approach, mechanical motion is transduced to magnetic flux, which couples into a superconducting quantum interference device (SQUID). The SQUID forms the inductor of a superconducting microwave circuit and the coupling strength between the microwave circuit and the mechanical displacement is tunable and scales with the magnitude of the magnetic transduction field. Due to the linear scaling behavior, this flux-mediated approach has been predicted to have the realistic potential to reach the fully nonlinear regime of the optomechanical coupling, opening the door for the preparation of mechanical quantum states and a new generation of optomechanical devices.

TT 69.2 Fri 10:00 HSZ 03

Magnetoelastic readout concepts — •Daniel Schwienbacher[1,2,3], Nynke Vlietstra[1,2], Thomas Luschmann[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany

Nanostring resonators are prime candidates for mechanical sensing applications. Typically, they are used for mass and force sensing. However, it is also possible to use these resonators for the investigation of solid state properties of materials, like magnetoelastics. We investigated the mechanical motion of a 60 μm long SiN/Co bi-layer nanostring resonator with a resonance frequency in the MHz range. Here, we simultaneously use optical and electrical readout techniques. We observe the well known impact of the magnetoelastics, due to the presence of Co, on the resonance frequency of the nanostring. In addition, we study the impact of electrical transport through the string resonator on the mechanical properties of the system.

TT 69.3 Fri 10:15 HSZ 03

Magnetomechanical Crystals — •T. Luschmann[1,2,3], D. Schwienbacher[1,2,3], J. Graf[4], F. Engelhardt[4], S. Viola Kusminskiy[4], R. Gross[1,2,3], and H. Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, München, Germany — [4]Max Planck Institute for the Science of Light, Erlangen, Germany

Optomechanical crystals have become an established platform for the investigation of light-matter interaction, specifically in the context of optomechanical interaction. The success of this concept is founded in the simultaneous localization of GHz frequency phonons alongside THz photons in a suspended nanostructure [1]. We expand this concept with the introduction of magnetic materials capable of supporting spin-wave resonances in the GHz frequency range. We present finite element studies of phononic crystal cavities alongside micromagnetic simulations of spin-waves in nanostructured magnetic materials to tailor the geometries towards the realization of resonant, artificial magnon-phonon coupling. In addition, we will quantitatively compare numerical simulations with early experimental data.

[1] Eichenfield et al. Nature **462**, 7882 (2009).

TT 70: Correlated Electrons: Charge Order

Time: Friday 9:30–10:45 Location: HSZ 103

TT 70.1 Fri 9:30 HSZ 103

Interplay of superconductivity and charge-density-wave in $NbSe_2$ at high pressures — •Owen Moulding, Israel Osmond, Takaki Muramatsu, and Sven Friedemann — University of Bristol, Bristol, UK

The transition metal dichalcogenide $NbSe_2$ has well-documented charge density wave (CDW) and superconducting transitions at 33 K and 7 K at ambient pressure. The CDW transition is suppressed under high pressure and is absent beyond its quantum critical point (QCP). 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, magnetic susceptibility, and X-ray measurements have explored the vicinity of this QCP and they indicate 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 and trace the CDW transition to higher pressures than previously measured with transport methods. The sign-change in the Hall coefficient marking the CDW transition is suppressed. Above the critical pressure of the CDW, the Hall effect remains hole-like consistent as observed by ARPES. We observe the superconducting temperature increase with pressure and then saturate beyond the critical pressure of the CDW at 4.8 GPa, indicating weak competition between superconductivity and charge order.

TT 70.2 Fri 9:45 HSZ 103

Collapse of layer-dimerization in 1T-TaS$_2$ — Quirin Stahl[1], Maximilian Kusch[1], Gaston Garbarino[2], Norman Kretzschmar[2], Kerstin Hanff[3], Kai Rossnagel[3], Jochen Geck[1], and •Tobias Ritschel[1] — [1]TU Dresden — [2]ESRF, Grenoble — [3]CA Universität zu Kiel

Photo-induced switching between collective quantum states of matter is a fascinating rising field with exciting opportunities for novel technologies. Presently very intensively studied examples in this regard are nanometer-thick single crystals of the layered material 1T-TaS$_2$, where picosecond laser pulses can trigger a fully reversible insulator-to-metal transition (IMT). This IMT is believed to be connected to the switching between metastable collective quantum states, but the microscopic nature of this so-called hidden quantum state remained largely elusive up to now. Here we determine the latter by means of state-of-the-art x-ray diffraction and show that the laser-driven IMT involves a marked rearrangement of the charge and orbital order in the direction perpendicular to the TaS$_2$-layers. More specifically, we identify the collapse of inter-layer molecular orbital dimers, which are a characteristic feature of the insulating phase, as a key mechanism for the non-thermal IMT in 1T-TaS$_2$, which indeed involves a collective transition between two truly long-range ordered electronic crystals.

TT 70.3 Fri 10:00 HSZ 103

The nature of the charge density wave in TiSe$_2$ — •Adam Kłosiński[1], Jans Henke[2], Krzysztof Wohlfeld[1], and Jasper van Wezel[2] — [1]University of Warsaw, Krakowskie Przedmieście 26/28, 00-927, Warsaw, Poland — [2]University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands

Recently a charge density wave (CDW) was observed in a momentum resolved EELS (M-EELS) experiment on TiSe$_2$. According to the model proposed for TiSe$_2$ the CDW present in the system is transversal [1]. However, it is known that M-EELS is not sensitive to transverse CDWs [2]. Here we calculate the M-EELS response of TiSe$_2$ using a minimal model. We show that one can observe not only longitudinal but also transversal components of a CDW, for M-EELS is a surface-sensitive technique.

[1] F. J. Di Salve et al., Phys. Rev. B 14, 4321 (1976)
[2] S. Vig et al., SciPost Phys. 3, 026 (2017)

TT 70.4 Fri 10:15 HSZ 103

Strain-induced charge ordering in LiV$_2$O$_4$: Phase competition in a geometrically frustrated system — •Ulrike Niemann[1,2], Yu-Mi Wu[1], Minu Kim[1,2], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solide State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

LiV$_2$O$_4$ has been attracting considerable interest over two decades as the first heavy fermion system hosted by a 3d transition metal oxide. Nevertheless, the underlying physics, leading to this exotic heavy fermion state is yet unknown, but is frequently discussed in the framework of geometric frustration.

We stabilised thin films of LiV$_2$O$_4$ with different levels of strain-induced lattice deformations in order to directly probe the importance of the geometric frustration on the heavy fermion phase. Under such anisotropic strain, we found a transition from a heavy-fermion metal in a fully relaxed thin film to a charge-ordered insulator in a moderately strained thin film, proving the underlying phase competition and criticality. This demonstrates the importance of geometric frustration inherited in the spinel lattice as origin of this unconventional heavy fermion and further establishes LiV$_2$O$_4$ as an ideal model system for tuneable charge ordering.

TT 70.5 Fri 10:30 HSZ 103

Disorder-Free Localisation and Mobility Edges in a Long Ranged Falikov-Kimball Model — •Thomas Hodson[1] and Johannes Knolle[1,2] — [1]Imperial College London — [2]Technische Universität München

We study the interplay of long range interactions and disorder-free localisation in a generalised Falikov-Kimbal model. The power law interactions induce a charge density wave (CDW) phase transition at non-zero temperature in the ionic degrees of freedom. The CDW splits the spectrum of the electronic degrees of freedom and thermal fluctuations about it lead to an unusual mobility edge in one dimension for the electronic degrees of freedom. The two point correlator of this emergent disorder potential can be tuned via the temperature of the system.

Using a combination of exact diagonalisation and Markov Chain Monte Carlo we compute the energy resolved localisation properties of the electrons in one dimension. The finite size scaling of the energy resolved inverse participation ratio and the localisation length computed via a transfer matrix approach both provide numerical evidence for the existence of a mobility edge in the system. We compare the localisation behaviour to a simple Anderson model with spatially correlated binary disorder potential.

TT 71: Correlated Electrons: Other Theoretical Topics

Time: Friday 9:30–12:00 Location: HSZ 304

TT 71.1 Fri 9:30 HSZ 304

GW calculations of electron momentum densities and Compton profiles — •Eddie Harris-Lee[1], Alyn James[1], John Kay Dewhurst[2], and Stephen Dugdale[1] — [1]H. H. Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom — [2]Max-Planck Institute of Microstructure Physics, Halle, Germany

Compton scattering gives direct access to the single-particle momentum density, which contains information about the ground state wave functions of the many-body system. Theoretical calculations of electron momentum densities and Compton profiles, using Kohn-Sham density functional theory, don't fully agree with experimental measurements [1]. This could be partly due to the approximate description of correlation and partly because the Kohn-Sham wave functions are chosen to reproduce the density in real space, not in momentum space [2]. There is therefore good motivation to try alternative first principles theories. GW methods are an obvious choice [3], since these employ quasiparticle wave functions and use a different, non-local, description of exchange and correlation [4]. A method for obtaining a set of wave functions and occupation numbers from the output of a GW calculation will be described. The resulting electron momentum densities will be compared to experimental measurements for various materials.

[1] W. Schülke et al., Phys. Rev. B **54** 14381 (1996)
[2] L. Lam and P.M. Platzman, Phys. Rev. B **9** 5122 (1974)
[3] V. Olevano et al., Phys. Rev. B **86** 195123 (2012)
[4] F. Aryasetiawan and O. Gunnarsson, Rep. Prog. Phys. **61** 237 (1998)

TT 71.2 Fri 9:45 HSZ 304

Constrained Random Phase Approximation: Why and When it Works — •Erik van Loon[1], Malte Rösner[2], Mikhail Katsnelson[2], and Tim Wehling[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Germany — [2]Radboud University, Nijmegen, the Netherlands

The constrained Random Phase Approximation (cRPA) is an important part of the modern theory of correlated electron materials. In the downfolding from the full band structure to an effective low-energy (Hubbard) model, the cRPA provides a way to calculate the Hubbard parameter U for the low-energy model, taking into account screening by the other electronic states. Although it is a popular tool, a formal justification for the cRPA has been lacking. Here, we show when the cRPA is a good approximation.

TT 71.3 Fri 10:00 HSZ 304

Nonergodic Observables in the Hubbard Model at finite tem-

peratures — •Clemens Watzenböck, Anna Kauch, Alessandro Toschi, and Karsten Held — Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

We show the appearance of nonergodic observables in specific regions of the phase-diagram for the Hubbard-Model. The nonergodicity can be quantified by the difference between the static isolated susceptibility and the isothermal suszeptibility. This is equivalent to the infinite time limit of <A(t) B> - <A><B> [1,2]. We present various ways to extract the nonergodic term from numerical data (e.g. quantum Monte Carlo simulations performed in imaginary time [3,4]). Our results are relevant for numerical analytic continuation of susceptibilities, and also give insight into symmetry broken phases.

[1] Wilcox et al. (1968) Phys. Rev., 174, 624-629
[2] Suzuki (1971) Physica, 51(2), 277 - 291
[3] Georges et al. (1996) Rev. Mod. Phys., 68, 13-125
[4] Wallerberger et al. (2019) Comput. Phys. Commun., 235, 388 - 399

TT 71.4 Fri 10:15 HSZ 304

Ground-state properties and enhancement of pairing correlations in an asymmetric Hubbard ladder — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Germany

We investigate ground-state properties and correlation functions of an asymmetric two-leg Hubbard ladder using the density matrix renormalization group method. The ladder consists in a Hubbard chain (Hubbard leg) and a tight-binding chain (Fermi leg) connected by a single-particle hopping between the adjacent sites. This two-leg ladder system is a generalization of the asymmetric ladder investigated in [1,2] by allowing the hopping terms in the Hubbard leg and the Fermi leg to be unequal. We determine the excitation gaps and the corresponding charge and spin densities as well as several correlation functions. For strong on-site interactions at half filling, we observe finite pair-binding energies for range of intra-leg hopping terms in the Hubbard leg and rung hopping terms larger than the intra-leg hopping term in the Fermi leg. There is no enhancement of pairing correlations at half filling. For dopped ladders, the pair-binding energies reduce but persist and we observe strong enhancement of pairing correlations that decay in power-law. The exponent of the dcay is close to one for some parameter sets.

[1] A. Abdelwahab, E. Jeckelmann, M. Hohenadler, Phys. Rev. B 91, 155119 (2015)
[2] A. Abdelwahab, E. Jeckelmann, Eur. Phys. J. B 91, 207 (2018)

TT 71.5 Fri 10:30 HSZ 304

Influence of lattice geometry and dimensionality on the critical properties of magnetic transitions: A dynamical vertex approximation analysis — •Andreas Hausoel[1], Georg Rohringer[2], Thomas Schäfer[3], Giorgio Sangiovanni[1], and Alessandro Toschi[4] — [1]University of Würzburg, Germany — [2]University of Hamburg, Germany — [3]École Polytechnique and Collège de France, Paris, France — [4]Technical University of Vienna, Austria

We present a fundamental analysis of the effects of non-local spatial correlations on the magnetic transitions in different lattice types. To this aim, we have applied the dynamical vertex approximation (DΓA), a non-perturbative diagrammatic extension [1] of the dynamical mean-field theory (DMFT), to the simple, the body-centered and face-centered cubic lattices to the corresponding DMFT ones.

While an overall reduction of the differences in the transition temperatures and critical properties w.r.t. DMFT for lattices with increasing coordination number is expected, our analysis will elucidate the underlying aspects of this trend. In particular, we investigate the difference between an increase of the coordination number by changing the lattice type (i.e., keeping space dimension fixed) and by increasing the space dimensions (for a selected lattice type).

[1] Rohringer, Toschi, et al., Rev. Mod. Phys. 90, 025003 (2018)

15 min. break.

TT 71.6 Fri 11:00 HSZ 304

Nonlocal Exchange Interactions in Strongly Correlated Electron Systems — •Edin Kapetanović[1,2], Malte Schüler[1,2], Gerd Czycholl[1], and Tim Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen — [2]Bremen Center for Computational Materials Science, Universität Bremen

We study the influence of ferromagnetic nonlocal exchange on correlated electrons in terms of a SU(2)-Hubbard-Heisenberg model and address the interplay of on-site interaction induced local moment formation and the competition of ferromagnetic direct and antiferromagnetic kinetic exchange interactions. In order to simulate thermodynamic properties of the system in a way that largely accounts for the on-site interaction driven correlations, we advance the correlated variational scheme introduced in [M. Schüler et al., Phys. Rev. Lett. 111, 036601 (2013)] to account for explicitly symmetry broken electronic phases by introducing an auxiliary magnetic field. After benchmarking the method against exact solutions of a finite system, we study the SU(2)-Hubbard-Heisenberg model on a square lattice. We obtain the U-J finite temperature phase diagram of a SU(2)-Hubbard-Heisenberg model within the correlated variational approach and compare to static mean field theory (MFT). While the generalized variational principle and MFT yield similar transitions, we find that the nature of the associated phase transitions differs between the two approaches. The fluctuations accounted for in the variational approach render the transitions continuous, while MFT predicts discontinuous transitions between ferro- and antiferromagnetically ordered states.

TT 71.7 Fri 11:15 HSZ 304

How to recognize confinement of a hole in a string-like potential in doped antiferromagnets? — Krzysztof Bieniasz[1,2], •Piotr Wrzosek[3], Andrzej M. Oleś[2,4], and Krzysztof Wohlfeld[3] — [1]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, British Columbia, Canada V6T 1Z4 — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Prof. S. Łojasiewicza 11, PL-30348 Kraków, Poland — [3]Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [4]Max Planck Institute for Solid State Research, Heisenbergstraße 1, D-70569 Stuttgart, Germany

We study the problem of a single hole doped to the antiferromagnet and using analytical methods and state of the art numerics we establish (model independent) signature of the hole confinement in an antiferromagnetic spin background [1]. We show that once the hole is subject to a string-like potential its wave function coefficients need to decay faster than exponentially ('super-exponentially'). As the latter coefficients can be observed in recent cold atoms simulations of the Fermi-Hubbard model [2], we verify whether the hole confinement is realized in doped antiferromagnets.

[1] K. Bieniasz et al., SciPost Phys. 7, 066 (2019)
[2] C. S. Chiu et al., Science 365, 251-256 (2019)

TT 71.8 Fri 11:30 HSZ 304

Dynamical DMFT susceptibility at second orderphase transitions — •Abuduaini Niyazi, Dominique Geffroy, and Jan Kuneš — Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

We present a dynamical mean-field study (DMFT) of dynamical susceptibility in two-band Hubbard model. By varying model parameters(band asymmetry, crystal field, temperature) we realize transitions between various phases such as triplet excitonic condensate, spin-state order(solid), supersolid or antiferromagnetic solid. We analyze the behavior of relevant dynamical susceptibilities across these transitions, which break either continuous or discrete symmetries. Besides revealing the rich physics of the studied model, our results show how DMFT susceptibilities can be used to identify approximate (weakly broken) symmetries and incipient instabilities.

TT 71.9 Fri 11:45 HSZ 304

Plasmons In Doped Mott Insulators — •Andrej Lehmann, Evgeny Stepanov, and Alexander Lichtenstein — I. Institut für Theoretische Physik, Hamburg, Deutschland

Plasmons play an important role in nanophotonics and different metamaterials applications exhibiting interesting phenomena like negative refraction, superlensing and more. Plasmons are usually studied in the metallic regime, where the mobility of charge carrier density is large. Recently, correlated plasmons attracted a lot of attention in Mott-like insulating oxides showing a low loss in the visible optical range. In order to study plasmons in insulators, one has to apply doping to induce fluctuations of a charge density. Theoretically, plasmons can be described by the Lindhardt dielectric function using the random phase approximation (RPA). However, the RPA is applicable only in the weakly interacting regime, which corresponds to small-gap or metallic systems. For description of plasmons in Mott insulating regime one have to use more elaborated methods, such as the Dual Boson (DB) theory. In this work we study correlated plasmons in a single band

Mott insulator with a prototype of C2F and C2H materials. For this aim we apply a ladder DB approach that considers the polarization operator in the two-particle ladder form written in terms of local three- and four-point vertex functions. Recently, it has been shown that two-particle vertex functions can be drastically simplified in the regime of strong collective fluctuations in the system. In this case the DB theory can be reduced to a much simpler RPA+EDMFT approach. Thus, we finally compare our results with results of the RPA method.

TT 72: Graphene II: Adsorption, Intercalation and Doping (joint session O/TT)

Time: Friday 10:30–12:30 Location: GER 37

TT 72.1 Fri 10:30 GER 37

Ab initio thermodynamics of hydrocarbons relevant to graphene growth at solid and liquid Cu surfaces — •Mie Andersen, Juan Santiago Cingolani, and Karsten Reuter — Theoretical Chemistry, Technische Universität München, Germany

High quality graphene can be synthesized through chemical vapor deposition (CVD) at liquid Cu [1]. However, the role of the liquid catalyst surface is not yet well understood, and the role of hydrogen in the reactant mixture is still debated [2]. Here [3], we use *ab initio* thermodynamics to study the stability of a wide range of hydrocarbons under various CVD conditions (temperature, methane and hydrogen pressures) used in experimental growth protocols at solid and liquid Cu surfaces. We compare various low-index Cu facets and make use of hindered translator/rotator or ideal 2D gas models [4] to describe the adsorbate free energies. We find that smaller hydrocarbons will completely dehydrogenate under most CVD conditions. For larger graphene-like clusters, metal-terminated and hydrogen-terminated edges have very similar stabilities. While both cluster types might thus form during the experiment, we show that the low binding strength of clusters with hydrogen-terminated edges could result in instability towards desorption.

[1] D. Geng *et al.*, PNAS **109**, 7992 (2012)
[2] X. Zhang *et al.*, JACS **136**, 3040 (2014)
[3] M. Andersen, J.S. Cingolani, K. Reuter, J. Phys. Chem. C **123**, 22299 (2019)
[4] L.H. Sprowl *et al.*, J. Phys. Chem. C **120**, 9719 (2016)

TT 72.2 Fri 10:45 GER 37

Graphene on liquid Cu, a multiscale model rationalizing mesoscale flake alignment — •Juan Santiago Cingolani, Karsten Reuter, and Mie Andersen — Chair of Theoretical Chemistry, Technical University of Munich, Germany

In recent years the use of liquid Cu as a catalyst during chemical vapor deposition (CVD) has emerged as a promising method for the continuous production of high-quality single layer graphene. The processes involved, such as carbon nucleation, defect healing, or flake alignment, remain largely unexplored or lack convincing atomic-scale rationalization. Of particular interest is the reported meso-scale interaction between growing flakes that leads to an ordering into 2D lattices.

To address the latter, we engage in a multiscale modeling study, hierarchically combining molecular dynamics (MD) simulations with continuum theory. Using a third-generation charge optimized many body potential (COMB3), the MD simulations reveal a strong interaction of graphene flakes with the liquid substrate, leading even to their partial immersion. On the basis of thus determined material parameters like surface energy, charge transfer or average flake height above the surface, we then set up a simple continuum model assuming the flakes to be spherically charged particles. Within an order of magnitude, this model rationalizes the experimental observation of a coalescence of the growing hexagonal flakes into a close-packed structure with well-defined inter-flake separation in terms of long-range capillary and electrostatic interactions.

TT 72.3 Fri 11:00 GER 37

Experimental access to thermodynamics and kinetics predicting the CVD growth of graphene on Cu — •Paul Leidinger, Jürgen Kraus, and Sebastian Günther — TUM, Dept. Chemie, Lichtenbergstr. 4, D-85748 Garching

Most Graphene growth recipes by chemical vapor deposition (CVD) on copper in a reactive CH_4/H_2 atmosphere are results of parameter variations optimized by trial and error. Many existing growth models described in the literature are qualitative or contain phenomenological parameters to describe the growth process. In our study, we aim at analyzing the key processes during CVD at 900-1050 °C while maintaining the defined geometry of a growing graphene flake surrounded by graphene free copper. For this purpose, it is essential to control the flake nucleation before and, more importantly, during the entire CVD growth. Systematic variation of the CVD parameters provides the experimental data used to formulate a kinetic model which predicts the graphene growth velocity as function of the chosen mass action constant Q. Determining experimentally the thermodynamic equilibrium of the CH_4 decomposition reaction enables us to use the equilibrium as reference point to which any chosen CVD parameter set can be related quantitatively. With experimental validation of our growth model we can understand both, the thermodynamics and kinetics of graphene growth on copper. Furthermore, we can also predict the growth rate of single graphene flakes formed during any CVD experiment on copper at high precision.

TT 72.4 Fri 11:15 GER 37

Stacking Relations and Substrate Interaction of Graphene on Copper Foil — •Philip Schädlich[1], Florian Speck[1], Stiven Forti[2], Camilla Coletti[2], and Thomas Seyller[1] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy

Graphene-based device production requires graphene sheets of perfect crystallinity and low defect density on a large scale. Beyond mechanical exfoliation, where the flake size is uncontrollable, there are two promising approaches for high-quality wafer-scale graphene growth: (i) the sublimation growth on silicon carbide (SiC) by thermal decomposition of the substrate [1] and (ii) the chemical vapour deposition (CVD) on metal substrates such as copper [2].

In the present study we investigate the crystallinity of CVD grown graphene and the orientation with respect to the underlying copper foil by means of low-energy electron microscopy (LEEM) and diffraction (LEED). We find a lattice match within $\pm 1°$ between the graphene and the Cu(111) surface, which shows a surface facetting depending on the graphene thickness on top. Recently, stress-induced stacking domains in bi- and multilayer graphene were found for epitaxial graphene on SiC [3], revealing a much less homogeneous system than believed. Our LEEM dark field images and reflectivity spectra suggest a similar decomposition into domains of different stacking order for the CVD grown graphene flakes. [1] K. V. Emtsev et al., Nature Mater. 8, 203 (2009). [2] X. S. Li et al., Science 324, 1312 (2009). [3] T. A. de Jong et al., Physical Review Materials 2, 104005 (2018).

TT 72.5 Fri 11:30 GER 37

Sidewall epigraphene investigated by STEM — •Markus Gruschwitz, Steffen Schulze, and Christoph Tegenkamp — TU Chemnitz, Chemnitz, Germany

Epitaxial graphene nanoribbons (GNR) grown on SiC facets reveal ballistic transport channels. The structure and growth were studied intensively by STM, LEED and LEEM [1]. Spatially resolved transport measurements and tight-binding calculations suggest that the bonding of the ribbons to the SiC substrate plays an important role [2]. In this study, cross-section STEM on similar structures were performed in order to characterize the interface and bonding between graphene and SiC in more detail.

Indeed, the zig-zag GNRs, grown along the [1100] direction, are delaminated from the SiC facet as seen by high resolution C_S corrected STEM. Mini steps at the top and the bottom of the sidewalls define the edges of the GNRs. Atomically resolved EELS and EDX confirm that the top part of the freestanding GNR merges into a bufferlayer. The SiC facet reveals a silicon deficiency in the three topmost substrate layers. These SiC imperfections were found already for epitaxial graphene on SiC(0001) and result from the sublimation processes [3]. The lower edge merges into SiC and shows a sp^3-hybridization. Moreover, differential phase contrast measurements allow the calculation of charge density maps and therefore the visualization of space charge distributions in the substrate. References: [1] Zakharov et al., ACS Appl Nano Mat., 2, 156 (2019) [2] Aprojanz et al., Nat. Comm. 9, 4426, (2018). [3] Gruschwitz et al., PRM 3, 094004 (2019).

TT 72.6 Fri 11:45 GER 37

Epitaxial growth of high-quality armchair graphene nanoribbons — •H. Karakachian[1], J. Aprojanz[2], T. T. N. Nguyen[2], A. A. Zakharov[3], R. Yakimova[4], P. Rosenzweig[1], C. M. Polley[3], T. Balasubramanian[3], C. Tegenkamp[2], and U. Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut für Physik, Technische Universität Chemnitz — [3]MAX IV laboratory, Lund — [4]IFM, Linköping University

Graphene nanoribbons (GNRs) are considered to be the fundamental building blocks for future carbon-based nanoelectronics. The functionality of GNRs is governed by the detailed atomic structure of their edges. Namely, a GNR terminated by armchair edges develops a bandgap in its electronic structure driven by quantum confinement effects, where the size of the bandgap scales with the width of the ribbon itself. Thus, the controlled growth of armchair GNRs (AC-GNRs) may solve the long-lasting problem of graphene, which is its inability to be embedded in modern quantum integrated circuitry. Here, we grow high-quality AC-GNRs on the sidewalls of 6H-SiC mesa structures. Using angle-resolved photoelectron spectroscopy we study the electronic structure of the one-dimensionally (1D) confined AC-GNRs which truly reveals a width-dependent bandgap formation. We observe a set of well-resolved sub-bands and a Fermi surface that consists strictly of a straight line which are characteristic features of 1D confined systems. Our findings provide a solid ground for further theoretical assessment and a deeper understanding of quantum confinement phenomena.

TT 72.7 Fri 12:00 GER 37

Monodispersed graphene nanoribbons on Ag(111) by electrospray controlled ion beam deposition: their self-assembly and on-surface extension visited by STM — •Wei Ran[1], Andreas Walz[1], Karolina Stoiber[1], Peter Knecht[1], Anthoula C. Papageorgiou[1], Annette Huettig[1], Diego Cortizo-Lacalle[2], Juan P. Mora-Fuentes[2], Aurelio Mateo-Alonso[2,3], Hartmut Schlichting[1], Joachim Reichert[1], and Johannes V. Barth[1] — [1]Physics Department E20, Technical University of Munich, Germany — [2]POLYMAT, University of the Basque Country UPV/EHU, Spain — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Graphene nanoribbons (GNRs) are of interest due to their potential in electronics, energy conversion, and storage. For atomically precise GNRs, elaborate bottom-up fabrication protocols have been developed, utilising the reactivity of a metallic support.[1] However this approach often results in GNR arrays with a variety of lengths. Here we employ a different approach for the preparation and study of GNRs on surfaces: chemical synthesis and purification of well-defined nanoribbons[2] followed by processing with electrospray controlled ion beam deposition (ES-CIBD). With this method, we can deposit well-defined GNRs on any solid support under ultra-high vacuum conditions. The quality of the films produced is exemplified for a $\sim$ 3 nm GNR on Ag(111). We explore their self-assembly and thermally activated polymerisation reactions by means of scanning tunnelling microscopy.

1) Fasel et al. *Adv. Mater.* **2016**, *28*, 6222.
2) Mateo-Alonso et al. *Angew. Chem., Int. Ed.* **2018**, *57*, 703.

TT 72.8 Fri 12:15 GER 37

Understanding trends in lithium binding at 2D materials — •Zeljko Sljivancanin[1,2], Srdjan Stavric[2], and Zoran S. Popovic[2] — [1]Serbian Academy of Sciences and Arts, Belgrade, Serbia — [2]Vinca Institute of Nuclear Sciences, Belgrade, Serbia

Employing density functional theory we studied microscopic mechanisms governing binding of metal atoms and their nanostructures at selected 2D materials. We considered the interaction of a Li adatom with monolayers of several transition metal oxides and dichalcogenides, carbides of group XIV elements, functionalized graphene, silicene and germanene, as well as black phosphorus and Ti_2C MXene. We found that the general trend in Li binding can be estimated from positions of conduction band minima of 2D materials, since the the energy of the lowest empty electronic states shows a nice correlation with the strength of Li adsorption [1]. At variance to the majority of studied surfaces where occurs a simple electron transfer from Li to the substrate, in monolayers of carbides of group XIV elements Li adsorbates profoundly modify substrates, creating well-localized mid-gap states. This gives rise to their capability to accommodate Li structures with the nearly constant binding energy of alkaline atoms over Li coverages ranging from well-separated adatoms to a full monolayer.

TT 73: Topology: Other Topics

Time: Friday 11:00–12:15 Location: HSZ 103

TT 73.1 Fri 11:00 HSZ 103

Electronic transport in one-dimensional Floquet topological insulators via topological-and non-topological edge states — •Niclas Müller[1], Dante M. Kennes[1], Jelena Klinovaja[2], Daniel Loss[2], and Herbert Schoeller[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52074 Aachen,Germany — [2]Department of Physics, University of Basel, Klingelbergstr. 82, CH-4056 Basel, Switzerland

Based on probing electronic transport properties, we study the recently discovered phase diagram of 1D Floquet topological insulators [Kennes et al., Phys. Rev. B 100, 041103(R) (2019)]. Using Keldysh formalism, we compute transport properties of this model, where we consider a setup in which states with a large relative edge-weight primarily contribute to the transport, which grants experimental access to the topological phase diagram. Surprisingly, we find conductance values similar in magnitude to those corresponding to topological edge states, when tuning the lead Fermi energy to special values in the bulk, which coincide with bifurcation points of the dispersion relation in quasimomentum space. These peaks reveal the presence of bands of states whose wave functions are linear combinations of delocalized bulk states and exponentially localized edge states, where the amplitude of the edge-state component is sharply peaked at the bifurcation point, resulting in an unusually large relative edge-weight. We discuss the emergence of these states in terms of an intuitive yet quantitative physical picture, which is not specific to the model, suggesting that they may be present in a wide class of systems.

TT 73.2 Fri 11:15 HSZ 103

Topological Sign Problems — •Adam Smith[1] and Zohar Ringel[2] — [1]Technical University Munich, Garching, Germany — [2]Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Sign-problems are one of the major obstacles for the numerical study of complex many-body quantum systems. They render such models intractable to otherwise powerful techniques, most famously demonstrated by the exponential difficultly of quantum Monte Carlo methods. Here we provide a simple criterion to diagnose incurable sign-problems in topologically ordered systems – that is, whether the model has a sign-problem that cannot be removed by any local unitary transformation. Explicitly, if the exchange statistics of the anyonic excitations do not form complete sets of roots of unity, then the model has an incurable sign-problem. This establishes a concrete connection between the statistics of anyons, contained in the modular S and T matrices, and the presence of a sign-problem in a microscopic Hamiltonian. We prove this criterion for the large set of bosonic non-chiral models described by an abelian topological quantum field theory at low-energy, and offer evidence that it applies more generally.

TT 73.3 Fri 11:30 HSZ 103

Interacting topological frequency converter — •Simon Körber[1], Lorenzo Privitera[1], and Björn Trauzettel[1,2] — [1]Institute of Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

Driving with a periodic force effectively raises the dimensionality of a system since each eigenstate can be expanded with respect to the harmonics of the drive frequency, with the Fourier amplitudes acting as additional coordinates. This extension opens a new approach to engineer and explore novel topological phases in synthetic dimensions. In this context, it has been shown that a two-level system coupled to two circularly polarized drives can act as the temporal analog of a Chern insulator, where the Hall response translates into a quantized frequency conversion between the dynamical drives.

In this talk, we extend this idea by analyzing a two-spin model with spin-spin interactions in addition to external fields. We demonstrate that the interplay of interaction and synthetic dimension gives rise to striking topological phenomena that have no counterpart in the non-interacting regime. By calculating the topological phase diagrams as a function of interaction strength, we show that this can lead to an enhancement of the frequency conversion as a direct manifestation of the correlated topological response.

TT 73.4 Fri 11:45 HSZ 103

Quantum robustness of three-dimensional fracton codes — •Matthias Mühlhauser[1], Matthias Walther[1], David A. Reiss[2], and Kai P. Schmidt[1] — [1]Institute for Theoretical Physics I, FAU Erlangen-Nürnberg, Germany — [2]Dahlem Center for Complex Quantum Systems and Physics Department, FU Berlin, Germany

We investigate zero-temperature phase transitions out of three-dimensional fracton phases. For this reason exactly solvable fracton codes like the X-Cube model, which features fracton topological order of type I, are studied in the presence of an external homogeneous magnetic field. We apply high order linked-cluster expansions to calculate the ground-state energy as well as excitation energies of fractonic quasi-particles in order to determine the ground-state phase diagram quantitatively. To this end a full graph decomposition is performed for these three-dimensional quantum many-body systems.

TT 73.5 Fri 12:00 HSZ 103

Parafermions and Z_3 Charge-Flux attachment — •Peng Rao and Inti Sodemann — Max Planck Institute for the Physics of Complex System, Dresden

A recent construction (Ann. Phys. 393, 234 (2018)) has introduced an interesting route to bosonization of fermions in two spatial dimensions by implementing a precise lattice version of flux-charge binding. The idea is to modify Kitaev's Toric code so that the electric charge (e) and magnetic flux (m) are always created in a tight “dipolar" pair ε ($=e \times m$) which is a fermion, providing a way to represent any local fermionic Hamiltonian as a local Hamiltonian of spins. We discuss an extension of these ideas to the case of a Z_N toric code which allows a bosonization of anyons with more general statistical angles. We have focused particularly in the case of N=3. We will prove that ground states in the torus in this case are at least three-fold degenerate, and, discuss a model featuring a topological phase transition between a 3-fold degenerate state and a 9-fold degenerate ground state featuring parafermionic excitations.