Low Temperature Physics Division
Fachverband Tiefe Temperaturen (TT)

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Overview of Invited Talks and Sessions

(Lecture halls HSZ 101, HSZ 103, HSZ 201, HSZ 204, and HSZ 304; Poster P2/2OG, P2/3OG, and P2/4OG)

Tutorial "Physics Meets Machine Learning (joint session DY/TT)"

TT 1.1	Sun	16:00–16:45	HSZ 01	**Machine Learning for Quantum Technologies** — •Florian Marquardt
TT 1.2	Sun	16:45–17:30	HSZ 01	**The Unreasonable Effectiveness of Gaussians in the Theory of Deep Neural Networks** — •Zohar Ringel
TT 1.3	Sun	17:30–18:15	HSZ 01	**Computing learning curves for large machine learning models using the replica approach** — •Manfred Opper

Plenary Talk

PLV X	Thu	14:00–14:45	HSZ 02	**Single-electron-spin-resonance detection by microwave photon counting** — •Patrice Bertet

Invited Talks of the joint Symposium SKM Dissertation Prize 2023 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ 04	**Diffusion of antibodies in solution: from individual proteins to phase separation domains** — •Anita Girelli
SYSD 1.2	Mon	10:00–10:30	HSZ 04	**Intermediate Filament Mechanics Across Scales** — •Anna V. Schepers
SYSD 1.3	Mon	10:30–11:00	HSZ 04	**Ultrafast Probing and Coherent Vibrational Control of a Surface Structural Phase Transition** — •Jan Gerrit Horstmann
SYSD 1.4	Mon	11:00–11:30	HSZ 04	**Electro-active metasurfaces employing metal-to-insulator phase transitions** — •Julian Karst
SYSD 1.5	Mon	11:30–12:00	HSZ 04	**The role of unconventional symmetries in the dynamics of many-body systems** — •Pablo Sala

Invited Talks of the joint Symposium Ultrafast Excitation Pathways of Quantum Materials (SYUE)

See SYUE for the full program of the symposium.

SYUE 1.1	Wed	9:30–10:00	HSZ 01	**Dynamics and control in quantum materials using multi-terahertz spectroscopy** — •Richard Averitt
SYUE 1.2	Wed	10:00–10:30	HSZ 01	**Accessing the nonthermal phonon populations in 2D materials with femtosecond electron diffuse scattering** — •Hélène Seiler
SYUE 1.3	Wed	10:30–11:00	HSZ 01	**Exciting potentials – Exploring the realms of ultrafast phase transitions** — •Laurenz Rettig
SYUE 1.4	Wed	11:15–11:45	HSZ 01	**Sub-cycle multidimensional spectroscopy of strongly correlated materials** — •Olga Smirnova
SYUE 1.5	Wed	11:45–12:15	HSZ 01	**Witnessing many-body entanglement in light-driven quantum materials** — •Matteo Mitrano
SYUE 1.6	Wed	12:15–12:45	HSZ 01	**Optical responses of photoexcited materials: from parametric amplification to photoinduced superconductivity** — •Eugene Demler

Invited Talks of the joint Symposium Topology in Quantum and Classical Physics – From Topological Insulators to Active Matter (SYQC)

See SYQC for the full program of the symposium.

SYQC 1.1	Wed	15:00–15:30	HSZ 01	**Topological magnetic whirls for computing** — •Karin Everschor-Sitte
SYQC 1.2	Wed	15:30–16:00	HSZ 01	**Topological waves from solids to geo/astrophysical flows** — •Pierre Delplace
SYQC 1.3	Wed	16:00–16:30	HSZ 01	**Topological Phase Transitions in Population Dynamics** — •Erwin Frey
SYQC 1.4	Wed	16:45–17:15	HSZ 01	**Topological invariants protect robust chiral currents in active matter** — •Evelyn Tang
SYQC 1.5	Wed	17:15–17:45	HSZ 01	**Topological defects in biological active matter** — •Amin Doostmohammadi

Invited Talks of the joint Symposium Real-Time Measurements of Quantum Dynamics (SYQD)

See SYQD for the full program of the symposium.

SYQD 1.1	Thu	9:30–10:00	HSZ 01	**Real-time measurement and control of spin dynamics in quantum dots** — •Seigo Tarucha
SYQD 1.2	Thu	10:00–10:30	HSZ 01	**Quantum Dot arrays for Quantum Information Transfer** — •Gloria Platero
SYQD 1.3	Thu	10:30–11:00	HSZ 01	**Optical Detection of Real-Time Quantum Dynamics in Quantum Dots** — •Martin Geller
SYQD 1.4	Thu	11:30–12:00	HSZ 01	**Cooper Pair Splitting in Real-Time** — •Christian Flindt
SYQD 1.5	Thu	12:00–12:30	HSZ 01	**Trajectory-based detection in stochastic and quantum thermodynamics** — •Jukka Pekola

Invited Talks of the joint Symposium Topological Superconductor-Magnet Heterostructures (SYTS)

See SYTS for the full program of the symposium.

SYTS 1.1	Thu	15:00–15:30	HSZ 01	**Blending of superconductivity and magnetism via topological solitons** — •Christos Panagopoulos
SYTS 1.2	Thu	15:30–16:00	HSZ 01	**Topological landscaping in magnet-superconductor heterostructures** — •Sebastián A. Díaz
SYTS 1.3	Thu	16:00–16:30	HSZ 01	**Experimental study of minigaps and end states in bottom-up designed multi-orbital Shiba chains** — •Jens Wiebe
SYTS 1.4	Thu	16:45–17:15	HSZ 01	**Quantum spins and hybridization in artificially-constructed chains of magnetic adatoms on superconducting 2H-NbSe$_2$** — •Katharina J. Franke
SYTS 1.5	Thu	17:15–17:45	HSZ 01	**Braiding of Majorana zero modes** — •Stephan Rachel

Invited Talks of the joint Symposium Physics of van der Waals 2D Heterostructures (SYHS)

See SYHS for the full program of the symposium.

SYHS 1.1	Fri	9:30–10:00	HSZ 01	**Novel moiré excitons and ultrafast optical dynamics in van der Waals 2D heterostructures** — •Steven G. Louie
SYHS 1.2	Fri	10:00–10:30	HSZ 01	**Interaction induced magnetism in 2D semiconductor moiré superlattices** — •Xiaodong Xu
SYHS 1.3	Fri	10:30–11:00	HSZ 01	**Ions in tight places: intercalation and transport of ions in van der Waals heterostructures** — •Irina Grigorieva
SYHS 1.4	Fri	11:15–11:45	HSZ 01	**Spin-orbit proximity in van der Waals heterostructures** — •Felix Casanova
SYHS 1.5	Fri	11:45–12:15	HSZ 01	**Plethora of many-body ground states in magic angle twisted bilayer graphene** — •Dmitri Efetov

Invited Talks of the Focus Session "Physics Meets ML I - Machine Learning for Complex Quantum Systems (joint session DY/TT)"

TT 2.1	Mon	9:30–10:00	HSZ 03	**Enhanced variational Monte Carlo for Rydberg atom arrays** — •Stefanie Czischek
TT 2.2	Mon	10:00–10:30	HSZ 03	**Data mining the output of quantum simulators – from critical behavior to algorithmic complexity** — •Marcello Dalmonte
TT 2.3	Mon	10:30–11:00	HSZ 03	**Reinforcement learning for quantum technologies** — •Florian Marquardt
TT 2.4	Mon	11:00–11:30	HSZ 03	**Machine learning of phase transition** — •Christof Weitenberg

Invited Talks of the Focus Session "Physics Meets ML II - Understanding Machine Learning as Complex Interacting Systems (joint session DY/TT)"

TT 13.1	Mon	15:00–15:30	ZEU 250	**The challenge of structured disorder in statistical physics** — •Marc Mezard
TT 13.2	Mon	15:30–16:00	ZEU 250	**The emergence of concepts in shallow neural-networks** — •Elena Agliari
TT 13.3	Mon	16:00–16:30	ZEU 250	**Adaptive Kernel Approaches to Feature Learning in Deep Neural Networks** — •Zohar Ringel
TT 13.5	Mon	17:00–17:30	ZEU 250	**Analysing the dynamics of message passing algorithms** — •Manfred Opper
TT 13.6	Mon	17:30–18:00	ZEU 250	**Deep Learning Theory Beyond the Kernel Limit** — •Cengiz Pehlevan

Invited Talks of the Focus Session "New Perspectives for Adiabatic Demagnetization Refrigeration in the Kelvin and sub-Kelvin Range (joint session TT/MA)"

TT 19.1	Tue	9:30–10:00	HSZ 03	**Self-cooling molecular spin quantum processors** — •Marco Evangelisti
TT 19.2	Tue	10:00–10:30	HSZ 03	**Triangular rare-earth borates for milli-Kelvin adiabatic demagnetization refrigeration** — •Philipp Gegenwart
TT 19.3	Tue	10:30–11:00	HSZ 03	**A millikelvin scanning tunnelling microscope in ultra-high vacuum with adiabatic demagnetisation refrigeration** — •Ruslan Temirov
TT 19.4	Tue	11:15–11:45	HSZ 03	**ADR cryostats in low temperature physics and their applications** — •Doreen Wernicke
TT 19.5	Tue	11:45–12:15	HSZ 03	**Frustrated dipolar materials for low-temperature magnetic refrigeration** — •Mike Zhitomirsky

Invited Talks of the Focus Session "Unconventional Transport Phenomena in Low-Dimensional Superconducting Heterostructures"

TT 27.1	Wed	9:30–10:00	HSZ 03	**Superconducting diode effect in Rashba superlattice** — •Teruo Ono
TT 27.2	Wed	10:00–10:30	HSZ 03	**Quasiparticle-based and Cooper-pair based superconducting diodes** — •Maria Spies
TT 27.3	Wed	10:30–11:00	HSZ 03	**Non-reciprocal superconductivity and the field free Josephson diode** — •Mazhar Ali

Invited Talks of the Focus Session "Correlations in Moiré Quantum Matter"

TT 35.1	Wed	15:00–15:30	HSZ 03	**Strongly correlated excitons in atomic double layers** — •Phuong Nguyen
TT 35.2	Wed	15:30–16:00	HSZ 03	**The Quantum Twisting Microscope** — •Shahal Ilani
TT 35.3	Wed	16:00–16:30	HSZ 03	**Light-driven phenomena in two-dimensional and correlated quantum materials** — •Angel Rubio
TT 35.4	Wed	16:45–17:15	HSZ 03	**Cascade of transitions in twisted and non-twisted graphene layers within the van Hove scenario** — •Laura Classen

TT 35.5	Wed	17:15–17:45	HSZ 03	**Topology and strong correlation: From twisted bilayer graphene to the boundary zeros of Mott insulators** — •Giorgio Sangiovanni

Invited Talks of the Focus Session "Superconducting Nickelates"

TT 44.1	Thu	9:30–10:00	HSZ 03	**Atomic-scale insights to lattice and electronic structure in superconducting nickelates** — •Berit Goodge
TT 44.2	Thu	10:00–10:30	HSZ 03	**Nickelate and cuprate superconductors: Similar yet different** — •Vamshi Mohan Katukuri
TT 44.3	Thu	10:30–11:00	HSZ 03	**Superconducting instabilities in strongly-correlated infinite-layer nickelates** — •Andreas Kreisel
TT 44.5	Thu	11:45–12:15	HSZ 03	**Superconducting layered square-planar nickelates: Synthesis, properties, and progress** — •Grace Pan
TT 44.4	Thu	11:15–11:45	HSZ 03	**Infinite-layer nickelate thin films: From synthesis to spectroscopy** — •Daniele Preziosi

Invited Talks not included in Focus Sessions

TT 8.1	Mon	15:00–15:30	HSZ 103	**Molecules on a superconductor: Inducing magnetism and resonance-enhanced vibrational spectroscopy** — •Richard Berndt
TT 17.3	Mon	17:15–17:45	HSZ 304	**Noise signatures of anyon statistics and Andreev scattering in the $\nu = 1/3$ fractional quantum Hall regime** — •Anne Anthore
TT 22.6	Tue	11:00–11:30	HSZ 204	**Higgs spectroscopy of superconductors in nonequilibrium** — •Dirk Manske
TT 28.6	Wed	10:45–11:15	HSZ 103	**Studying the Fulde-Ferrell-Larkin-Ovchinnikov order parameter in quasi-2D organic superconductors** — •Tommy Kotte
TT 39.1	Wed	15:00–15:30	HSZ 304	**Sensing and control of MHz photons with microwave photon-pressure** — •Daniel Bothner
TT 66.1	Fri	9:30–10:00	HSZ 304	**Towards ultrasensitive calorimetric detection in superconducting quantum circuits** — •Bayan Karimi

Sessions

TT 1.1–1.3	Sun	16:00–18:15	HSZ 01	**Tutorial: Physics Meets Machine Learning (joint session DY/TUT/TT)**
TT 2.1–2.9	Mon	9:30–13:00	HSZ 03	**Focus Session: Physics Meets ML I – Machine Learning for Complex Quantum Systems (joint session TT/DY)**
TT 3.1–3.13	Mon	9:30–13:00	HSZ 103	**Superconductivity: Properties and Electronic Structure**
TT 4.1–4.13	Mon	9:30–13:00	HSZ 201	**f-Electron Systems and Heavy Fermions I**
TT 5.1–5.14	Mon	9:30–13:15	HSZ 204	**Correlated Electrons: Method Development**
TT 6.1–6.13	Mon	9:30–13:00	HSZ 304	**Topological Semimetals**
TT 7.1–7.14	Mon	9:30–13:00	HSZ 403	**Spin Transport and Orbitronics, Spin-Hall Effects (joint session MA/TT)**
TT 8.1–8.8	Mon	15:00–17:15	HSZ 103	**Yu-Shiba-Rusinov Systems**
TT 9.1–9.8	Mon	15:00–17:00	HSZ 201	**f-Electron Systems and Heavy Fermions II**
TT 10.1–10.12	Mon	15:00–18:15	HSZ 204	**Correlated Electrons: Other Materials**
TT 11.1–11.6	Mon	15:00–16:30	HSZ 304	**Spintronics, Spincalorics and Magnetotransport**
TT 12.1–12.8	Mon	15:00–17:15	HSZ 403	**Topological Insulators (joint session MA/TT)**
TT 13.1–13.8	Mon	15:00–18:30	ZEU 250	**Focus Session: Physics Meets ML II – Understanding Machine Learning as Complex Interacting Systems (joint session DY/TT)**
TT 14.1–14.5	Mon	15:00–17:45	POT 361	**Focus Session: Graphene Quantum Dots (joint session HL/TT)**
TT 15.1–15.7	Mon	15:00–17:15	POT 251	**Quantum Transport and Quantum Hall Effects I (joint session HL/TT)**
TT 16.1–16.18	Mon	15:00–18:00	P2/OG4	**Poster: Transport**
TT 17.1–17.7	Mon	16:45–18:45	HSZ 304	**Topology: Quantum Hall Systems**
TT 18.1–18.5	Mon	17:15–18:30	HSZ 201	**Nano- and Optomechanics**

TT 19.1–19.9	Tue	9:30–13:15	HSZ 03	**Focus Session: New Perspectives for Adiabatic Demagnetization Refrigeration in the Kelvin and sub-Kelvin Range (joint session TT/MA)**
TT 20.1–20.13	Tue	9:30–13:00	HSZ 103	**Superconductivity: Tunnelling and Josephson Junctions**
TT 21.1–21.9	Tue	9:30–11:45	HSZ 201	**Correlated Electrons: Electronic Structure Calculations**
TT 22.1–22.13	Tue	9:30–13:15	HSZ 204	**Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)**
TT 23.1–23.13	Tue	9:30–13:00	HSZ 304	**Kagome Systems**
TT 24.1–24.9	Tue	9:30–12:15	POT 151	**Quantum Dots: Transport (joint session HL/TT)**
TT 25.1–25.4	Tue	12:00–13:00	HSZ 201	**Molecular Electronics and Photonics (joint session TT/CPP)**
TT 26	Tue	14:00–15:30	HSZ 304	**Members' Assembly**
TT 27.1–27.10	Wed	9:30–13:00	HSZ 03	**Focus Session: Unconventional Transport Phenomena in Low-Dimensional Superconducting Heterostructures**
TT 28.1–28.6	Wed	9:30–11:15	HSZ 103	**Unconventional Superconductors**
TT 29.1–29.14	Wed	9:30–13:15	HSZ 201	**Frustrated Magnets: General**
TT 30.1–30.13	Wed	9:30–13:00	HSZ 204	**Complex Oxides**
TT 31.1–31.12	Wed	9:30–12:45	HSZ 304	**Topology: Majorana Physics**
TT 32.1–32.11	Wed	9:30–12:30	GÖR 226	**Molecular Electronics and Excited State Properties (joint session CPP/TT)**
TT 33.1–33.12	Wed	9:30–13:00	MOL 213	**Many-Body Quantum Dynamics (joint session DY/TT)**
TT 34.1–34.6	Wed	11:30–13:00	HSZ 103	**Fe-based Superconductors**
TT 35.1–35.7	Wed	15:00–18:15	HSZ 03	**Focus Session: Correlations in Moiré Quantum Matter I**
TT 36.1–36.10	Wed	15:00–17:45	HSZ 103	**Topological Insulators**
TT 37.1–37.13	Wed	15:00–18:30	HSZ 201	**Ruthenates**
TT 38.1–38.13	Wed	15:00–18:30	HSZ 204	**Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)**
TT 39.1–39.11	Wed	15:00–18:15	HSZ 304	**Superconducting Electronics**
TT 40.1–40.8	Wed	15:00–18:30	POT 81	**Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)**
TT 41.1–41.6	Wed	15:00–17:00	POT 251	**Quantum Transport and Quantum Hall Effects II (joint session HL/TT)**
TT 42.1–42.22	Wed	15:00–18:00	P2/OG2	**Poster: Correlated Electrons I**
TT 43.1–43.33	Wed	15:00–18:00	P2/OG3	**Poster: Correlated Electrons II**
TT 44.1–44.8	Thu	9:30–13:00	HSZ 03	**Focus Session: Superconducting Nickelates I**
TT 45.1–45.10	Thu	9:30–12:15	HSZ 103	**Correlated Electrons: 1D Theory**
TT 46.1–46.13	Thu	9:30–13:00	HSZ 201	**Frustrated Magnets: Spin Liquids**
TT 47.1–47.13	Thu	9:30–13:00	HSZ 204	**Quantum-Critical Phenomena**
TT 48.1–48.7	Thu	9:30–11:15	HSZ 304	**Topological Superconductors**
TT 49.1–49.6	Thu	11:30–13:00	HSZ 304	**Quantum Coherence and Quantum Information Systems I**
TT 50.1–50.8	Thu	15:00–17:00	HSZ 03	**Focus Session: Superconducting Nickelates II**
TT 51.1–51.9	Thu	15:00–17:30	HSZ 103	**Correlated Electrons: Charge Order**
TT 52.1–52.9	Thu	15:00–17:30	HSZ 201	**Frustrated Magnets: Strong Spin-Orbit Coupling**
TT 53.1–53.10	Thu	15:00–17:45	HSZ 204	**Graphene**
TT 54.1–54.10	Thu	15:00–17:45	HSZ 304	**Quantum Coherence and Quantum Information Systems II**
TT 55.1–55.9	Thu	15:00–17:30	MOL 213	**Dynamics and Chaos in Many-Body Systems I (joint session DY/TT)**
TT 56.1–56.11	Thu	15:00–18:30	WIL A317	**Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management I (joint session O/TT)**
TT 57.1–57.28	Thu	15:00–18:00	P2/OG2	**Poster: Superconductivity I**
TT 58.1–58.31	Thu	15:00–18:00	P2/OG3	**Poster: Superconductivity II**
TT 59.1–59.18	Thu	15:00–18:00	P2/OG4	**Poster Session: Topology**
TT 60.1–60.7	Thu	17:15–19:00	HSZ 03	**Quantum Dots, Quantum Wires, Point Contacts**
TT 61.1–61.5	Thu	17:45–19:00	HSZ 201	**Focus Session: Correlations in Moiré Quantum Matter II**
TT 62.1–62.8	Fri	9:30–11:45	HSZ 03	**Ultrafast Dynamics of Light-Driven Systems**
TT 63.1–63.14	Fri	9:30–13:15	HSZ 103	**Superconductivity: Theory**
TT 64.1–64.8	Fri	9:30–11:30	HSZ 201	**Topology: Other Topics**
TT 65.1–65.10	Fri	9:30–12:15	HSZ 204	**Correlated Electrons: Other Theoretical Topics**
TT 66.1–66.7	Fri	9:30–11:30	HSZ 304	**Cryogenic Detectors**
TT 67.1–67.11	Fri	9:30–12:30	MOL 213	**Dynamics and Chaos in Many-Body Systems II (joint session DY/TT)**

TT 68.1–68.11	Fri	9:30–12:45	WIL A317	**Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management II (joint session O/TT)**

Annual Meeting of the Low Temperature Physics Division

Tuesday 14:00–15:30 HSZ 304
All members of the Low Temperature Physics Division are welcome to attend!

- Report
- Elections
- Miscellaneous

TT 1: Tutorial: Physics Meets Machine Learning (joint session DY/TUT/TT)

Machine learning has revolutionized many application fields such as computer vision and natural language processing. In physics there is a growing interest in using machine learning to enhance the analysis of experimental data and to devise and optimize experiments or numerical simulations. On the other hand physicists use their intuition and methods from statistical physics and complex systems theory to better understand the working principles of modern machine learning methods. This tutorial session introduces some subfields within this area and the basic methods involved.

Organized by Sabine Andergassen (Tübingen), Martin Gärttner (Heidelberg), Moritz Helias (Jülich), and Markus Schmitt (Cologne)

Time: Sunday 16:00–18:15 Location: HSZ 01

Tutorial TT 1.1 Sun 16:00 HSZ 01

Machine Learning for Quantum Technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Machine learning is revolutionizing science and technology. In the past few years, it has become clear that it promises significant benefits as well for the development of quantum technologies. In this tutorial I will first give a brief introduction to neural networks. I will then discuss a number of areas and examples in which machine learning is being successfully applied in this context. These include measurement data analysis and quantum state representation, approximate quantum dynamics, parameter estimation, discovering strategies for hardware-level quantum control, the optimization of quantum circuits, and the discovery of quantum experiments, discrete quantum feedback strategies, and quantum error correction protocols.

Reference: "Artificial intelligence and machine learning for quantum technologies", M. Krenn, J. Landgraf, T. Foesel, and F. Marquardt, Phys. Rev. A 107, 010101 (2023).

Tutorial TT 1.2 Sun 16:45 HSZ 01

The Unreasonable Effectiveness of Gaussians in the Theory of Deep Neural Networks — •Zohar Ringel — Racah Institute of Physics, Hebrew University in Jerusalem

Physical Sciences are in many ways the success story of explaining fundamental phenomena using simple math [1]. The fact that physical phenomena could be arranged in that manner is remarkable. Yet this simplicity does not necessarily carry over to life sciences or data sciences. Indeed prominent authors have argued against our desire to rely on neat mathematical structures when analyzing big data [2].

In the past half-decade several results have emerged which balance mathematical simplicity with data-induced complexity. These could be seen as a middle ground between the above juxtaposing views. The common divider here is the use of Gaussian distributions as approximants of various different quantities in deep neural networks (DNNs). Specifically these Gaussians emerge when describing outputs of DNNs with random weights, outputs of trained DNNs at random times, outputs of fixed DNNs over random input data, and fluctuations of hidden DNN pre-activations. In this tutorial I will present these quantities, provide arguments supporting their Gaussianity, and outline several theoretical implications.

[1] The Unreasonable Effectiveness of Mathematics in the Natural Sciences. Wigner (1960)

[2] The Unreasonable Effectiveness of Data. Halevy, Norvig, Pereira (2009)

Tutorial TT 1.3 Sun 17:30 HSZ 01

Computing learning curves for large machine learning models using the replica approach — •Manfred Opper — Inst. für Softwaretechnik und Theor. Informatik, TU Berlin — Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, UK

Methods of statistical physics have been used for a long time to mathematically analyse the typical performance of machine learning models in the limit where both the number of data and the number of parameters (such as network weights) is large. By defining Boltzmann-Gibbs probability distributions over parameters where the cost function of the machine learning problem plays the role of a hamiltoninan, one can derive analytical expressions for training errors and generalisation errors using the corresponding partition functions and free energies in terms of a usually small number of order parameters.

Since the models depend on a set of random data to be learnt, additional appropriate statistical (so-called quenched) averages of free energies over this 'disorder' have to be performed. The replica approach is a prominent analytical tool from the statistical physics of disordered systems to solve this nontrivial technical challenge.

In this tutorial I will give an introduction to this approach. Starting with an explicit calculation for simple single layer perceptrons, I will then argue how the method can be applied to more complex problems such as kernel machines (support vector machines and Gaussian processes) and multilayer networks.

TT 2: Focus Session: Physics Meets ML I – Machine Learning for Complex Quantum Systems (joint session TT/DY)

Modern machine learning methods open new perspectives on the high-dimensional data arising naturally in complex quantum systems. The applications range from the analysis of experimental observations over optimal control to the enhancement of numerical simulations in and out of equilibrium. This focus session brings together experts in the field to discuss recent progress and promising directions for future research.

Organizers: Markus Schmitt (University of Cologne), Martin Gärttner (University of Heidelberg)

Time: Monday 9:30–13:00 Location: HSZ 03

Invited Talk TT 2.1 Mon 9:30 HSZ 03
Enhanced variational Monte Carlo for Rydberg atom arrays — •Stefanie Czischek — Department of Physics, University of Ottawa, Ottawa, Canada, K1N 6N6

Rydberg atom arrays are promising candidates for high-quality quantum computation and quantum simulation. However, long state preparation times limit the amount of measurement data that can be generated at reasonable timescales. This restriction directly affects the estimation of operator expectation values, as well as the reconstruction and characterization of quantum states.

Over the last years, neural networks have been explored as a powerful and systematically tuneable ansatz to represent quantum wave functions. Via tomographical state reconstruction, such numerical models can significantly reduce the amount of necessary measurements to accurately reconstruct operator expectation values. At the same time, neural networks can find ground state wave functions of given Hamiltonians via variational energy minimization.

While both approaches experience individual limitations, a combination of the two leads to a significant enhancement in the variational ground state search by naturally finding an improved network initialization from a limited amount of measurement data. Additional specific modifications of the neural network model and its implementation can further optimize the performance of variational Monte Carlo simulations for Rydberg atom arrays and provide significant insights into their behaviour.

Invited Talk TT 2.2 Mon 10:00 HSZ 03
Data mining the output of quantum simulators – from critical behavior to algorithmic complexity — •Marcello Dalmonte — Abdus Salam International Centre for Theoretical Physics, Trieste (I)

Recent experiments with quantum simulators and noisy intermediate-scale quantum devices have demonstrated unparalleled capabilities of probing many-body wave functions, via directly probing them at the single quantum level via projective measurements. However, very little is known about to interpret and analyse such huge datasets. In this talk, I will show how it is possible to provide such characterisation of many-body quantum hardware via a direct and assumption-free data mining. The core idea of this programme is the fact that the output of quantum simualtors and computers can be construed as a very high-dimensional manifold. Such manifold can be characterised via basic topological concepts, in particular, by their intrinsic dimension. Exploiting state of the art tools in non-parametric learning, I will discuss theoretical results for both classical and quantum many-body spin systems that illustrate how data structures undergo structural transitions whenever the underlying physical system does, and display universal (critical) behavior in both classical and quantum mechanical cases. I will conclude with remarks on the applicability of our theoretical framework to synthetic quantum systems (quantum simulators and quantum computers), and emphasize its potential to provide a direct, scalable measure of Kolmogorov complexity of output states.

Invited Talk TT 2.3 Mon 10:30 HSZ 03
Reinforcement learning for quantum technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Complex quantum devices require sophisticated control. Discovering such control strategies from scratch with the help of machine learning will enable us to keep pace with the ever-increasing demands encountered when scaling up quantum computers. In this talk, I will describe how the field of reinforcement learning can deliver on this promise. I will present examples ranging from the optimization of quantum circuits to the model-based discovery of better quantum feedback strategies. Moreover, in a recent collaboration with our experimental colleagues, we could show how to train a novel latency-optimized neural network by reinforcement learning in an experiment, acting on a superconducting qubit in cycles of less than one microsecond.

Invited Talk TT 2.4 Mon 11:00 HSZ 03
Machine learning of phase transition — •Christof Weitenberg — Universität Hamburg, Institut für Laserphysik, Hamburg, Germany

Machine learning is emerging as vital tool in many sciences. In quantum physics, notable examples are neural networks for the efficient representation of quantum many-body states and reinforcement learning of preparation and read-out routines. In this talk, I will present our results on machine learning of quantum phase transitions using classification techniques. This approach works very well even on noisy experimental data both with supervised and unsupervised machine learning, as we demonstrate for quantum simulators based on ultracold atoms. Next to the practical advantages, such techniques might in the future reveal phase transitions, for which conventional order parameters are not known.

15 min. break

TT 2.5 Mon 11:45 HSZ 03
Machine learning optimization of Majorana hybrid nanowires — •Matthias Thamm and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig

As the complexity of quantum systems such as quantum bit arrays increases, efforts to automate expensive tuning are increasingly worthwhile. We investigate machine learning based tuning of gate arrays using the CMA-ES algorithm for the case study of Majorana wires with strong disorder. We find that the algorithm is able to efficiently improve the topological signatures, learn intrinsic disorder profiles, and completely eliminate disorder effects. For example, with only 20 gates, it is possible to fully recover Majorana zero modes destroyed by disorder by optimizing gate voltages.

TT 2.6 Mon 12:00 HSZ 03
Model-independent learning of quantum phases of matter with quantum convolutional neural networks — •Yu-Jie Liu[1], Adam Smith[2], Michael Knap[1], and Frank Pollmann[1] — [1]Technical University of Munich, 85748 Garching, Germany — [2]University of Nottingham, Nottingham, NG7 2RD, UK

Quantum convolutional neural networks (QCNNs) have been introduced as classifiers for gapped quantum phases of matter. Here, we propose a model-independent protocol for training QCNNs to discover order parameters that are unchanged under phase-preserving perturbations. We initiate the training sequence with the fixed-point wavefunctions of the quantum phase and then add translation-invariant noise that respects the symmetries of the system to mask the fixed-point structure on short length scales. Without the translational invariance or other additional symmetries, we prove that a phase-classifying QCNN cannot exist. We illustrate this approach by training the QCNN on phases protected by time-reversal symmetry in one dimension, and test it on several time-reversal symmetric models exhibiting trivial, symmetry-breaking, and symmetry-protected topological order. The QCNN discovers a set of order parameters that identifies all three phases and accurately predicts the location of the phase boundary. The proposed protocol paves the way towards hardware-efficient training of quantum phase classifiers on a programmable quantum processor.

TT 2.7 Mon 12:15 HSZ 03

Simulating spectral functions of two-dimensional systems with neural quantum states — •Tiago Mendes Santos[1], Markus Schmitt[2], and Markus Heyl[1] — [1]University of Augsburg, Augsburg, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Spectral functions are key tools to characterize and probe condensed matter systems. Simulating such quantities in interacting two-dimensional quantum matter is, however, still an outstanding challenge. This work presents a numerical approach to simulate spectral functions using Neural Quantum States. As the key aspect, our scheme leverage the flexibility of artificial-neural-network wave functions to access spectral properties by simulating the dynamics of localized excitations with the time-dependent variational Monte Carlo. For demonstration, we study the dynamical structure factor (DSF) of models describing two-dimensional quantum phase transitions, namely, the quantum Ising and a square-lattice Rydberg Atom Arrays model in a regime of parameters relevant to quantum simulators. When combined with deep network architectures whose number of variational parameters increase at a mild polynomial expense with the number of spins, we showcase that our approach reliably describes the DSF for unprecedented system sizes and time scales.

TT 2.8 Mon 12:30 HSZ 03

Efficient optimization of deep neural quantum states toward machine precision — •Ao Chen and Markus Heyl — Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Neural quantum states (NQSs) have emerged as a novel promising numerical method to solve the quantum many-body problem. However, it has remained a central challenge to train modern large-scale deep network architectures, which would be key to utilize the full power of NQSs and to make them competitive or superior to conventional numerical approaches. Here, we propose a minimum-step stochastic reconfiguration (MinSR) method that reduces the optimization complexity by orders of magnitude while keeping similar accuracy as compared to conventional stochastic reconfiguration. In this talk, I will show MinSR allows for an accurate training on unprecedentedly deep NQS with up to 64 layers and more than 10^5 parameters in the spin-1/2 Heisenberg J_1-J_2 models on the square lattice. With limited numerical resources, partly obtained on single workstations, we find that this approach yields better variational energies as compared to existing NQS results and we further observe that the accuracy of our ground state calculations approaches different levels of machine precision on modern GPU and TPU hardware.

TT 2.9 Mon 12:45 HSZ 03

Time-dependent variational principle for quantum and classical dynamics — •Moritz Reh[1], Markus Schmitt[2], and Martin Gärttner[1,3,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [3]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [4]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany

The solution of many-body quantum dynamics is a challenging feat due to the curse of dimensionality, hindering the exploration of dynamics beyond a mediocre number of qubits. Neural Networks can variationally approximate the state of interest and therefore present a promising tool as they allow to efficiently represent the quantum state at the expense of truncating the Hilbert space.

We present such a scheme that is aimed at solving dissipative quantum dynamics using a probabilistic framework, i.e. the so-called POVM-formalism and demonstrate it for spin chains of up to 40 spins. We then show that the generality of the approach allows us to translate this formalism directly to the case of partial differential equations in high dimensions, defeating the exponential growth of grid cells when adding dimensions.

TT 3: Superconductivity: Properties and Electronic Structure

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

TT 3.1 Mon 9:30 HSZ 103

Band-selective quasiparticle scatterers in a two-band superconductor — •Thomas Gozlinski[1], Qili Li[1], Nola Warwick[1], Janic Beck[1], and Wulf Wulfhekel[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie (KIT) — [2]Institute for Quantum Materials and Technologies (IQMT), Karlsruher Institut für Technologie (KIT)

We study stacking fault tetrahedra (SFTs) in a bulk Pb crystal by mK scanning tunnelling microscopy and spectroscopy and find that the Bogoliubons of the two superconducting bands produce different quasiparticle interference patterns owed to the respective Fermi surface anisotropy. We believe that such extended crystal defects provide a platform to experimentally study interband couplings and scattering rates in a multiband superconductor.

TT 3.2 Mon 9:45 HSZ 103

Symmetry breaking and emergent phases in a noncentrosymmetric superconductor — •Feifan Wang[1], Xianghan Xu[2], Sang-Wook Cheong[2], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Dept. of Physics and Astronomy, Rutgers University, USA

Symmetry breaking raises rich physics in condensed matters, such as Rashba splitting, Weyl fermions, unconventional superconducting, multiferroic ordering, etc. Nonlinear optical processes, being extremely sensitive to material symmetries, offer a direct access to the observation of subtly broken or even hidden symmetries. Here we discover emergant phases in a noncentrosymmetric superconductor, Mo_3Al_2C, and resolve the symmetry lowering using second harmonic generation measurements. Together with temperature-dependent electronic conductivity measurements, the phase transition from a normal metal at high temperatures to a charge-density-wave state is proposed. In the former, all mirror symmetries are broken bringing in the structural chirality. The correlation between superconductivity/charge-density-wave transition and noncentrosymmetry/chirality will then be discussed. Exotic properties in a low-symmetry system such as Mo_3Al_2C may add new ingredients to the strong-correlation physics.

TT 3.3 Mon 10:00 HSZ 103

Hunt for FFLO superconductivity in transition metal dichalcogenides — •Jiawei Zhang[1], Dennis Huang[1], Yosuke Matsumoto[1], Masahiko Isobe[1], Thomas Palstra[1,2], and Hidenori Takagi[1,3,4] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70569 Stuttgart, Germany — [4]Department of Physics, University of Tokyo, 113-0033 Tokyo, Japan

The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state was proposed almost half a century ago. In contrast to the Bardeen-Cooper-Schrieffer state, the FFLO state hosts Cooper pairs with finite center-of-mass momentum, giving rise to a modulation of the superconducting gap in real space. Two-dimensionality plays an essential role in the materialization of the FFLO state. With 1T buffer layers that reduce the interlayer coupling between successive 1H superconducting layers, $4H_b$-TaS_2 is a promising FFLO candidate. I will talk about the two-dimensional nature of superconductivity in this system as revealed by the Berezinskii-Kosterlitz-Thouless transition. Electrical transport measurements with in-plane magnetic field show that the superconductivity survives above the Pauli limit, providing a high-field regime in the phase diagram to host a possible FFLO state.

TT 3.4 Mon 10:15 HSZ 103

Tuning metal/superconductor to insulator/superconductor coupling via control of proximity enhancement between $NbSe_2$ monolayers — •O. Chiatti[1], K. Mihov[1], T. Griffin[1], C. Grosse[1], L. Grote[1], K. Hite[2], D. Hamann[2], M. B. Alemayehu[2], A. Mogilatenko[3], D. C. Johnson[2], and S. F. Fischer[1] — [1]Novel

Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Solid State Chemistry, University of Oregon, Eugene OR 97403-1253, U.S.A. — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, 12489 Berlin, Germany

The interplay between charge transfer and electronic disorder in transition-metal dichalcogenide multilayers [1] gives rise to superconductive coupling driven by proximity enhancement, tunneling and superconducting fluctuations. Artificial spacer layers introduced with atomic precision change the density of states by charge transfer. Here, we tune the superconductive coupling between $NbSe_2$ monolayers from proximity-enhanced to tunneling-dominated and correlate normal and superconducting properties in $[(SnSe)_{1+\delta})]_m[NbSe_2]_1$ tailored multilayers with varying SnSe layer thickness (m=1-15). We show crossovers between three regimes: metallic with proximity-enhanced coupling, disordered-metallic with intermediate coupling and insulating with Josephson tunneling. [1] A. Devarakonda *et al.*, Science **370**, 231 (2020) [2] M. Trahms *et al.*, Supercond. Sci. Technol. **31**, 065006 (2018)

TT 3.5 Mon 10:30 HSZ 103

Higgs-CDW hybrid mode in coherently-driven 2H-$NbSe_2$ and $La_{2-x}Sr_xCuO_4$ — •Liwen Feng[1,2,3,4], Jiayuan Cao[2], Tim Priessnitz[1], Gennady Logvenov[1], Bernhard Keimer[1], Yuan Huang[7], Jan-Christoph Deinert[5], Sergey Kovalev[5], Tao Dong[6], Stefan Kaiser[1,3,4], and Hao Chu[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Shanghai Jiaotong University, Shanghai, China — [3]University of Stuttgart, Stuttgart, Germany — [4]Technical University Dresden, Dresden, Germany — [5]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [6]Peking University, Beijing, China — [7]Beijing Institute of Technology, Beijing, China

Superconductivity and a charge-density-wave (CDW) are often found as close neighbors in the thermodynamic phase diagram of many materials at low temperatures. A prototypical system showing the coexistence of the two orders is 2H-$NbSe_2$. Here, we coherently drive collective oscillations by terahertz radiation and report on third harmonic generation (THG) from both CDW amplitude oscillations and Higgs oscillations. We find the interaction between two orders leads to a Fano interference of THG signals, which displays as an out-of-phase interference in the time-domain. This we characterize as Higgs-CDW hybrid that can be controlled by the THz driving field. Additionally, a similar phenomenon manifestes in the underdoped cuprate $La_{2-x}Sr_xCuO_4$ ($x \sim 0.12$) under non-perturbative drive. As such non-linear THz drives of order parameter oscillations opening up possibilities of investigating intertwined orders in the future.

TT 3.6 Mon 10:45 HSZ 103

Clean-limit superconductivity at 197 K in high-pressure sulfur hydride — •Sam Cross[1], Israel Osmond[1], Owen Moulding[1], Takaki Muramatsu[1], Annabelle Brooks[1], Oliver Lord[2], Timofey Fedotenko[3], Jonathan Buhot[1], and Sven Friedemann[1] — [1]HH Wills Physics Laboratory, University of Bristol, UK — [2]School of Earth Sciences, University of Bristol, UK — [3]Photon Science, DESY, Germany

The search for room temperature superconductivity in hydrogen rich compounds has accelerated since the discovery of superconductivity in sulfur hydride, H_3S, in 2015 [1]. Controlled synthesis of hydrides remains a challenge, and further work on the formation pathways will prove vital in the search for room temperature superconductivity in such compounds. Here we confirm the synthesis of cubic $Im\bar{3}m$ H_3S by laser heating elemental sulfur and hydrogen donor ammonia borane, NH_3BH_3. Superconductivity is characterised using electrical transport measurements in a diamond anvil cell, confirming a transition temperature T_c = 197 K at 153 GPa, in agreement with previous studies. The coherence length extracted from measurements of the critical field H_{c2} together with estimations of the carrier mean free path from the normal state resistance suggest that H_3S follows clean-limit behaviour. The work further highlights the potential for in-situ synthesis of clean hydrides using ammonia borane, a more accessible synthesis alternative to pure hydrogen.

[1] A.P. Drozdov et al., Nature 525, 73 (2015)

TT 3.7 Mon 11:00 HSZ 103

Unraveling charge transfer to understand superconductivity in MgB_2 — •Simon Marotzke[1,2], Jan Oliver Schunck[1,3], Amina Alic[4], Octave Duros[4], Moritz Hoesch[1], Alessandro Nicolaou[5], Gheorghe Sorin Chiuzbaian[4], and Martin Beye[1] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [3]Universität Hamburg, Hamburg, Germany — [4]Sorbonne Université, Paris, France — [5]Synchrotron SOLEIL, Saint-Aubin, France

Magnesium diboride (MgB_2) holds the world-record for the highest transition temperature (T_C = 39 K) in a conventional Bardeen-Cooper-Schrieffer (BCS)-type, i.e., phonon-mediated, superconductor. The undoped electron configuration of MgB_2 is still disputed as contradicting results on the appearance of charge transfer upon crossing T_C have been reported. To settle this question, we conducted high-resolution resonant X-ray emission spectroscopy (XES) as well as X-ray absorption spectroscopy (XAS) measurements around the boron K-edge at the SEXTANTS beamline at the synchrotron SOLEIL. In order to investigate the charge transfer between in-plane and out-of-plane states, we varied the polarization of the incoming photons as well as the incidence and emission angle. We report on differences in the spectral intensity for both the absorption and emission spectra upon crossing T_C to be first indications of changes in the density of the boron $2p$ states. Complementary density of states calculations showing good agreement with the experimental data were performed.

15 min. break

TT 3.8 Mon 11:30 HSZ 103

Emergence of incipient superconductivity in CrB_2 under anisotropic strain — Alexander Regnat[1], •André Deyerling[1], Christoph Resch[1], Jan Spallek[1], Alfonso Chacon[1], Philipp G. Niklowitz[1,2], Andreas Bauer[1], Marc A. Wilde[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technical University of Munich, D-85748 Garching, Germany — [2]Department of Physics, Royal Holloway, University of London, Egham TW20 0EX, UK

Resistivity studies of the hexagonal C32 diborides MoB_2[1], WB_2[2], and CrB_2[3,4] under ultra-high pressures of the order 100 GPa have recently revealed superconducting transitions, where the precise pressure conditions are unknown. We report a study of the electrical resistivity of the itinerant-electron antiferromagnet CrB_2 [5,6] under uniaxial, hydrostatic, and quasi-hydrostatic pressures up to 0.5 GPa, 2.2 GPa and 8 GPa, respectively. Tracking the magnetic transition temperature and the onset of incipient superconductivity we derive a phase diagram as a function of the ratio of lattice constants c/a. Supported by detailed electronic structure calculations, we suggest that the reduction of lattice constant c controls the suppression of magnetic order and concomitant emergence of superconductivity in CrB_2.

[1] C. Pei et al., arXiv:2105.13250 (2021)
[2] J. Lim et al., arXiv:2109.11521 (2021)
[3] C. Pei et al., arXiv:2109.15213 (2021)
[4] S. Biswas et al. arXiv:2211.01054 (2022)
[5] M. Brasse et al., PRB **88**, 155138 (2013)
[6] A. Bauer et al., PRB **90**, 064414 (2014)

TT 3.9 Mon 11:45 HSZ 103

Annaleing microstructured crystals of cuprate superconductor $Tl_2Ba_2CuO_{6-x}$ — •Ayanesh Maiti[1,2,3], Seunghyun Khim[1], Carsten Putzke[2], and Andrew P Mackenzie[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Max Planck Institute for Structure and Dynamics of Matter, Hamburg — [3]University of St Andrews, Scotland

Cuprates exhibit a variety of interesting physics that is not well understood, ranging from unconventional superconductivity to strange metal behaviour. Past experiments have mostly focused on underdoped cuprates that have complex phases due to competing orders. Studies with overdoped samples were limited by the rarity of candidate materials and the difficulty to probe crystals with surface reconstructions. $Tl_2Ba_2CuO_{6-x}$ is a naturally overdoped cuprate that can be grown with high enough purity to show quantum oscillations, and we can suppress the effects of surface reconstructions by using focused ion beam (FIB) microstructuring techniques. However, FIB procedures remove oxygen from the crystal surface and introduces inhomogeneities in samples, making it hard to study their intrinsic behavior. We are developing annealing techniques to re-homogenize our microstructures, using measurements of the doping-dependent high-temperature resistivity to monitor their oxygen content. This will allow us to study the overdoped part of the cuprate phase diagram and hence improve our understanding of unconventional superconductivity. Our techniques will also enable studies with the full range of doping on a single specimen, eliminating sample-to-sample variations from future experiments.

TT 3.10 Mon 12:00 HSZ 103

Vortex matching at 6 T in $YBa_2Cu_3O_{7-\delta}$ by imprinting an ultradense hexagonal pinning array with focused helium ion irradiation — •Bernd Aichner[1], Lucas Backmeister[1], Max Karrer[2], Katja Wurster[2], Christoph Schmid[2], Reinhold Kleiner[2], Edward Goldobin[2], Dieter Koelle[2], and Wolfgang Lang[1] — [1]Fakultät für Physik, Universität Wien, Wien, Österreich — [2]Physikalisches Institut, Center for Quantum Science (CQ) and LISA+, Universität Tübingen, Tübingen, Deutschland

The focused beam of a helium ion microscope (HIM) is used to locally suppress superconductivity in thin films of the prototypical copper-oxide superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO). In these pillar-shaped regions, the critical temperature T_c is reduced or entirely suppressed due to pair-breaking by point defects.

The narrow spacing of these nanopillars leads to vortex commensurability effects at high magnetic fields, which appear as pronounced maxima of the critical current and corresponding resistance minima. In accordance with the calculation, these effects appear at an unprecedented high magnetic field of 6 T in a hexagonal nanopillar lattice with 20 nm spacing. In contrast to previous observations, matching phenomena persist in the whole accessible temperature range, from the onset of superconductivity down to a temperature of 2 K. At the matching field, we observe a novel behavior in voltage-current isotherms, which we attribute to an ordered Bose glass phase. These results establish the HIM as a versatile platform for creating ultradense vortex pinning landscapes with complex designs in copper-oxide superconductors.

TT 3.11 Mon 12:15 HSZ 103

Quantum interference in a finite-width mesoscopic ring with superconducting vortices — Gian Paolo Papari[1,2,3] and •Vladimir M. Fomin[4,5] — [1]Dipartimento di Fisica, Università di Napoli "Federico II", I-80126 Napoli, Italy — [2]CNR-SPIN, UOS Napoli, I-80126 Napoli, Italy — [3]Istituto Nazionale di Fisica Nucleare (INFN), Naples Unit, I-80126 Napoli, Italy — [4]Institute for Integrative Nanosciences (IIN), Leibniz IFW Dresden, D-01069 Dresden, Germany — [5]Moldova State University, MD-2009, Chişinău, Republic of Moldova

We analyze the origin of the parabolic background of magnetoresistance oscillations measured in finite-width superconducting mesoscopic rings with input and output stubs and in patterned films. The transmission model [1] explaining the sinusoidal oscillation of magnetoresistance is extended to address the background as a function of the magnetic field. Apart from the interference mechanism activated by the ring, pinned superconducting vortices as topological defects introduce a further interference-based distribution of supercurrents that affects, in turn, the voltmeter-sensed quasiparticles. The onset of vortices changes the topology of the superconducting state in a mesoscopic ring in a such a way that the full magnetoresistance dynamics can be interpreted owing to the interference of the constituents of the order parameter induced by both the ring itself and the vortex lattice in it.

[1] G. P. Papari and V. M. Fomin, Phys. Rev. B 105, 144511 (2022)

TT 3.12 Mon 12:30 HSZ 103

Frequency-locking effect in Nb open nanotubes — Igor Bogush[1,2], Oleksandr V. Dobrovolskiy[3], and •Vladimir M. Fomin[1,2] — [1]Institute for Integrative Nanosciences (IIN), Leibniz IFW Dresden, D-01069 Dresden, Germany — [2]Department of Theoretical Physics, Moldova State University, MD-2009 Chişinău, Republic of Moldova — [3]University of Vienna, Faculty of Physics, Nanomagnetism and Magnonics, Superconductivity and Spintronics Laboratory, 1090 Vienna, Austria

We study alternating voltage generation in Nb open nanotubes under weakly modulated transport current and magnetic field by numerically solving the time-dependent Ginzburg-Landau equation [1]. Under stationary currents and fields, as a rule, an alternating voltage with a fixed frequency is generated in the nanotube. The frequency is associated with the period of the vortex nucleation at the nanotube edges. If the transport current is modulated by a weak ac component with a frequency close to the nucleation frequency, we reveal the effect of frequency-locking of the vortex nucleation, i.e., the nucleation frequency becomes equal to the external frequency of the modulated transport current. The frequency-locking width is discussed as a function of the modulation depth. Its sensitivity to the magnetic field variation opens up opportunities for the experimental examination of the effect.

[1] I. Bogush and V. M. Fomin, Phys. Rev. B 105, 094511 (2022)

TT 3.13 Mon 12:45 HSZ 103

Superconductivity in curved 3D nanoarchitectures — •Vladimir M. Fomin[1,2] and Oleksandr V. Dobrovolskiy[3] — [1]Institute for Integrative Nanosciences (IIN), Leibniz IFW Dresden, D-01069 Dresden, Germany — [2]Laboratory of Physics and Engineering of Nanomaterials, Department of Theoretical Physics, Moldova State University, MD-2009 Chişinău, Republic of Moldova — [3]University of Vienna, Faculty of Physics, Nanomagnetism and Magnonics, Superconductivity and Spintronics Laboratory, 1090 Vienna, Austria

In recent years, superconductivity and vortex matter in curved 3D nanoarchitectures have turned into a vibrant research avenue because of the rich physics of the emerging geometry- and topology-induced phenomena and their prospects for applications in (electro)magnetic field sensing and information technology. We outline the experimental techniques capable of the fabrication of curved 3D nanostructures and present a selection of own results on the intertwined dynamics of screening superconducting currents, Abrikosov vortices and slips of the phase of the superconducting order parameter therein. We share our vision regarding the prospect directions and current challenges in this research domain, arguing that curved 3D nanoarchitectures open a new dimension in superconductors research and possess great potential for magnetic field sensing, bolometry, and fluxonic devices [1].

[1] V. M. Fomin, O. V. Dobrovolskiy, Appl. Phys. Lett. 120, 090501 (2022)

TT 4: f-Electron Systems and Heavy Fermions I

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

TT 4.1 Mon 9:30 HSZ 201

The potential of resonant x-ray scattering for the study of Kondo lattices — •Marein Rahn — Institute for Solid State and Materials Physics, Technical University of Dresden, 01062 Dresden, Germany

Kondo lattices represent a pivotal point of quantum matter - where local-itinerant correlations start being shaped by a material's lattice character and their consequences can no longer be reduced to local/mean-field models. Many traditional experimental probes cannot provide insights "beyond the mean field" because they themselves average this phenomenon over time and space. In this talk, I will showcase recent advances in momentum-resolved spectroscopies that can reveal the fine structure and dynamics of Kondo quasiparticles in unprecedented detail. Synchrotron-based techniques like resonant inelastic x-ray scattering provide a particularly interesting new perspective. Their experimental possibilities in f-electron systems have been hardly exploited, which should also be a strong motivation for progress in computational approaches.

TT 4.2 Mon 9:45 HSZ 201

Kondo screening and coherence on the Kagome lattice: Energy scales of the Kondo effect in the presence of at bands — •Christos Kourris and Matthias Vojta — Institut für Theoretische Physik, TU Dresden, Dresden, Germany

The formation of a heavy Fermi liquid in metals with local moments is characterized by multiple energy and temperature scales, most prominently the Kondo temperature and the coherence temperature, characterizing the onset of Kondo screening and the emergence of Fermi-liquid coherence, respectively. In the standard setting of a wide conduction band, both scales depend exponentially on the Kondo coupling. Here we discuss how the presence of flat, i.e., dispersionless, conduction bands modifies this situation. The Kagome Kondo-lattice model, due to its rich band structure, leads to a plethora of non-conventional Kondo behaviour emerging at different fillings. We utilize a parton mean-field approach to determine both the Kondo temperature and the coherence temperature as function of the conduction-band filling n_c, both numerically and analytically. For n_c values corresponding to the flat conduction band, we show that the exponential is replaced by linear and quadratic dependences for the Kondo and coherence temperature respectively, while a cubic power law emerges in the coherence temperature at n_c corresponding to the band edge between the flat and dispersive bands. We discuss implications of our results for pertinent experimental data.

TT 4.3 Mon 10:00 HSZ 201

Uniaxial strain tuning the signature of Kondo effect in the electrical resistance of heavy-fermion metals — •Soumendra Panja, Anton Jesche, Bin Shen, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

Physical properties of Kondo lattices are determined by the interplay of the Kondo effect and the RKKY interaction, which both depend sensitively on the antiferromagnetic exchange J between f- and conduction electrons. This competition is extremely sensitive to pressure, as evidenced by very large Gruneisen parameters found in these materials. We intend to tune the Kondo-maximum signature in the electrical resistance of such materials with tensile and compressive strain by utilizing a commercial piezo-strain device. In this talk, first results will be discussed under experimentally accessible strains.

TT 4.4 Mon 10:15 HSZ 201

Kondo breakdown transitions and phase-separation tendencies in valence-fluctuating heavy-fermion materials — •Pedro Monteiro Cônsoli and Matthias Vojta — Institut für Theoretische Physik, TU Dresden

The breakdown of the lattice Kondo effect in local-moment metals can lead to nontrivial forms of quantum criticality and a variety of non-Fermi-liquid phases. Given indications that Kondo-breakdown transitions involve criticality not only in the spin but also in the charge sector, we investigate the interplay of Kondo breakdown and strong valence fluctuations in generalized Anderson lattice models. We employ a parton mean-field theory to describe the transitions between deconfined fractionalized Fermi liquids and various confined phases. As a result, we find that rapid valence changes near Kondo breakdown can render the quantum transition first order. This leads to phase-separation tendencies which, upon inclusion of longer-range Coulomb interactions, will produce intrinsically inhomogeneous states near Kondo-breakdown transitions. We connect our findings to unsolved aspects of experimental data.

TT 4.5 Mon 10:30 HSZ 201

Quantum spin liquid in an RKKY-coupled two-impurity Kondo system — •Krzysztof P. Wójcik[1,2,3] and Johann Kroha[3] — [1]M. Curie-Skłodowska University, 20-031 Lublin, Poland — [2]Institute of Molecular Physics, PAS, 60-179 Poznań, Poland — [3]Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany

We consider a 2-impurity Anderson model with spin-exchange coupling within the conduction-band sector of the Hamiltonian. Our numerical renormalization group calculations show that for strong intraband spin correlations their competition with the Kondo spin screening stabilizes a metallic spin-liquid phase of the localized spins, even without geometric frustration. It is characterized by nonuniversal impurity spectral density, fractionalization of the phase shift between the local and conduction-band parts, and large but not complete spin-spin correlations. For weak Kondo coupling the spin liquid and the Kondo singlet phase are separated by two quantum phase transitions and an intermediate RKKY spin-dimer phase, while beyond a critical coupling they are connected by a crossover. The results suggest how a quantum spin liquid may be realized in heavy-fermion systems near a spin-density wave instability.

TT 4.6 Mon 10:45 HSZ 201

Epitaxial $EuPd_2$ and $EuPd_3$ thin films — •Sebastian Kölsch and Michael Huth — Goethe Universität, Frankfurt (Main)

Europium-based binary compounds reveal a variety of interesting phenomena, which are attributed to strong electronic correlations and a competition between two different valence states of the europium ion, which lie close in energy [1]. As a result Eu forms intermetallic compounds usually either in a divalent (e.g. $EuPd_2$) or trivalent (e.g. $EuPd_3$) state, depending on the surrounding environment, whereas most other rare earth elements are always trivalent. Some ternary compounds even exhibit a change between both valence states, which may be tuned by temperature, pressure or high magnetic fields. As one of these rare candidates, $EuPd_2Si_2$ gained much interest due to a temperature driven valence transition from nearly Eu^{2+} above 200 K to Eu^{3+} below 50 K [2]. Recently we achieved for the first time the growth of epitaxial $EuPd_2Si_2$ thin films, where the valence transition was completly suppressed due to biaxial strain [3]. Epitaxial thin films thus offer the possibility to manipulate the strongly correlated Eu-based systems. Here we present the successful growth of $EuPd_2$ and $EuPd_3$ as epitaxial thin films and report on first results regardings their properties.

[1] Y. Onuki et al., Phil. Mag. 97, 36 (2017)
[2] K. Kliemt et al., Crys. Grow. & Des., 2022
[3] S. Kölsch et al., PRM 6, 2022

TT 4.7 Mon 11:00 HSZ 201

Single crystal growth of $EuPd_2Si_2$ under enhanced gas pressure — •Alexej Kraiker, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany

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 $EuPd_2Si_2$ crystallizing in the $ThCr_2Si_2$ structure type. Because of the the high vapor pressure of Eu, high-quality single crystals of EuT_2X_2-compounds are very challenging to grow in larger size. One way to prevent Eu from evaporating out of the melt, is growing the crystals in argon overpressure. In this contribution, we present the crystal growth of $EuPd_2Si_2$ single crystals with a 20 bar and a 150 bar Czochralski-furnace. We show that the argon overpressure slows down the evaporation process of the Eu and leads to crystals with higher quality compared to Bridgman grown samples [1].

[1] K. Kliemt at al. Cryst. Growth Des. 2022, 9, 5399

15 min. break

TT 4.8 Mon 11:30 HSZ 201

Tuning the ground state of $EuPd_2(Si_{1-x}Ge_x)_2$ using He-gas pressure — •Bernd Wolf, Theresa Lundbeck, Marius Peters, Kristin Kliemt, Cornelius Krellner, and Michael Lang — Physikalisches Institut, Goethe University, 60438 Frankfurt/Main, Germany

The strongly correlated intermetallic compound $EuPd_2Si_2$ shows a strong valence-change crossover in a small temperature range. This valence change is accompanied by pronounced lattice effects together with significant changes in the magnetic properties. The material is located on the high-pressure side (crossover range) of the second-order critical endpoint (CEP) where novel collective phenomena which originate from a particularly strong coupling between electronic-, magnetic- and lattice degrees of freedom can be expected. We present magnetic susceptibility measurements data taken on high-quality single crystals of $EuPd_2(Si_{1-x}Ge_x)_2$ for nominal Ge-concentrations $0 \leq x_{nom} \leq 0.2$ in the temperature range 2 K $\leq$ T $\leq$ 300 K and He-gas pressure up to 0.5 GPa. For x = 0 at ambient pressure we observe a pronounced valence crossover centered around $T_V \sim 160$ K. As expected, T_V shifts to lower temperatures with increasing Ge-concentration, reaching $T_V \sim 90$ K for $x_{nom} = 0.1$, while still showing a non-magnetic ground state. For $x_{nom} = 0.2$ we observe long-range antiferromagnetic order setting in below $T_N = 47.3$ K. The important finding is that the application of a weak pressure as low as 0.2 GPa the long-range magnetic order can be suppressed giving way to a non-magnetic ground state with pronounced valence fluctuations.

TT 4.9 Mon 11:45 HSZ 201

Search for a critical endpoint in $Eu(Pd_{1\text{-}x}Au_x)_2Si_2$ single crystals — •Robert Möller, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, Germany

In a general phase diagram for Eu compounds [1], the intermediate valent $EuPd_2Si_2$, T_V ~ 150 K, is located very close, but slightly at the high-pressure side of a second order critical endpoint [2]. The analysis of polycrystalline samples of $Eu(Pd_{1\text{-}x}Au_x)_2Si_2$ revealed that in this series a critical endpoint can be found which separates the region of continuous from first order transitions. It was shown that the valence state of the material can be tuned via Au substitution and that for x between 0.04 and 0.2 the transition becomes a first order phase transition [3]. Using single crystals grown with the Czochralski method, several characterisations were done to understand the main factors affecting the valence transition of $Eu(Pd_{1\text{-}x}Au_x)_2Si_2$.

[1] Y. Onuki et al., Phil. Mag. 97, 3399 (2017)
[2] B. Batlogg et al., in: Wachter, Boppart (eds.): Valence Instabilities, North-Holland publishing company (1982)
[3] C. U. Segre et al., Phys. Rev. Lett. 49, 1947 (1982)

TT 4.10 Mon 12:00 HSZ 201

Orbital selective coupling in $CeRh_3B_2$: co-existence of high Curie and high Kondo temperature — Andrea Amorese[1,2], Philipp Hansmann[3], Andrea Marino[2], Peter Körner[1], Thomas Willers[1], Andrew Walters[4], Kejin Zhou[4], Kurt Kummer[5], Nickolas B. Brooks[5], Hong-Ji Lin[6], Chien-Te Chen[6], Pascal Lejay[7], Maurits W. Haverkort[8], Liu Hao Tjeng[2], and •Andrea Severing[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]MPI-CPfS, Dresden, Germany — [3]Department of Physics, University of Erlangen-Nürnberg, Germany — [4]Diamond Light Source, Didcot, UK — [5]ESRF, Grenoble, France — [6]NSRRC, Hsinchu, Taiwan — [7]Institut Neel, CNRS, Grenoble, France — [8]Institute for Theoretical Physics, Heidelberg University, Germany

$CeRh_3B_2$ combines seemingly exclusive properties of strong intermediate valence and high temperature ferromagnetism below 116K with strongly reduced magnetic moments. Utilizing recent advances in synchrotron techniques (XAS & RIXS) in combination with ab-initio density functional calculations, we find that the Rh states are irrelevant for the high temperature ferromagnetism and the Kondo effect, and that the crystal-field strength is not sufficiently strong to account for the Ce moment reduction. Instead our investigation reveals that different Ce $4f$ orbitals contribute differently to the magnetic coupling and the Kondo-type hybridization in $CeRh_3B_2$. The manifestation of such selective orbital coupling is a new aspect in the world of the strongly correlated 4f intermetallics.

TT 4.11 Mon 12:15 HSZ 201

Superconductivity beyond the Pauli limit in high-pressure $CeSb_2$ — •Oliver Squire, Stephen Hodgson, Jiasheng Chen, Vitaly Fedoseev, Christian de Podesta, Theodore Weinberger, Patricia Alireza, and Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

The Kondo lattice system $CeSb_2$ has been recently found to undergo a structural transition under applied pressure. Here, we focus on the low-temperature properties in the new high-pressure structure which hosts an ultra-heavy fermion electronic state and antiferromagnetic order.

We have accessed the high-pressure structure of $CeSb_2$ using both piston-cylinder and anvil pressure cells at mK temperatures, and suppressed the magnetic order to a quantum critical point. In the vicinity of the quantum critical point, we have discovered a superconducting dome with $T_c = 250\,\mathrm{mK}$. The upper critical field exceeds the conventional Pauli limit by almost an order of magnitude and displays an unusual S-shaped temperature dependence. We will discuss the relationship between the upper critical field, the locally non-centrosymmetric crystal structure and the strong electronic mass enhancement in $CeSb_2$.

TT 4.12 Mon 12:30 HSZ 201

Structural and electronic instabilities in high pressure $CeSb_2$ — •Christian K. de Podesta[1], Theodore I. Weinberger[1], Oliver P. Squire[1], Stephen A. Hodgson[1], Jiasheng Chen[1], Rustem Khasanov[2], Christine Beavers[3], Patricia L. Alireza[1], and F. Malte Grosche[1] — [1]Uniersity of Cambridge, UK — [2]Paul Scherrer Institut, Switzerland — [3]Diamond Light Soure, UK

The Kondo-lattice material $CeSb_2$ undergoes a cascade of at least three magnetic transitions below 16 K and - unusually for a Ce system - settles on a ferromagnetic ground state. Whereas these transitions are initially hardly affected by applied pressure, they disappear abruptly above 18 kbar. We find that this disappearance is caused by a pressure induced structural change. The high pressure structure of $CeSb_2$ is profoundly different. It hosts a highly renormalised heavy fermion state which itself undergoes further magnetic transitions at very low temperature. Magnetic order within the high pressure structure extrapolates to zero at a pressure tuned quantum critical point, inducing a new superconducting phase with an anomalous field dependence[1].

We present the first detailed account of the high pressure crystal structure of $CeSb_2$ from X-ray diffraction, alongside a comprehensive study of the associated magnetic order, using μSR, AC-heat capacity and resistivity measurements. This provides the foundation on which to understand the anomalous superconducting properties which are thought to emerge from the quantum critical point.

[1] O. P. Squire et al., arXiv:2211.00975 (2022)

TT 4.13 Mon 12:45 HSZ 201

Observation of anomalous magneto-transport properties in $CeAl_2$ — •Christian Oberleitner, Christian Franz, Alexander Regnat, Jan Spallek, Michael Petrov, Georg Benka, Andreas Bauer, Marc Wilde, and Christian Pfleiderer — Physik-Department, Technische Universität München, D-85748 Garching, Germany

Rare-earth compounds historically have attracted great interest due to their diverse low-temperature properties comprising complex magnetic order, superconductivity, and heavy fermion behaviour. We report a study of the electrical transport properties of non-centrosymmetric $CeAl_2$ at low temperatures and large magnetic fields. For our study single crystals were grown by means of optical float-zoning, where Laue and powder x-ray diffraction as well as low residual resistivities confirm excellent sample quality. Measurements of the magnetization, specific heat, and torque magnetization were used to map out the magnetic phase diagram for different crystallographic orientations. In the regime of the antiferromagnetic order, which supports multi-k antiferromagnetic structures, the magnetoresistance and Hall effect are highly anomalous suggestive of an intricate interplay of anomalous and topological contributions.

TT 5: Correlated Electrons: Method Development

Time: Monday 9:30–13:15 Location: HSZ 204

TT 5.1 Mon 9:30 HSZ 204

Generalized Bogoliubov-Hartree-Fock theory for the Hubbard model — •Chris Koschenz[1] and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

We present the phase diagram of the Hubbard model on the square lattice up to a four-site unit cell derived via a generalized Bogoliubov-Hartree-Fock theory. Our approach allows to study magnetic ordering, charge ordering, and superconductivity on the same footing and gives additional information about the so-called mixed phases [1]. These phases emerge in parameter ranges where the system is potentially strongly affected by fluctuations and cannot be described by any set of usual Hartree-Fock states (Slater determinants) [1,2]. Furthermore, we show how to obtain the self-consistent set of order parameters by straightforward unrestricted global minimization of the appropriate Landau functional [3]. This method allows us to study the coexistence and competition of various magnetic orders and can be used to study the possibility of additional phase transitions in the coexistence regime. [1] E. Langmann and M. Wallin, J. Stat. Phys. **127**, 825 (2007) [2] V. Bach *et al.*, J. Stat. Phys. **76**, 3 (1994) [3] R. Agra *et al.*, Eur. J. Phys. **27**, 407 (2006)

TT 5.2 Mon 9:45 HSZ 204

Competing instabilities with fRG in highly symmetric triangular lattice Hubbard models — •Hannes Braun — Max Planck Institute for Solid State Research

Motivated by, e.g., simulations via cold atomic gases and twisted multilayer transition metal dichalcogenides, we consider Hubbard models with SU(N)*SU(M) symmetry. Such highly symmetric systems with additional degrees of freedom offer possibilities for novel types of symmetry-broken phases and their competition. To analyse the competing correlated phases of the resulting Hubbard models, we generalise the functional Renormalization Group (fRG) approach for correlated fermionic systems to efficiently incorporate the high symmetries. The truncated unity fRG provides us with unbiased fluctuation diagnostics and allows us to analyse the interplay between charge, spin, and pairing instabilities on equal footing. We present the new set of SU(N)*SU(M)-symmetric fRG equations and first results for the two-dimensional Hubbard model on the triangular lattice.

TT 5.3 Mon 10:00 HSZ 204

Functional renormalization group without functional integrals — Peter Kopietz, Rüdiger Krämer, and •Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

We show that exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within a Hamiltonian operator formalism without using functional integrals. This can be useful for teaching FRG methods to students unfamiliar with functional integrals and also opens new possibilities for applying FRG methods to quantum systems with projected Hilbert spaces such as quantum spin models or strongly interacting fermionic lattice models. In particular, by representing the Hubbard model and the $t-J$-model in terms of so-called Hubbard X-operators we construct a new strong-coupling FRG approach to these models.

TT 5.4 Mon 10:15 HSZ 204

Reduced basis modeling of quantum spin systems based on DMRG — •Paul Brehmer[1], Michael Herbst[2], Matteo Rizzi[3,4], Benjamin Stamm[5], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Applied and Computational Mathematics, RWTH Aachen University, 52062 Aachen, Germany — [3]FZ Jülich GmbH, Institute of Quantum Control, Peter Grünberg Institut (PGI-8), 52425 Jülich, Germany — [4]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [5]Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, 70569 Stuttgart, Germany

Within the reduced basis modeling approach, an effective low-dimensional subspace of a quantum many-body Hilbert space is constructed in order to investigate, e.g., the ground-state phase diagram. The basis of this subspace is built from solutions of snapshots, i.e., ground states corresponding to particular and well-chosen parameter values. Here, we show how a greedy strategy to assemble the reduced basis and thus to select the parameter points can be implemented based on density-matrix-renormalization-group (DMRG) calculations. Once the reduced basis is computed, observables required for the computation of phase diagrams can be computed with a computational complexity independent of the underlying Hilbert space for any parameter value. We illustrate the efficiency and accuracy of this approach for different one-dimensional quantum spin-S models with both $S = 1/2$ and $S = 1$, including anisotropic as well as biquadratic exchange interactions, leading to rich quantum phase diagrams.

TT 5.5 Mon 10:30 HSZ 204

Novel degrees of freedom in cluster Mott insulators — •Vaishnavi Jayakumar and Ciarán Hickey — Institute for Theoretical Physics, University of Cologne, Germany

The Hubbard model provides a playground for investigating the physics of a wide range of strongly correlated systems. An important feature of these systems is the Mott insulating phase, where at half-filling, an electron gets localised on a single lattice site. In this work, we study cluster Mott insulators – where electrons are now localised on clusters of sites. To that end, we study an extended Hubbard-Kanamori model on a plethora of clusters with multiple orbitals per site, at different electron fillings. We then explore different regimes of interplay between strong correlations and hopping within these clusters, and the effective degrees of freedom that emerge. It is seen, for example, that high ground-state degeneracies are possible that are due to a combination of both spatial and orbital symmetries. We further include crystal field splitting and spin-orbit coupling to bring our model closer to real materials. Once a blueprint for these building blocks has been established, the clusters can be connected through inter-cluster terms, giving rise to potentially novel Hamiltonians.

TT 5.6 Mon 10:45 HSZ 204

Numerical linked cluster expansions for the ordered low-field phase of the transverse-field Ising model — •Matthias Mühlhauser, Max Hörmann, and Kai Phillip Schmidt — Institute for Theoretical Physics I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We present a hypergraph approach to numerical linked cluster expansions (NLCEs) in the low-field limit of the transverse-field Ising model (TFIM) where the Z2-Symmetry of the TFIM is spontaneously broken and the ground state is magnetically ordered.

Conventional NLCEs in this limit are performed as site expansions where the magnetic order of the ground state is taken into account by longitudinal boundary fields on the graphs.

Here, using an isospectral dual description of the TFIM where the ordered phase is mapped to an effective (symmetry unbroken) polarized phase in the dual desciption, we demonstrate that a straightforward hypergraph expansion can be executed so that no boundary fields are necessary. This allows us to obtain competitive results for the ground-state energy of the ordered low-field phase of the TFIM.

TT 5.7 Mon 11:00 HSZ 204

Projective cluster-additve block-diagonalisation method — •Max Hörmann and Kai Phillip Schmidt — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

We present an efficient block-diagonalisation method that only relies on the lowest eigenvectors and eigenvalues and allows for a linked-cluster expansion. The method is applied to a low-field expansion of the transverse-field Ising model on the square lattice. Both the single spin-flip and bound-state dispersion is calculated perturbatively and non-perturbatively. The origin of the breakdown of the non-perturbative linked-cluster expansion for the bound-state dispersion at a critical field value is discussed and potential solutions to overcome this problem are examined.

15 min. break

TT 5.8 Mon 11:30 HSZ 204

Series expansions with multiple quasi-particle types for the

dual Dicke-Ising model — •Andreas Schellenberger, Lea Lenke, and Kai Phillip Schmidt — FAU Erlangen-Nürnberg, Erlangen, Deutschland

The established approach of perturbative continuous unitary transformations (pCUT) constructs effective quantum many-body Hamiltonians in a perturbative series that conserve the number of one quasiparticle type. We extend the pCUT method to similarity transformations – dubbed pcst^{++} – allowing for multiple quasi-particle-types with complex-valued energies. This enlarges the field of application to closed and open quantum many-body systems with unperturbed operators corresponding to arbitrary superimposed ladder spectra. To illustrate the new possibility of the pcst^{++} method to specifically tackle interacting light-matter systems, we discuss the dual Dicke-Ising model. We determine low-energy spectral properties and investigate potential conversion processes between different quasi-particle types.

TT 5.9 Mon 11:45 HSZ 204

Series expansions in open and non-Hermitian quantum many-body systems with multiple quasi-particle types — •Lea Lenke, Andreas Schellenberger, and Kai Phillip Schmidt — FAU Erlangen-Nürnberg

The established approach of perturbative continuous unitary transformations (pCUT) constructs effective quantum many-body Hamiltonians in a perturbative series that conserve the number of one quasiparticle type. We extend the pCUT method to similarity transformations – dubbed pcut^{++} – allowing for multiple quasi-particle-types with complex-valued energies. This enlarges the field of application to closed and open quantum many-body systems with unperturbed operators corresponding to arbitrary superimposed ladder spectra. To this end a generalized counting operator is combined with the quasi-particle generator for open quantum systems recently introduced by Schmiedinghoff and Uhrig [1]. The pcut^{++} then yields model-independent quasiparticle conserving effective Hamiltonians and Lindbladians allowing a linked-cluster expansion similar to the conventional pCUT method. We illustrate the application of the pcut^{++} method by discussing representative open and non-Hermitian quantum systems. [1] G. Schmiedinghoff and G. S. Uhrig, arXiv:2203.15532 [cond-mat.quant-ph].

TT 5.10 Mon 12:00 HSZ 204

Multi-scale space-time ansatz for correlation functions of quantum systems — •Hiroshi Shinaoka[1], Markus Wallerberger[2], Yuta Murakami[3], Kosuke Nogaki[4], Rihito Sakurai[1], Philipp Werner[5], and Anna Kauch[2] — [1]Department of Physics, Saitama University, Saitama 338-8570, Japan — [2]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [3]Center for Emergent Matter Science, RIKEN, Wako, Saitama 351-0198, Japan — [4]Department of Physics, Kyoto University, Kyoto 606-8502, Japan — [5]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Correlation functions of quantum systems are central objects in quantum field theories, which may be defined in high-dimensional spacetime domains. The numerical treatment of these objects suffers from the curse of dimensionality, which hinders the application of sophisticated many-body theories to interesting problems.

In this talk, we propose a quantum-algorithms-inspired Multi-Scale Space-Time Ansatz (MSSTA) for correlation functions of quantum systems [1]. The space-time dependence is mapped to auxiliary qubit (S = 1/2 spin) degrees of freedom describing exponentially different length scales, and the ansatz assumes a separation of length scales. We numerically verify the ansatz for various equilibrium and nonequilibrium systems and show essential building blocks of diagrammatic equations, such as convolutions or Fourier transforms are formulated in the compressed form using tensor networks.

[1] H. Shinaoka et al., arXiv:2210.12984v2

TT 5.11 Mon 12:15 HSZ 204

Efficient flow equations for dissipative systems — •Gary Schmiedinghoff and Götz S. Uhrig — Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Open quantum systems provide an essential theoretical basis for the development of novel quantum technologies, since any real quantum system inevitably interacts with its environment. Lindblad master equations capture the effect of Markovian environments. Closed quantum systems can be treated using flow equations with the particle conserving generator. We generalize this generator to non-Hermitian matrices and open quantum systems governed by Lindbladians, comparing our results with recently proposed generators by Rosso et al. In comparison, we find that our advocated generator provides an efficient flow with good accuracy in spite of truncations.

TT 5.12 Mon 12:30 HSZ 204

Dynamical mean-field study of a photon-mediated ferroelectric phase transition — •Katharina Lenk[1], Jiajun Li[2,3], Philipp Werner[2], and Martin Eckstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, 22607 Hamburg — [2]Department of Physics, University of Fribourg, 1700 Fribourg Switzerland — [3]Paul Scherrer Institute, Condensed Matter Theory, PSI Villigen, Switzerland

The interplay of light and matter gives rise to intriguing cooperative effects in quantum many-body systems. This is even true in thermal equilibrium, where the electromagnetic field can hybridize with collective modes of matter, and virtual photons can induce interactions in the solid. Here, we treat these light-mediated interactions using dynamical mean-field theory. We consider a minimal model of a two-dimensional material that couples to a surface plasmon polariton mode of a metal-dielectric interface. Within the mean-field approximation, the system exhibits a ferroelectric phase transition that is unaffected by the light-matter coupling. Bosonic dynamical mean-field theory provides a more accurate description and reveals that the photon-mediated interactions enhance the ferroelectric order and stabilize the ferroelectric phase.

TT 5.13 Mon 12:45 HSZ 204

Energy correlations of excited states in localization landscape theory — •Torsten Weber, Johannes Dieplinger, Christoph Forster, Lucas Resch, Ferdinand Evers, and Klaus Richter — Universität Regensburg, Regensburg, Deutschland

The localization landscape method, first described in [1], is a method that enables the prediction of the localization regions of eigenfunctions of a localized system. Additionally, the method gives a prediction of the energy of low-lying localized eigenfunctions by defining an effective potential from the landscape function [2]. This energy prediction, although providing good results for low energy eigenfunctions, ceases to work for higher energy states. Studying the method for a one-dimensional disordered system we observe a characteristic form of the ratio of the predicted eigenvalue by the landscape method and the actual eigenvalue for this region of the spectrum. We provide a possible explanation for this behaviour by extending the method leading to the energy prediction by including excited states of the effective potential. By harnessing the universal technique of quantifying excited states by counting nodes we observe a correspondence of the n-th excited states with the n-th repetition of a substructure of the characteristic behaviour described above. We go further to also find an analytic estimate for the structures.

[1] M. Filoche and S. Mayboroda, PNAS 109, 14761 (2012)
[2] D. N. Arnold et al., SIAM Journal on Scientific Computing, 41(1) (2019)

TT 5.14 Mon 13:00 HSZ 204

Extended quasiparticle Padé approximation for non-Fermi liquids — •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 extended quasiparticle picture is adapted to non-Fermi systems by suggesting a Padé approximation which interpolates between the known small scattering-rate expansion and the deviation from the Fermi energy. The first two energy-weighted sum rules are shown to be fulfilled independent of the interpolating function. For various models of one-dimensional Fermions scattering with impurities the quality of the Padé approximation for the spectral function is demonstrated and the reduced density matrix or momentum distribution is shown to be reproduced not possessing a jump at the Fermi energy. Though the two-fold expansion is necessary to reproduce the spectral function and reduced density it is shown that for the description of transport properties the extended quasiparticle approximation is sufficient. The T-matrix approximation leads to the delay time as the time two particles spend in a correlated state. This contributes to the reduced density matrix and to an additional part in the conductivity which is presented at zero and finite temperatures. Besides a localization at certain impurity concentrations, the conductivity shows a maximum at small temperatures interpreted as onset of superconducting behaviour triggered by impurities. The Tan contact reveals the same universal behaviour as known from electron-electron scattering.

[1] arXiv:2208.11971

TT 6: Topological Semimetals

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

TT 6.1 Mon 9:30 HSZ 304

Anomalous Hall and Nernst effects in Kane fermions — •Karun Gadge[1,3], Sumanta Tewari[2], and Girish Sharma[3] — [1]Institute for Theoretical Physics University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Department of Physics and Astronomy, Clemson University, Clemson, South Carolina, 29634, USA — [3]School of Basic Sciences, Indian Institute of Technology, Mandi, Mandi 175005, India

Kane fermions are characterized by a linear Dirac cone intersecting with a flat band, resembling a pseudo-spin-1 Dirac semimetal. Similar to relativistic Dirac fermions, Kane fermions satisfy a linear energy-momentum relation and can be classified as being pseudorelativistic. Unlike Dirac fermions, they are not protected by symmetry or by topology, but respect time-reversal symmetry, and can emerge by suitable band engineering, for example, in mercury-telluride compounds. Here we discuss the reminiscences of Berry-phase physics in Kane fermions that emerge in the presence of broken time-reversal symmetry. We discuss anomalous transport in Kane fermions and show its similarity to transport in a Dirac semimetal. Furthermore, we study anisotropy in their response that can be probed in current experiments.

[1] PRB 105, 235420 (2022)

TT 6.2 Mon 9:45 HSZ 304

Automatic generation and topological classification of low-energy Hamiltonians at multi-fold degeneracies — •Kirill Alpin — Max Planck Institute for Solid State Research, Stuttgart, Germany

In this talk, we show a method of generating general high-symmetry Hamiltonian with the goal of topologically classifying all possible multi-fold crossings in bandstructures of condensed matter systems. To do so, we found all higher-dimensional irreducible representations at all high-symmetry points in all space groups. The topological phase diagrams of the automatically generated low-energy Hamiltonian at these k-points were mapped out. During this process, we identified a prevalent topological phase with an unusually high Chern number of 5 in multi-fold point crossings. A material was found featuring this topological phase. Further ab-initio calculations of this materials surface DOS showed a high number of Fermi arcs.

TT 6.3 Mon 10:00 HSZ 304

Finite-size effects in a two-dimensional non-symmorphic wallpaper group lattice — •Miguel Ángel Jiménez Herrera[1] and Dario Bercioux[1,2] — [1]Donostia International Physics Center, 20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

We investigate the spectral properties of a two-dimensional electronic lattice belonging to the non-symmorphic wallpaper group: the herringbone lattice. Specifically, we focus on the cases of ribbons and flakes geometry. Within a tight-binding description, we study how the different states localize inside the system both for ribbons and flakes. We apply different perturbations and symmetry breaking distortions to the lattice and investigate the robustness of the spectral features. Similarly to the bulk case, where we can gap the band structure or merge the Dirac cones into semi-Dirac cones [1], we recover the same properties along the two main directions that ribbons can be constructed. Finally, we study the finite size effects on this lattice, both on ribbon and flake geometries, and report a spectral flow of states across the bulk-like bands.

[1] Herrera & Bercioux, arXiv:2209.11653.

TT 6.4 Mon 10:15 HSZ 304

Landau quantization in the topological semimetal WTe_2 — •R. Sanchez-Barquilla[1], F. Martin-Vega[1], J. J. Baldovi[2], M. Ochi[3], R. Arita[4], N. H. Jo[5], S. L. Bud'ko[5], P. C. Canfield[5], H. Suderow[1], and I. Guillamon[1] — [1]Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, UAM, E-28049, Spain — [2]ICMol, UV, 46980 Paterna, Spain. — [3]Department of Physics, Osaka University, Osaka 560-0043, Japan — [4]RIKEN Center, Saitama 351-0198, Japan — [5]Department of Physics and Astronomy, Ames, IA 50011

WTe_2 is a layered semimetal which has sparked much interest due to the non-saturating linear MR and possible non-trivial band structure properties, such as Weyl type-II fermions. Quantum oscillations under magnetic fields signal the passage of Landau levels (LL) through the Fermi level and are easily observed in macroscopic measurements, providing a rather complete view of the FS. However, the Landau quantization of the band structure above and below the Fermi energy has not yet been resolved in detail. We present mK STM measurements up to 14T. We have obtained the band structure close to the Fermi level and identified the main electron and hole pockets thanks to QPI experiments at 0T. When applying magnetic field, the spatially averaged tunneling conductance is devoid of LL and shows no field dependence. Atomically resolved measurements present however Landau quantization. We show that the contribution from the electron and hole pockets to the tunneling density of states (DOS) compensates LL peaks in the spatially averaged DOS. We describe Landau quantization at atomic scale and show a non-trivial energy shift of the LL structure.

TT 6.5 Mon 10:30 HSZ 304

Landau levels in NbAs as seen in magneto-optics: experiment versus modeling — S. Polatkan[1], M. Orlita[2], C. Shekhar[3], C. Felser[3], M. Dressel[1], and •A. V. Pronin[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]LNCMI, CNRS-UGA-UPS-INSA-EMFL, 38042 Grenoble, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

We measured the inter-Landau-level transitions the Weyl semimetal NbAs in magneto-optical experiments and found that the fits with pure Weyl bands do not lead to a satisfactory agreement between theory and experiment. We thus propose a coupled hyperbolic band model, supplemented by detailed 2D band structure cuts, attributing a secondary role to the presence of Weyl points. We argue that this minimalist model is sufficient to describe the measured magneto-optical spectra.

TT 6.6 Mon 10:45 HSZ 304

Static and dynamic magnetic properties of *R*AlSi Weyl semimetals — •Tillmann Weinhold[1], Hank Wu[2,3], Rajib Sarkar[1], George Gill[2], Vadim Grinenko[4], Fazel Tafti[5], Stephen Blundell[2], and Hans-Henning Klauss[1] — [1]TU Dresden, Germany — [2]University of Oxford — [3]MPI for Solid State Research, Stuttgart, Germany — [4]Shanghai JiaoTong University, China — [5]Boston College, MA, USA

Weyl semimetals show interesting electronic transport behavior like anomalous Hall effect and negative magnetoresistance. In the magnetic semimetal NdAlSi spin-density wave order was found below 7.2 K. It is proposed that the magnetic order is driven by RKKY interaction of Weyl fermions on narrow Fermi pockets.

We used NMR and μSR experiments to gain information about local static and dynamic magnetic properties of NdAlSi and discuss the results in comparison with diamagnetic LaAlSi and canted ferromagnetic CeAlSi.

TT 6.7 Mon 11:00 HSZ 304

Optically enhanced terahertz harmonic generation in the Dirac semimetal Cd_3As_2 — •Patrick Pilch[1], Changqing Zhu[1], Renato M. A. Dantas[2], Anneke Reinold[1], Yunkun Yang[3], Faxian Xiu[3], and Zhe Wang[1] — [1]TU Dortmund University, Germany — [2]University of Basel, Switzerland — [3]Fudan University, Shanghai, China

High harmonic generation provides an efficient tool to investigate nonequilibrium dynamics of a driven system, and is also very interesting for applications. Cd_3As_2 is a well-established three-dimensional Dirac semimetal with a topologically protected crossing of linear bands at the Fermi level. Terahertz harmonic generation is observed in Cd_3As_2 due to field-driven intraband kinetics [1]. By optically pumping the electron-doped Cd_3As_2, we observe a strong enhancement of the terahertz third harmonic generation. By investigating the dependence of the terahertz third harmonic generation on the pump fluence and time delay, we can ascribe this enhancement to the kinetics of a long-lived nonequilibrium state which corresponds to a population inversion of electrons and holes in the Dirac cone with a characteristic relaxation time $\tau \leq 10$ ps.

[1] Kovalev, S. et al. Nature Commun. 11, 2451 (2020).

15 min. break

TT 6.8 Mon 11:30 HSZ 304

Signatures of a magnetic-field-induced Lifshitz transition in the ultra-quantum limit of the topological semimetal $ZrTe_5$ — •Stanislaw Galeski[1,2] and Henry Legg[3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, germany — [2]Physics Institute, Universität Bonn, Bonn, Germany — [3]Department of Physics, University of Basel, Basel, Switzerland

The quantum limit (QL) of an electron liquid, realised at strong magnetic fields, has long been proposed to host a wealth of strongly correlated states of matter. Electronic states in the QL are, for example, quasi-one dimensional (1D), which implies perfectly nested Fermi surfaces prone to instabilities. Whereas the QL typically requires unreachably strong magnetic fields, the topological semimetal $ZrTe_5$ has been shown to reach the QL at fields of only a few Tesla. Here, we characterize the QL of $ZrTe_5$ at fields up to 64 T by a combination of electrical-transport and ultrasound measurements. We find that the Zeeman effect in $ZrTe_5$ enables an efficient tuning of the 1D Landau band structure with magnetic field. This results in a Lifshitz transition to a 1D Weyl regime in which perfect charge neutrality can be achieved. Since no instability-driven phase transitions destabilise the 1D electron liquid for the investigated field strengths and temperatures, our analysis establishes $ZrTe_5$ as a thoroughly understood platform for potentially inducing more exotic interaction-driven phases at lower temperatures.

TT 6.9 Mon 11:45 HSZ 304

The anomalous photo-Nernst effect in a Dirac semimetal — •Maanwinder Partap Singh[1,2], Jonas Kiemle[1,2], Waldemar Schmunk[1,2], Alexander Holleitner[1,2], and Christoph Kastl[1,2] — [1]Walter Schottky Institut, Technical University of Munich, Am Coulombwall 4a, 85748 Garching, Germany. — [2]Munich Center of Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany.

The 3D Dirac semimetal $HfTe_5$ is a model system to study unconventional Hall transport phenomena, such as quasi quantized and anomalous Hall efects, in the limit of very low charge carrier densities. Here, we report on anomalous photocurrents in $HfTe_5$, which are intimately linked to the anomalous Hall and the related Nernst conductivities. As the dominant mechanism of photocurrent generation, we establish a, hitherto hidden, anomalous photo-Nernst effect of 3D Dirac electrons. The anomalous photo-Nernst effect manifests itself as a long-range, photoresponse along the crystal edge arising from a Shockley-Ramo type response and the local symmetry breaking at the edge. The observed temperature and density dependences of the anomalous photo-Nernst currents are consistent with a dominating intrinsic Berry curvature mechanism.

TT 6.10 Mon 12:00 HSZ 304

Field-tunable inverted band gap in GdPtBi: A magneto-optical study — •S. Polatkan[1], E. Uykur[1], A. V. Pronin[1], M. Orlita[2], I. Mohelsky[2], J. Wyzula[2], C. Shekhar[3], C. Felser[3], and M. Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]LNCMI, CNRS-UGA-UPS-INSA-EMFL, 38042 Grenoble, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

GdPtBi is a half-Heusler compound that was suggested to host triple-point fermions. Such fermions may be transformed into Weyl fermions in magnetic fields. We present magneto-optical data alongside a $\mathbf{k} \cdot \mathbf{p}$ model, evidencing the exchange-interaction mediated pseudo-Zeeman splitting of the parabolic band touching at the Γ point predicted by DFT, and thus prove the existence of highly tunable Weyl cones.

TT 6.11 Mon 12:15 HSZ 304

Anisotropic optics and gravitational lensing of tilted Weyl fermions — •Viktor Könye[1], Lotte Mertens[1,2], Corentin Morice[3], Dmitry Chernyavsky[1], Ali G. Moghaddam[4,5], Jasper van Wezel[2], and Jeroen van den Brink[1,6] — [1]Institute for Theoretical Solid State Physics, IFW Dresden and Wurzburg-Dresden Cluster of Excellence ct.qmat, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands — [3]Laboratoire de Physique des Solides, CNRS UMR 8502, Universite Paris-Saclay, F-91405 Orsay Cedex, France — [4]Department of Physics, Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan 45137-66731, Iran — [5]Computational Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, FI-33014 Tampere, Finland — [6]Institute for Theoretical Physics, TU Dresden, 01069 Dresden, Germany

We show that tilted Weyl semimetals with a spatially varying tilt provide a platform for studying analogues to problems in anisotropic optics as well as curved spacetime. Considering particular tilting profiles, we numerically evaluate the time evolution of wave packets. We demonstrate that electron trajectories in such systems can be obtained from Fermat's principle in the presence of an inhomogeneous, anisotropic effective refractive index. On the other hand, we show how the electrons dynamics reveal gravitational features and use them to simulate gravitational lensing around a synthetic black hole.

TT 6.12 Mon 12:30 HSZ 304

Black hole mirages: Electron lensing and Berry curvature effects in inhomogeneously tilted Weyl semimetals — •Andreas Haller[1], Suraj Hedge[2], Chen Xu[2], Christophe De Beule[1,3], Thomas L. Schmidt[1], and Tobias Meng[2] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg — [2]Institute of Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01069 Dresden, Germany — [3]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia PA 19104, USA

In this talk, I present our recent study about electronic transport in Weyl semimetals with spatially varying nodal tilt profiles. We discuss two complementary approaches that characterise the electron flow: solutions of the semiclassical equations of motion, in analogy to those encountered in black hole spacetimes, and large-scale microscopic simulations of a scattering region surrounded by semi-infinite leads. We show that the two approaches lead to equivalent results when the wave packet is sufficiently far from the center of the tilt. The two methods are arguably a powerful toolset in the pursuit of tiltronic devices such as e.g. electronic lenses.

TT 6.13 Mon 12:45 HSZ 304

Weyl-type parallel spin-momentum locking in a chiral topological semimetal — •Niels B. M. Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Orthogonal Rashba-type spin-momentum locking is well-known from semiconductors and topological insulator surface states and has inspired many theoretical proposals for technological applications. In contrast, Weyl-type purely parallel spin-momentum locking – which can be considered the natural counterpart of the Rashba-type – has remained elusive in experiments because all experimentally confirmed Weyl-fermion are described by Pauli matrices that act on an orbital pseudospin rather than the proper electron spin. Recently, chiral topological semimetals (CTS) that host single- and multifold band crossings [1,2] have been predicted to realize parallel spin-momentum locking. Here, we use spin-resolved photoemission to probe the spin-texture Fermi-arc surface states in the CTS PtGa. We find that the electron spin points orthogonal to the Fermi surface contour for momenta close to the projection of a bulk multifold fermion, which is consistent with parallel spin-momentum locking of the latter [3]. We anticipate that our discovery of parallel spin-momentum locking of multifold fermions will lead to the integration of chiral topological semimetals in novel spintronic devices that can be used for field-free switching of magnets with perpendicular magnetic anisotropy, and other novel phenomena.

[1] Schröter et al., Nat. Phys 8 759-65 (2019)
[2] Schröter et al., Science 369, 179-83 (2020)
[3] Krieger et al., arXiv.2210.08221 (2022)

TT 7: Spin Transport and Orbitronics, Spin-Hall Effects (joint session MA/TT)

Time: Monday 9:30–13:00 Location: HSZ 403

TT 7.1 Mon 9:30 HSZ 403

Topological information device operating at the Landauer limit — •Ahmet Mert Bozkurt[1,2,3], Alexander Brinkman[4], and Inanc Adagideli[3,4] — [1]QuTech, Delft University of Technology, 2600 GA Delft, The Netherlands — [2]Kavli Institute of Nanoscience, Delft University of Technology, 2600 GA Delft, The Netherlands — [3]Faculty of Engineering and Natural Sciences, Sabanci University, Orhanli-Tuzla, Istanbul, Turkey — [4]MESA+ Institute for Nanotechnology, University of Twente, The Netherlands

We propose and theoretically investigate a novel Maxwell's demon implementation based on the spin-momentum locking property of topological matter. We use nuclear spins as a memory resource which provides the advantage of scalability. We show that this topological information device can ideally operate at the Landauer limit; the heat dissipation required to erase one bit of information stored in the demon's memory approaches $k_BT\ln 2$. Furthermore, we demonstrate that all available energy, $k_BT\ln 2$ per one bit of information, can be extracted in the form of electrical work. Finally, we find that the current-voltage characteristics of the topological information device satisfy the conditions of an ideal memristor.

TT 7.2 Mon 9:45 HSZ 403

Controlling 3D spin textures by manipulating sign and amplitude of interlayer DMI with electrical current — •Fabian Kammerbauer[1], Won-Young Choi[1], Freimuth Frank[1,2], Robert Frömter[1], Yuriy Mokrousov[1,2], and Mathias Kläui[1] — [1]Institute of Physics, Joahnnes Gutenberg University, Staudingerweg 7, 55128 Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The recently discovered interlayer Dzyaloshinskii-Moriya interaction (IL-DMI) in multilayers with perpendicular magnetic anisotropy favors a canting of spins in the in-plane direction [1]. It could thus stabilize exciting spin textures such as Hopfions. A key requirement for nucleation is to control the IL-DMI and so, we investigate the influence of an electric current on the strength of the IL-DMI, as previously found for FMI. The IL-DMI is quantified using out-of-plane hysteresis loops while applying a static in-plane magnetic field at varied azimuthal angles. We observe a shift in the azimuthal dependence with increasing current, which is concluded to originate from the additional in-plane symmetry breaking introduced by the current flow. Fitting the angular dependence we demonstrate the presence of an additive current-induced term [3]. With this, an easily accessible possibility to manipulate 3D spin textures by current is realized.

[1] Han et al., Nat. Mater. 18, 703-708 (2019)
[2] Karnad et al., Phys. Rev. Lett. 121, 147203 (2018)
[3] Kammerbauer et al, arXiv:2209.01450 (2022)

TT 7.3 Mon 10:00 HSZ 403

Nonequilibrium dynamics in a spin valve with noncollinear magnetization — •Rudolf Smorka[1], Pavel Baláž[2], Michael Thoss[1], and Martin Žonda[3,1] — [1]University of Freiburg, Germany — [2]Institute of Physics of the Czech Academy of Sciences Prague, Czech Republic — [3]Charles University Prague, Czech Republic

Manipulation of magnetization by electric currents enables novel functions for spin-transfer torque devices. We study the nonequilibrium spin dynamics and spin-transfer torques in noncollinear spin-valve heterojunctions using a mixed quantum-classical Ehrenfest approach.

In an isolated valve for short spacer layers and weak spin-electron couplings, magnetization dynamics of the ferromagnetic layers is in agreement with the macrospin approximation. For large spacer layers, our quantum-classical approach predicts electron-induced spin relaxation. For intermediate electron-spin couplings, a change in the localization character of the electronic eigenstates from metallic-like to insulator-like leads to a reduced indirect exchange interaction between spins mediated by the conduction electrons. In a spin valve coupled to leads, spin relaxation times differ by several orders of magnitude depending on whether the DC bias is introduced by shifting the electrochemical potentials of both leads symmetrically about the equilibrium Fermi level of the spin valve (reminiscent of a gate-tunable junction) or by shifting the chemical potential of only one lead (as realized in a scanning tunneling microscope geometry).

[1] R. Smorka, P. Baláž, M. Thoss, M. Žonda, Phys. Rev. B 2022, 106, 144435.

TT 7.4 Mon 10:15 HSZ 403

Nonrelativistic spin currents in altermagnets — •Rodrigo Jaeschke-Ubiergo, Jairo Sinova, and Libor Šmeijkal — Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany

Altermagnetism has emerged recently as a third basic collinear magnetic phase [1], in addition to ferromagnets and antiferromagnets. Conventional antiferromagnets exhibit two sublattices with opposite magnetic moment related by translation or inversion. In altermagnets the magnetic sublattices are connected by a rotation or a mirror operation. The particular symmetry causes that altermagnets display time-reversal (T) symmetry breaking and spin split band structure even in absence of spin-orbit coupling [2]. In this work, we study the spin conductivity tensor in altermagnets by using spin group theory formalism [1]. We also use Kubo's linear response to calculate the spin conductivity tensor in all the altermagnetic spin point groups models. Additionally, we identify and sort 200 altermagnetic candidates into spin conductivity tensor classes. We will discuss some spin point groups that allow for a transverse spin current in detail. This is the case of spin splitter current in RuO2 [3,4], which is a nonrelativistic effect that conserves spin unlike in general magnetic spin Hall effect in noncollinear magnets. Moreover, the spin conductivity tensor is symmetric and T-odd, which makes it different from the conventional spin Hall effect. [1] Šmejkal et al., PRX, 12, 031042 (2022). [2] Šmejkal, et al. Sci.Adv 2020. [3] Gonzalez- Hernandez, et al. PRL 2021. [4] Šmejkal, et al. PRX 12, 011028 (2022).

TT 7.5 Mon 10:30 HSZ 403

Quantification and modulation of intrinsic spin transport in 5d transition metals — •Akash Bajaj, Reena Gupta, Andrea Droghetti, and Stefano Sanvito — School of Physics and CRANN, Trinity College Dublin, Dublin 2, Ireland

Spin-Hall effect (SHE) enables charge-to-spin conversion in heavy transition metals, such as Ta and Pt, with strong spin-orbit coupling (SOC) strengths. It has been extensively studied as a viable mechanism for the development of next-generation spintronics-based non-volatile memory devices. Numerous experimental and first-principles approaches have been devised to quantify the charge-to-spin conversion efficiency i.e., the spin-Hall angle (SHA), for the SHE. However, such approaches unavoidably involve interface contributions and, in general, extrinsic effects such as disorder and impurities, which are known to be less dominant than the bandstructure-only intrinsic contribution in such heavy metals. In this work, we use density functional theory combined with a bond-current-based non-equilibrium Green's functions approach to quantify the intrinsic SHAs of bulk elemental and thin-film models of 5d transition metals. We then computationally demonstrate a strategy for modulating the SHA within the same device, using Pt and Au as contrasting examples. Our computational work not only provides a quantitative estimation of the intrinsic SHAs for these materials, but also enables its theoretical understanding aimed towards the development of higher performance and power-efficient spintronics-based non-volatile memory devices.

TT 7.6 Mon 10:45 HSZ 403

Influence of Disorder at Insulator-Metal Interface on Spin Transport — Mahsa Alsadat Seyed Heydari, Wolfgang Belzig, and •Niklas Rohling — Department of Physics, University of Konstanz

Motivated by experimental work showing enhancement of spin transport between yttrium iron garnet and platinum by the thin antiferromagnetic insulator NiO [1] between them, we consider spin transport trough the interface of a non-magnetic metal and a ferro- or antiferromagnetically ordered insulator. The spin transport is carried by spin-polarized electrons in the metal and by magnons in the insulator. Spin current can be generated by a spin accumulation in the metal due to the inverse spin Hall effect, a microwave field exciting magnons in the insulator, or by a thermal gradient (spin Seebeck effect). The spin current can be computed using Fermi's Golden Rule [2]. For a perfectly clean interface, the in-plane momentum is conserved for the electron-magnon scattering events which govern the spin transport through the interface. We calculate how disorder-induced broadening of the scatting matrix elements with respect to the in-plane momentum influences the spin current. As a general result, we observe that for many experimental setups, one should expect a rather small effect of interface disorder on the measured spin current.

[1] Wang et al., Phys. Rev. Lett. 113, 097202 (2014), Phys. Rev. B 91, 220410(R) (2015); Lin et al. Phys. Rev. Lett. 116, 186601 (2016)
[2] Bender et al., Phys. Rev. Lett. 108, 246601 (2012)

TT 7.7 Mon 11:00 HSZ 403

Long-range orbital-Hall torques in Nb(or Ru)/Ni Heterostructures — Arnab Bose[1], Fabian Kammerbauer[1], •Rahul Gupta[1], Dongwook Go[2], Yuriy Mokrousov[1,2], Gerhard Jakob[1], and Mathias Kläui[1,3] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, 55128 Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [3]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

We report a large orbital Hall torque (OHT) generated by Nb and Ru via strong dependence of torques on the ferromagnets, Ni, in Nb(Ru)/Ni heterostructures. We found the sign reversal of the damping-like torque in Nb/Ni. Moreover, the long-range orbital transport in the ferromagnet was revealed by the thickness dependences of Ni in Ni/Nb(or Ru) heterostructure, which are markedly different from the regular spin absorption in the ferromagnet that takes place within a few angstroms and thus it uniquely distinguishes OHT from the spin Hall torque. The experimentally measured effective orbital-Hall conductivities are found to be 6.1×10^4 $\frac{\hbar}{2e}$ $(\Omega\mathrm{m})^{-1}$ and 5.86×10^4 $\frac{\hbar}{2e}$ $(\Omega\mathrm{m})^{-1}$ for Nb and Ru, respectively, which is an order of magnitude higher than their measured spin Hall conductivities, as also confirmed by the density functional theory. This study opens a plethora of possibilities to further engineering the torques, utilizing the orbital degree of freedom.

TT 7.8 Mon 11:15 HSZ 403

Layer-resolved spin-orbit torque assisted magnetization dynamics in Pt/Co heterostructure — •Harshita Devda[1], András Deák[2], Leandro Salemi[3], Levente Rózsa[1], László Szunyogh[2], Peter M. Oppeneer[3], and Ulrich Nowak[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]Uppsala University, Uppsala, Sweden

It is well known that the spin-orbit torque (SOT) mechanism is more reliable for current induced magnetization dynamics than the spin-transfer torque. The key phenomenon behind the SOT in heavy metal/ferromagnet (HM/FM) bilayers is attributed to the spin Hall effect (SHE) and the spin Rashba-Edelstein effect (SREE). However, the exact mechanism is still under debate. So far various works have studied the SOT-driven magnetic behavior in different magnetic systems, but the layer-resolved understanding of the SOT effect in the HM/FM bilayer due to spin-orbit coupling (SOC) in heavy metal is still lacking. We focus on current-induced magnetization dynamics in a Pt/Co bilayer assisted by the SOC in Pt. We use a multiscale model which links ab initio calculations with atomistic spin dynamics simulations. We implement a linear-response formalism to compute the electrically induced magnetic moments, caused by SHE in bulk and SREE at the interface, and utilize these in atomistic spin dynamics simulations. We analyse the layer-resolved behavior of both field-like and damping-like torques in FM and determine how they affect magnetization dynamics in ferromagnets.

TT 7.9 Mon 11:30 HSZ 403

Spin and orbital Edelstein effect in a bi- and trilayer system with Rashba interaction — •Sergio Leiva[1], Jürgen Henk[1], Ingrid Mertig[1], and Annika Johansson[2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

The spin Edelstein effect has proved to be a promising phenomenon to generate spin polarization from a charge current in systems without inversion symmetry. In recent years, current-induced orbital magnetization, also called the orbital Edelstein effect, has also been predicted for several systems with broken inversion symmetry [1-6].

In the present work, we calculate the current-induced spin and orbital magnetization for a bilayer and a trilayer system with Rashba interaction for the interface and the free-standing slab configurations. We use the modern theory of orbital magnetization [7] and the Boltzmann transport theory. We found a significantly larger orbital than spin effect, with a strong dependence on the model parameters, such as effective mass and spin-orbit coupling per layer. This dependence allows us to enhance and even revert the sign of the orbital effect.

[1] T. Yoda *et al.*, Sci. Rep., **5**, 12024 (2015).
[2] D. Go *et al.*, Sci. Rep. **7**, 46742 (2017)
[3] T. Yoda *et al.*, Nano Lett., **18**, 916 (2018).
[4] L. Salemi *et al.*, Nat. Commun. **10**, 5381 (2019)
[5] D. Hara *et al.*, Phys. Rev. B, **102**, 184404 (2020).
[6] A. Johansson *et al.*, Phys. Rev. Research, **3**, 013275 (2021).
[7] T. Thonhauser *et al.* Phys. Rev Lett. **95**, 137205 (2005).

TT 7.10 Mon 11:45 HSZ 403

Optical detection of the orbital Hall effect in a light metal Ti — •Young-Gwan Choi[1,2], Daegeun Jo[3], Kyung-Hun Ko[1], Dongwook Go[4,5], Kyung-Han Kim[3], Hee Gyum Park[6], Changyoung Kim[7,8], Byoung-Chul Min[6], Uri Vool[2], Gyung-Min Choi[1,9], and Hyun-Woo Lee[3,10] — [1]DOES, SKKU, Suwon, Korea — [2]MPI-CPfS, Dresden, Germany — [3]Physics, POSTECH, Pohang, Korea — [4]PGI and IAS, FZJ and JARA, Julich, Germany — [5]GSE Mainz, Mainz, Germany — [6]Center for Spintronics, KIST, Seoul, Korea — [7]Physics, SNU, Seoul, Korea — [8]CCES, IBS, Seoul, Korea — [9]CINAP, IBS, Suwon, Korea — [10]APCTP, Pohang, Korea

Electrical generation of the angular momentum current enables the development of novel memory devices, similar to spin current generation. Recently, it has been theoretically proposed that the orbital angular momentum (OAM) current can be driven by a charge current, called as the orbital Hall effect (OHE). Here we report evidence of the OHE, measured by magneto-optical Kerr effect microscopy. We detect large Kerr signals in one of the 3d transition metals, Ti, in which the high orbital Hall conductivity is predicted. We also find that the large OAM is accumulated by the OHE with a relaxation length ~70 nm. Moreover, we present the torque results in Ti/Ni. The high torque efficiency shows that the OAM injection allows for the electrical control of the magnetization. We also propose magnetic imaging using a nitrogen-vacancy scanning probe to measure OAM accumulation directly. Our results can pave the way for a deep understanding and provide techniques for generating and detecting orbital transport.

TT 7.11 Mon 12:00 HSZ 403

Spin and orbital Edelstein effects at oxide interfaces — •Annika Johansson[1], Börge Göbel[2], Sara Varotto[3], Srijani Mallik[3], Ingrid Mertig[2], and Manuel Bibes[3] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany — [3]Unité Mixte de Physique, CNRS, Thales, Université Paris-Saclay, Palaiseau, France

The spin Edelstein effect (SEE) provides charge-spin interconversion in nonmagnetic systems with broken inversion symmetry [1,2]: An external electric field generates a charge current as well as a homogeneous spin density. Further, a finite current-induced magnetization originating from the electrons' orbital moments can be generated, which is called orbital Edelstein effect (OEE) [3-5]. In this talk, the SEE and OEE at $SrTiO_3$- and $KTaO_3$-based two-dimensional electron gases are discussed within a semiclassical Boltzmann approach [6-8]. The OEE is predicted to exceed its spin counterpart by one order of magnitude, which can be understood by a band-resolved analysis of the SEE and OEE. Further, we suggest design rules for Rashba-like systems to enhance spin-charge interconversion efficiencies.

[1] A. G. Aronov, Y. B. Lyanda-Geller, JETP Lett. **50**, 431 (1989) [2] V. M. Edelstein, Solid State Commun. **73**, 233 (1990) [3] T. Yoda *et al.*, Sci. Rep. **5**, 12024 (2015). [4] T. Yoda *et al.*, Nano Lett. **18**, 916 (2018). [5] L. Salemi *et al.*, Nat. Commun. **10**, 5381 (2019) [6] D. Vaz *et al.*, Nat. Materials **18**, 1187 (2019) [7] A. Johansson *et al.*, Phys. Rev. Research **3**, 013275 (2021) [8] S. Varotto *et al.*, Nat. Commun. **13**, 6165 (2022)

TT 7.12 Mon 12:15 HSZ 403

Anisotropic anomalous Hall effect in altermagnetic Mn_5Si_3 — •Miina Leiviskä[1], Rafael Lopes Seeger[1], Helena Reichlová[2,3], Ismaïla Kounta[4], Libor Šmejkal[5,3], Javier Rial[1], Sebastian Beckert[2], Antonín Badura[6,7], Isabelle Joumard[1], Dominik Kriegner[2,3], Eva Schmoranzerová[6], Jairo Sinova[5], Tomáš Jungwirth[3], Sebastian Goennenwein[7], Lisa Michez[4], and Vincent Baltz[1] — [1]Univ. Grenoble Alpes, CNRS, CEA, Grenoble INP, IRIG-SPINTEC, F-38000 Grenoble — [2]Institute of Solid State and Materials Physics, TU Dresden, Dresden, Germany —

[3]Institute of Physics, Czech Academy of Sciences, Prague, Czechia — [4]Aix-Marseille University, CNRS, CINaM, Marseille, France — [5]Institute for Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [6]Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University, Prague, Czechia — [7]Department of Physics, University of Konstanz, Konstanz, Germany

The altermagnetic epitaxial films of Mn_5Si_3 exhibit anomalous Hall effect (AHE) despite the vanishing net magnetization [1]. This can be explained by non-relativistic time-reversal symmetry breaking, which allows for momentum-locked alternating spin-splitting of the bands [2]. Here, we investigate the anisotropy of the AHE by varying both the external field and the current channel orientations. In both cases, we observe unconventional, anisotropic behaviour that deviates from the typical behaviour of ferromagnets.

[1] H. Reichlova et al. arXiv:2012.15651, (2020)
[2] L. Šmejkal et al. Phys Rev X 12, 031042 (2022)

TT 7.13 Mon 12:30 HSZ 403

Observation of nonreciprocal magnon Hanle effect — •Janine Gückelhorn[1,2], Sebastián de-la-Peña[3], Matthias Grammer[1,2], Monika Scheufele[1,2], Matthias Opel[1], Stephan Geprägs[1], Juan Carlos Cuevas[3], Rudolf Gross[1,2,4], Hans Huebl[1,2,4], Akashdeep Kamra[3], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]Physik-Department, School of Natural Sciences, TUM, Garching, Germany — [3]IFIMAC and Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain — [4]Munich Center for Quantum Science and Technology, München, Germany

The realization of the magnon Hanle effect, which is based on the precession of magnon pseudospin about the equilibrium pseudofield, via electrically injected and detected spin transport in an antiferromagnetic insulator demonstrates its high potential for devices and as a convenient probe for the underlying spin interactions in antiferromagnets. Here, we observe a nonreciprocity in the magnon Hanle signal measured in hematite (α-Fe_2O_3) using two spatially separated platinum electrodes as spin injector/detector [1]. Interchanging their roles was found to alter the detected magnon spin signal. The recorded difference depends on the applied magnetic field and reverses sign when the signal passes its nominal maximum at the so-called compensation field. We explain these observations in terms of a spin transport direction-dependent pseudofield. The latter leads to a nonreciprocity, which is found to be controllable via the applied magnetic field.

[1] J. Gückelhorn *et al.*, arXiv:2209.09040 (2022).

TT 7.14 Mon 12:45 HSZ 403

Spontaneous anomalous Hall effect arising from an unconventional compensated magnetic phase in a semiconductor — •Dominik Kriegner[1,2], Ruben Dario Gonzalez Betancourt[1,2,3,4], Jan Zubáč[1,3], Rafael Julian Gonzalez Hernandez[5], Kevin Geishendorf[4], Gunther Springholz[6], Kamil Olejník[1], Jakub Železný[1], Libor Šmejkal[7], Andy Thomas[2,4], Helena Reichlová[1,2], Sebastian Tobias Benedikt Goennenwein[8], and Tomas Jungwirth[1,9] — [1]Institute of Physics, AV ČR, Prague, Czech Republic — [2]IFMP, TU Dresden — [3]Charles University, Prague — [4]IFW Dresden — [5]Universidad del Norte, Barranquilla, Colombia — [6]JKU Linz, Austria — [7]JGU, Mainz — [8]University of Konstanz — [9]University of Nottingham, United Kingdom

The anomalous Hall effect, commonly observed in metallic magnets, has been established to originate from the time-reversal symmetry breaking by an internal macroscopic magnetization in ferromagnets or by a non-collinear magnetic order. Here we observe a spontaneous anomalous Hall signal in the absence of an external magnetic field in an epitaxial film of MnTe, which is a semiconductor with a collinear antiparallel magnetic ordering of Mn moments and a vanishing net magnetization. The anomalous Hall effect arises from an unconventional phase with strong time-reversal symmetry breaking and alternating spin polarization in real-space crystal structure and momentum-space electronic structure.

R. D. Gonzalez Betancourt et al., arXiv:2112.06805

TT 8: Yu-Shiba-Rusinov Systems

Time: Monday 15:00–17:15 Location: HSZ 103

Invited Talk TT 8.1 Mon 15:00 HSZ 103

Molecules on a superconductor: Inducing magnetism and resonance-enhanced vibrational spectroscopy — •Richard Berndt[1], Jan Homberg[1], Alexander Weismann[1], Manuel Gruber[2], and Troels Markussen[3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen, Germany — [3]Synopsys Denmark, Copenhagen, Denmark

Magnetic impurities can induce so-called Yu-Shiba-Rusinov (YSR) resonances in the energy gap of a superconductor. We use these resonances for spin detection in a scanning tunneling microscope and demonstrate that diamagnetic phthalocyanine molecules acquire a spin when they are arranged into supramolecular arrays on superconducting Pb(100). Spectroscopy and modeling reveal that the electrostatic fields of its neighbors render a molecule paramagnetic.

Inelastic tunneling spectroscopy of vibrational excitations usually suffers from low sensitivity and limited spectral resolution. We harness YSR resonances to enhance the inelastic signal by more than an order of magnitude and to improve the energy resolution beyond the thermal broadening limit. As a result, 46 vibrational peaks are resolved from Pb-phthalocyanine enabling a comparison with calculated modes. The method may help to further probe the interaction of molecules with their environment and to better understand selection rules for vibrational excitations.

TT 8.2 Mon 15:30 HSZ 103

Yu-Shiba-Rusinov impurity bound states in superconductors from first principles — •David Antognini Silva[1], Philipp Rüssmann[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Würzburg Universität, Germany

Materials that combine magnetism, spin-orbit interaction and conventional s-wave superconductivity are a suitable platform to study Majorana zero modes (MZM) [1], that can be used as building blocks of fault-tolerant topological qubits. In general, magnetic impurities in superconductors leads to localized Yu-Shiba-Rusinov (YSR) states at the impurity [2]. Understanding their interplay with MZMs is crucial to achieve topological quantum computers in the future.

In our work, we implemented the Bogoliubov-de Gennes (BdG) formalism in the juKKR Korringa-Kohn-Rostoker Green function impurity code (https://iffgit.fz-juelich.de/kkr/jukkr) to allow the material-specific description of defects perfectly embedded in superconductors from first principles. We apply it to an Fe impurity embedded in bulk Pb in the normal and superconducting state, then analyse the YSR states of different magnetic transition-metal adatoms placed on a superconducting Nb(110) surface where the influence of the impurity-substrate distance on the energy of the YSR states is discussed.

[1] Nadj-Perge *et al.*, Science **346**, 6209 (2014)
[2] L. Yu, Acta Physica Sinica **21**, 75 (1965)
H. Shiba, Prog. Theor. Phys. **40**, 435 (1968) A. I. Rusinov, Sov. J. Exp. Theor. Phys. **29**, 1101 (1969)

TT 8.3 Mon 15:45 HSZ 103

Yu-Shiba-Rusinov states of quantum impurities in spin-split superconductors — •Anastasiia Skurativska[1], Jon Ortuzar[2], Sebastian Bergeret[1,3], Dario Bercioux[1,4], and Miguel Angel Cazalilla[1,4] — [1]DIPC, 20018 San Sebastian, Spain — [2]CIC nanoGUNE-BRTA, 20018 San Sebastian, Spain — [3]CFM-MPC Centro Mixto CSIC-UPV/EHU, 20018 San Sebastian, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain

Yu-Shiba-Rusinov (YSR) states arise as a sub-gap excitations in a system of magnetic impurity coupled to a superconducting host. Despite the quantum nature of their spin degree of freedom, magnetic impurities in such systems are often described by a classical spin. Taking into account quantum nature of the impurity-spin has proven to give useful insights into the ground-state and excitation properties of the magnetic impurity-superconductor system.

Here, we report on the spectral properties of the YSR states of a magnetic impurity on a spin-split superconductor. Using the zero-bandwidth approximation we obtain the spectral function of the YSR states. Unlike the classical model which predicts full spin polarization for the YSR peaks, we find the quantum model predicts partial polarization. The parity-changing phase transition switches the spin polarization of the YSR peaks after crossing at the center of the superconducting gap. We discuss the possibility of using this effect as a tunable spin-filter in a quantum dot or a molecule in proximity to a spin-split superconductor.

TT 8.4 Mon 16:00 HSZ 103

Building crystalline topological superconductors from Shiba lattices — •Martina Ondina Soldini[1], Felix Küster[2], Glenn Wagner[1], Souvik Das[2], Amal Aldarawsheh[3,5], Ronny Thomale[4,6], Samir Lounis[3,5], Stuart S. P. Parkin[2], Paolo Sessi[2], and Titus Neupert[1] — [1]University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, Jülich, Germany — [4]Institut fur Theoretische Physik und Astrophysik, Universitat Wurzburg, Wurzburg, Germany — [5]Faculty of Physics, University of Duisburg-Essen and CENIDE, Duisburg, Germany — [6]Department of Physics and Quantum Centers in Diamond and Emerging Materials (QuCenDiEM) Group, Indian Institute of Technology Madras, Chennai, India

Majorana boundary modes are the key feature of topological superconductors. Lattices of Shiba bound states, arising from magnetic adatoms placed on the surface of a conventional superconductor, may host these topological excitations. With scanning tunneling microscopy we create and probe adatom lattices to create topological crystalline superconductors. We combine theoretical modeling and experimental analysis to reveal signatures consistent with mirror-symmetry protected topological superconductors, hosting edge and higher-order corner states. Our results show the immense versatility of Shiba lattices to design the topology of 2D superconductors.

TT 8.5 Mon 16:15 HSZ 103

Mn clusters on superconducting Ta(110) surface — •András Lászlóffy[1], Bendegúz Nyári[2,3], László Szunyogh[2], and Balázs Újfalussy[1] — [1]Wigner Research Centre for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]ELKH-BME Condensed Matter Physics Research Group, Hungary

Over the past decade, the formation of Yu-Shiba-Rusinov (YSR) states around magnetic impurities proximity coupled to superconducting materials raised considerable interest. The hybridization between these states leads to bands in magnetic chains being potential candidates for hosting Majorana edge states. In this work we solve the Bogoliubov-de Gennes equation as implemented in the first-principles Korringa-Kohn-Rostoker Green's function method. First, we provide an in-depth analysis of the YSR states of a single Mn adatom on Ta(110), and the hybridization between them in Mn dimers. We then study the formation of a minigap and zero energy states in chains with various directions and nearest-neighbor distances, making a strong implication that Majorana zero modes can emerge in these systems.

TT 8.6 Mon 16:30 HSZ 103

Effect of Fe impurities on the superconducting state of Ir/Nb overlayer — •Bendegúz Nyári[1,2], András Lászlóffy[3], Krisztián Palotás[3], László Szunyogh[1,2], Levente Rózsa[4], and Balázs Újfalussy[3] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Hungary — [2]ELKH-BME Condensed Matter Physics Research Group, Hungary — [3]Wigner Research Centre for Physics, Institute for Solid State Physics and Optics, Hungary — [4]Department of Physics, University of Konstanz, Germany

Artificial magnetic chains on top of superconducting surfaces, where in the presence of large spin-orbit coupling or non-collinear magnetic states a topological gap can appear, are potential candidates to host Majorana edge states. Iridium as an overlayer on various metallic substrates appeared to be a good platform for the formation of spin-spiral states in magnetic overlayers and chains.

By solving the relativistic Bogoliubov–de Gennes equations, first we investigate the superconducting properties of 10 monolayers of Ir on top of Nb(110) surface. In the Ir layer we observe a strong reduction of the superconducting order parameter, but the gap just slightly decreases as compared to bulk Nb. Then the effect of Fe impurities on the superconducting state is studied in different setups. For a single Fe impurity we find a huge spatial extension of the Yu–Shiba–Rusinov states. Disordered Fe impurities modelled within the coherent-potential approximation in the dilute concentration limit seem to rapidly destroy the superconducting state of the Ir overlayer.

TT 8.7 Mon 16:45 HSZ 103

Yu-Shiba-Rusinov states in small Fe clusters on Pb(111) — •Nora Kucska, Krisztián Palotás, Andras Laszloffy, and Balazs Ujfalussy — Wigner Research Centre for Physics, Budapest, Hungary

By solving the fully relativistic Bogoliubov-de Gennes equations by band-theoretical methods, we investigate the Yu-Shiba-Rusinov (YSR) states of single, double and triple magnetic Fe adatoms on the top of Pb(111) surface. First, we show that the local density of states in the normal state plays a key role in the formation of the YSR states that appear in the interior of the superconducting gap. We discuss the effects of different atomic arrangements, the role of lattice relaxations and various spin configurations on the YSR states, and we compare our results to recent experiments.

TT 8.8 Mon 17:00 HSZ 103

Yu-Shiba-Rusinov band dispersion of an infinite chain on a semi-infinite surface — •Rik Broekhoven, Artem Pulkin, Antonio Manesco, Sander Otte, Anton Ahkmerov, and Michael Wimmer — Delft University of Technology, Delft, the Netherlands

Chains of magnetic atoms on s-wave superconductors have been proposed to become topological superconductors, when their in-gap Yu-Shiba-Rusinov (YSR) band is p-wave gapped by for example spin-orbit coupling. As recently shown through STM experiment, however, realistic systems have many YSR bands and relatively small spin-orbit coupling limiting the topological phase. Ab initio models can help to increase our understanding and find regions of material and parameter space where the system is still predicted to be topological. These finite-size simulations must however overestimate the superconducting gap to ensure the system is smaller than the superconductor coherence length.

We combine ab initio calculation with multi-dimensional Green's functions formalism to extend the model beyond this limit. This allows us to do calculations with realistic gap size. We compute the dispersion of an infinite chain on top of a semi-infinite surface. We focus on Mn atoms on Nb(110) and show how our model compares with the dispersion measured by Schneider et al. in 2021.

TT 9: f-Electron Systems and Heavy Fermions II

Time: Monday 15:00–17:00 Location: HSZ 201

TT 9.1 Mon 15:00 HSZ 201

Quantum oscillations in heavy-fermion ferromagnet $YbNi_4P_2$ over many Zeeman induced Lifshitz transitions — •William Broad[1], Sven Friedemann[1], Owen Moulding[1], Takaki Muramatsu[1], Kristin Kliemt[2], and Cornelius Krellner[2] — [1]University of Bristol, Bristol, United Kingdom — [2]Goethe-Universität, Frankfurt am Main, Germany

$YbNi_4P_2$ is a heavy-fermion metal situated near a very rare ferromagnetic quantum critical point (FM QCP). Understanding the nature of this ferromagnetism requires knowledge of the Fermi surface; it has been speculated that this FM QCP is enabled by a quasi-1D Fermi surface. At the same time, the strongly renormalised band structure is readily modified by relatively small magnetic fields, with nine Lifshitz transitions below 20 T due to Zeeman splitting. Here, we present Shubnikov–de Haas oscillations up to 35T, including detailed rotation and mass studies. We present analysis over several of these Lifshitz transitions, observing frequency changes and appearances/disappearances. We model the band structure with DFT calculations of the local 4f reference compound $LuNi_4P_2$ and use rigid-band shifts to approximate the effect of the Kondo hybridisation. At highest fields, the Fermi surface is well modelled with a small shift to increase the Fermi volume. As the field is reduced, we find better agreement with a larger shift corresponding to stronger hybridisation of 4f electrons. Finally, we present models for the topology of the Lifshitz transitions.

TT 9.2 Mon 15:15 HSZ 201

Exploring the effect of different substitutions on the valence transition in $YbInCu_4$ single crystals — •Michelle Ocker, Bereket Ghebretinsae, Bernd Wolf, Kristin Kliemt, Michael Lang, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

At ambient pressure the compound $YbInCu_4$ undergoes a 1^{st} order valence transition at T_v = 42 K by changing the temperature [1]. Thus, ytterbium in the compound is present in the $Yb^{2.9+}$ state at high temperatures and as $Yb^{2.7+}$ at low temperatures [2]. In analogy to Eu compounds, the line of first order valence transitions might end in a second order critical endpoint [3]. In order to study the nature of the phase transition in more detail, single crystal samples can be prepared in In-Cu flux which are substituted with silver and gold [4]. With increasing substitution level, negative chemical pressure within the crystal is increased and the characteristics of the valence transition changes significantly. Here, we report on the single crystal growth with different substitution levels and the results of our structural, chemical and physical characterization.

[1] I. Felner et al., Phys. Rev. B 35, (1987) 6956
[2] H. Sato et al., Physica B 351, (2004) 298
[3] Y. Ōnuki et al., J. Phys. Soc. Jap. 89, (2020) 102001
[4] J. L. Sarrao et al., Phys. Rev. B 54, (1996) 12207.

TT 9.3 Mon 15:30 HSZ 201

Impact of Fe substitution on the electronic structure of URu_2Si_2 — •Andrea Marino[1], Denise S. Christovam[1], Chun-Fu Chang[1], Johannes Falke[1], Chang-Yang Kuo[2], Chi-Nan Wu[2], Martin Sundermann[1,3], Andrea Amorese[1,3], Hlynur Gretarsson[4,5], Camilla Moir[6], M. Brian Maple[6], Peter Thalmeier[1], Liu Hao Tjeng[1], and Andrea Severing[3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]University of Cologne, Cologne, Germany — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany — [5]PETRA III, DESY, Hamburg, Germany — [6]University of California, San Diego, USA

The application of pressure as well as the substitution of Ru with Fe in the hidden order (HO) compound URu_2Si_2 lead to the formation of the large moment antiferromagnetic phase (LMAFM), with the respective phase diagrams bearing similarities for low Fe content (<0.3). For higher Fe content (>1) $URu_{(2-x)}Fe_{(x)}Si_2$ adopts the Pauli paramagnetic ground state of UFe_2Si_2. However, the question remains open what causes the suppression of HO in favour of the LMAFM phase. We investigate the $URu_{(2-x)}Fe_{(x)}Si_2$ series with $4f$ core-level photoelectron spectroscopy. The $4f$ satellite features are enhanced at low Fe content (x<0.4) and suppressed as x increases, following the trend shown by the ordered moment. We discuss this in terms of the variation of the filling of the $5f$ shell. Implications for the exchange interaction in a Doniach phase diagram picture are then also considered.

TT 9.4 Mon 15:45 HSZ 201

High-resolution tender x-ray RIXS at the example of UGa_2 — •Martin Sundermann[1,2], Andrea Marino[1], Denise Christovam[1], Andrea Amorese[1,3], Ladislav Havela[4], Bernhard Keimer[5], Hlynur Gretarsson[1,2,5], Peter Thalmeier[1], Liu Hao Tjeng[1], and Andrea Severing[1,3] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]Condensed Matter Physics, Karls-Universität, Prag, Czech — [5]MPI-FKF, Stuttgart, Germany

The nature of the $5f$ electrons in U intermetallic compounds, usually thought to be on the verge between localization and itinerant states, still challenges the reach of well-established condensed matter physics' techniques. Yet, it is not uncommon that U-based compounds show no inelastic neutron scattering excitations, and the question remains, if these compounds are fully delocalized or if multiplet states are present but not observable. Cutting-edge instrumental developments enables us to perform tender x-ray high-resolution (150 meV) resonant inelastic X-ray scattering (RIXS) experiments at the strong U $M_{4,5}$ absorption edges. We demonstrate the potential of this technique at the example of the intermetallic high T_C ferromagnet UGa_2. We observe mutliplet excitations that are well reproduced with a full multiplet calculation that includes the crystal-electron field splitting and is based on an U $5f^2$ configuration. Further we show that, although crystal-field splittings are too small to be resolved, the directional dependence of the scattering cross-section gives access to the ground-state symmetry.

TT 9.5 Mon 16:00 HSZ 201

Electronic structure of UO_2 studied by high-resolution tender-x-ray RIXS — •Denise S. Christovam[1], Martin Sundermann[1,2], Andrea Marino[1], Daisuke Takegami[1], Andrea Amorese[1,3], Hlynur Gretarsson[2,4], Bernhard Keimer[4], Philipp Raison[5], Robertro Caciuffo[5], Andrea Severing[1,3], and Liu Hao Tjeng[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Institute of Physics II, University of Cologne, Germany — [4]MPI-FKF, Stuttgart, Germany — [5]Joint Research Centre, Euorpean Commission, Karlsruhe, Germany

The investigation of the $5f$ electronic states in uranium-based compounds is a great challenge for x-ray instrumentation. Recent instrumental developments in the tender x-ray regime enable us to carry out resonant inelastic x-ray scattering (RIXS) experiments at the strong U $M_{4,5}$ absorption edge with an experimental resolution of 150 meV. In this work, we studied the electronic structure of UO_2. We observe the excitations the U^{4+} $5f^2$ ionic multiplet states as well as the excitations involving the O $2p$ to U $5f$ charge transfer satellites. Detailed insight in the many-body nature of the ground state and excited states of UO_2 is obtained by analysing the data with full-multiplet cluster calculations which also take into account crystal field and hybridization effects.

TT 9.6 Mon 16:15 HSZ 201

Strain-tuning of charge frustration in the heavy $3d$ fermion oxide LiV_2O_4 — •Ryosuke Oka[1,2], Dennis Huang[1], Minu Kim[1], Peter Wochner[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Physics, University of Tokyo, Tokyo, Japan — [3]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany

The mixed-valent spinel LiV_2O_4 is the first discovered $3d$ electron system showing heavy fermion behavior without localized f moments, but its origin has remained a decades-old mystery. Amongst numerous scenarios proposed so far, including an analogy with a dense Kondo system, one of the leading scenarios is charge frustration inherent in the pyrochlore sublattice of the spinel. In this scenario, the ground state is composed of a macroscopic number of degenerate charge orderings (COs), and the frustration prevents the system from undergoing a metal-to-insulator transition, thereby enhancing the effective mass. By applying external perturbations that lift the degeneracy in different ways, various insulating COs can be selected out of the frustrated metallic ground state. For example, hydrostatic pressure and biaxial tensile strain in the (001) plane stabilize distinct [111]- and [001]-oriented COs, respectively. We have grown LiV_2O_4 thin films on various substrates, in order to apply uniaxial strain in different directions. We used synchrotron x-ray diffraction to characterize the applied strain and transport measurements to probe how the heavy fermion phase in LiV_2O_4 moves toward possible distinct charge-ordered states.

TT 9.7 Mon 16:30 HSZ 201

Evolution of the 4*f* states in $TmSe_{1-x}Te_x$ from semimetals to semiconductors — •Chul Hee Min[1], Simon Müller[2], Michael Heber[3], Lenart Dudy[4], Hendrik Bentmann[3], Matthias Kallåne[1], Markus Scholz[3], Woojae Choi[5], Yong Seung Kwon[5], Friedrich Reinert[2], and Kai Rossnagel[1,3] — [1]IEAP, CAU Kiel, Germany — [2]EP7 and ct.qmat, University of Würzburg, Germany — [3]DESY, Hamburg, Germany — [4]Synchrotron SOLEIL, Saint-Aubin, France — [5]Dep. of EMS, DGIST, South Korea

Localized $4f$ states are often considered to become coherent states at low temperatures by hybridizing with itinerant conduction $5d$ states. In the standard Anderson model, only one type of interaction between the two states is taken into account, which is sufficient to describe Kondo physics. However, additional interaction has been suggested for the mixed valence regime to satisfy the Friedel sum rule when two charge states exist on a short time scale [1]. Here we present photoemission results of mixed-valent Thulium monochalcogenide $TmSe_{1-x}Te_x$. This system allows us to study the evolution of the localized $4f$ states between semimetallic and semiconducting phases without applying external pressure and disturbing the periodicity of Tm ions. Our results show two different interactions between $4f$ and $5d$ states across the phase transition.

[1] F. Haldane, Phys. Rev. B 15, 2477 (1976)
C. Varma, Phys. Rev. B 102, 155145 (2022)

TT 9.8 Mon 16:45 HSZ 201

Orbital-selective Mott transition and heavy-fermion physics in the van der Waals ferromagnet $Fe_{3-x}GeTe_2$ — •Frank Lechermann[1], Xiaojian Bai[2], Yaohua Liu[2], Yongqiang Cheng[2], Alexander I. Kolesnikov[2], Feng Ye[2], Travis J. Williams[2], Songxue Chi[2], Tao Hong[2], Garrett E. Granroth[2], Andrew F. May[3], and Stuart Calder[2] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA — [3]Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The van der Waals ferromagnet $Fe_{3-x}GeTe_2$ is a fascinating material that attracts combined strong interest from magnetoelectronics as well as from strong correlation physics. While near room temperature, the possibilities to exfoliate conducting ferromagnetic layers is investigated, at temperatures below $T \sim 100$ K the system displays surprising signatures of heavy-fermion physics. By means of first-principles many-body calculations, we here show that the latter temperature regime is governed by a rare orbital-selective Mott phase. This leads to emergent Kondo(-lattice) behavior in an unique transition-metal $3d$ compound, accompanied by antiferromagnetic fluctuations within the ferromagnetic phase. These fluctuations are experimentally revealed by neutron scattering.

TT 10: Correlated Electrons: Other Materials

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

TT 10.1 Mon 15:00 HSZ 204

Towards a complete quantum oscillatory assessment of the Fermi surface of CoSi — •Nico Huber[1], Simon Röder[1], Georg Benka[1], Andreas Bauer[1], Sanu Mishra[2,3], Ilya Sheikin[2], Christian Pfleiderer[1], and Marc A. Wilde[1] — [1]Physik-Department, TU Munich, D-85748 Garching, Germany — [2]LNCMI-CNRS, Grenoble, France — [3]Los Alamos National Laboratory, Los Alamos, USA

The B20 compound CoSi has recently attracted great interest due to its electronic structure hosting multifold fermions at the Γ- and R-point [1] and topologically non-trivial nodal planes on the Brillouin zone boundary [2,3]. While quantum oscillations (QOs) arising from the Fermi surface (FS) around the R-point have been studied in great detail and are well understood [3,4], only limited information has been presented on QOs related to the FS around the Γ-point [5]. Here, we report the experimental identification of previously unobserved QOs arising from heavy FS sheets around Γ in the Shubnikov-de Haas and de Haas-van Alphen spectra of CoSi. The oscillation frequencies, their angular dispersion, and the associated effective masses are in good agreement with first principle calculations. Our observations confirm the calculated bandstructure of CoSi, thus completing the experimental verification of the Fermi surface based on quantum oscillations.

[1] Rao *et al.*, Nature **567**, 496 (2019)
Sanchez *et al.*, Nature **567**, 500 (2019)
[2] Wilde *et al.*, Nature **594**, 374 (2021)
[3] Huber *et al.*, PRL **129**, 026401 (2022)
[4] Guo *et al.*, Nat. Phys. **18**, 813 (2022)
[5] Wang *et al.*, PRB **102**, 115129 (2020)
Sasmal *et al.*, J. Phys.: Condens. Matter **34**, 425702 (2022)

TT 10.2 Mon 15:15 HSZ 204

Miniaturized setup for quantum oscillatory studies under temperature modulation — •Michelle Hollricher, Christian Pfleiderer, and Marc A. Wilde — Physik-Department, Technical University of Munich, D-85748 Garching, Germany

Measurements of the magnetization and its derivatives provide fundamental insights into the magnetic properties of metals. In particular this is true for magnetic quantum oscillations. We report the development of a miniaturized setup for direct measurements of the temperature derivative of the magnetization as a function of magnetic field and temperature, using a modular setup comprising AC heating with inductive signal pick-up. The dimensions of our setup have been optimized to permit use in combination with standard mechanical rotators, this way enabling measurements of the magnetization as a function of magnetic field orientation down to ultra-low temperatures. Following thorough characterization of the frequency response of our miniaturized setup, we revisited the de Haas-van Alphen effect in bismuth, focusing on the electronic structure of the electron pockets.

TT 10.3 Mon 15:30 HSZ 204

Torque magnetometry of FeSi at low temperatures — •Carolina Burger, Vivek Kumar, Andreas Bauer, and Christian Pfleiderer — Physik-Departement, Technical University of Munich, D-85748 Garching, Germany

We report a study of the torque magnetization of the correlated small-band-gap semiconductor FeSi in the regime of the saturation of the resistivity at temperatures below a few Kelvin. The magnetic field dependence of the electrical transport properties provides strong circumstantial evidence of a high-mobility surface conduction channel, that is insensitive to the additional presence of an impurity band in the bulk [1, 2]. The surface conduction channel shares great similarities with properties reported for topological insulators, but displays a striking lack of sensitivity to the presence of ferromagnetic impurities as studied by means of a series of single crystals with slightly different starting compositions. We discuss the torque magnetization observed in FeSi with respect to key characteristics observed in the field-polarized state of isostructural magnetic B20 compounds such as MnSi or $Fe_{1-x}Co_xSi$.

[1] Y. Fang, et al., Proc. Natl. Acad. Sci. 115, 8558 (2018)
[2] B. Yang, et al., Proc. Natl. Acad. Sci. 118, e2021203118 (2021)

TT 10.4 Mon 15:45 HSZ 204

Metal-insulator transition and onset of magnetic order in $Fe_{1-x}Co_xSi$ — •Julius Grefe[1], Philipp Herre[1], Yannis Hilgers[1], Felix Labbus[1], Nina Lüer[1], Mauricio de Melo[1,2], Jochen Litterst[1], Stefan Süllow[1], and Dirk Menzel[1] — [1]Inst. für Physik der Kondensierten Materie, Technische Universität Braunschweig, Germany — [2]Departamento de Fisica, Universidade Estadual de Maringá, Brazil

The B20 transition metal silicides (Fe,Co,Mn)Si have been under investigation for many decades. Although the general observations regarding the electronic and magnetic properties are similar, various details of the phase diagram of $Fe_{1-x}Co_xSi$ are not yet well-established. We have prepared a series of $Fe_{1-x}Co_xSi$ single crystals and investigated the metal-insulator transition as well as the onset of magnetic order in the low Co percentage range by means of transport and susceptibility measurements. In addition, we present for the first time single-crystal Mössbauer spectroscopy experiments in order to complement our study using a microscopic probe. Our investigation sheds light on the physics of quantum criticality and metal-insulator transition and their interplay in the regime of small Co concentrations.

TT 10.5 Mon 16:00 HSZ 204

Temperatur dependence of the lattice constants of $Mn_{1-x}Fe_xSi$ and $Mn_{1-x}Co_xSi$ — •Tobias Konrad, Alexander Engelhardt, Christoph Resch, Andreas Bauer, and Christian Pfleiderer — Physik Department, Technical University Munich, D-85748 Garching, Germany

When magnetic order in the chiral magnet MnSi is suppressed under hydrostatic pressure, topological non-Fermi-liquid behavior emerges, where neutron Larmor diffraction of the lattice constants establishes the absence of quantum criticality [1-3]. Magnetic order in MnSi may also be suppressed by substitutional replacement of iron or cobalt on the manganese sites [4,5]. Using powder x-ray diffraction, we have studied the temperature dependence of the lattice constants of $Mn_{1-x}Fe_xSi$ ($0 \leq x \leq 0.22$) and $Mn_{1-x}Co_xSi$ ($0 \leq x \leq 0.04$) between room temperature and $\sim 12\,K$. The evolution of the lattice constants as a function of iron and cobalt concentration is discussed in comparison to changes of the lattice constants of MnSi under hydrostatic pressure.

[1] C. Pfleiderer et al., Nature **414**, 427 (2001)
[2] C. Pfleiderer et al., Science **316**, 1871 (2007)
[3] R. Ritz et al., Nature **497**, 231 (2013)
[4] A. Bauer et al., Phys. Rev. B **82**, 064404 (2010)
[5] J. Kindervater et al., Phys. Rev. B **101**, 104406 (2020)

TT 10.6 Mon 16:15 HSZ 204

Effect of anion substitution on the Mott insulating instability in the organic conductors κ-(BEDT-TTF)$_2$X studied by magnetic quantum oscillations — •Shamil Erkenov[1,2], Florian Kollmannsberger[1,2], Werner Biberacher[1], Ilya Sheikin[3], Toni Helm[4], Natalia Kushch[1], Rudolf Gross[1,2], and Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Laboratoire National des Champs Magnétiques Intenses, Grenoble, France — [4]Hochfeld-Magnetlabor Dresden, HZDR, Dresden, Germany

The layered organic charge-transfer salts κ-(BEDT-TTF)$_2$X have been extensively employed as model systems for studying the Mott metal-insulator transition. The insulating instability in these materials is very sensitive to external pressure and to minor chemical changes, e.g., variation of the insulating anion. The anion substitution is broadly believed to act similarly to pressure, leading to a modification of the correlation strength ratio U/t. However, recent first-principles band-structure calculations [1] suggest that anion substitution in κ salts influences the ground state chiefly through the spin-frustration effect by changing the transfer-integral anisotropy ratio t'/t rather than through U/t. Here we report on comparative studies of magnetic quantum oscillations in the salts with X = NCS, Cl, and Br, aiming at disentangling the roles of the electronic correlations and spin frustration in the insulating instability within this family.

[1] T. Koretsune and C. Hotta, Phys. Rev. B **89**, 045102 (2014).

15 min. break

TT 10.7 Mon 16:45 HSZ 204

Mott criticality in the deuterated variant of κ-(BEDT-TTF)$_2$ Cu[N(CN)$_2$]Br studied by thermal expansion under He-gas pressure — •Yassine Agarmani, Harald Schubert, Bernd Wolf, and Michael Lang — PI, GU Frankfurt, CRC/TRR288, DE

The understanding of the nature of the critical behavior at the Mott transition has recently been given a new twist by thermodynamic measurements on the Mott insulator κ-(ET)$_2$Cu[N(CN)$_2$]Cl (κ-Cl)]. While so far mainly electronic scenarios have been considered to describe the Mott transition, the observations of strong non-linearities in the strain-stress relation around the Mott critical endpoint in κ-Cl showed that the lattice degrees of freedomn play a crucial role [1]. This behavior has been found to be consistent with the proposed scenario of critical elasticity [2], which considers a non-perturbatively strong coupling of the elastic- to the electronic degrees of freedom, causing a softening of the lattice. These observations raise the question of the implication of critical elasticity for our understanding of the general phase diagram of the κ-(ET)$_2$X family. To address this question, we have chosen a system related to κ-Cl, namely the fully deuterated κ-(ET)$_2$Cu[N(CN)$_2$]Br, which is known to be near the Mott critical endpoint at ambient pressure. By using an extension [3] of the setup used in [1], which enables us to fine-tune the He-gas pressure while performing high-resolution measurements of length changes, we aim to compare our results with those on κ-Cl in terms of the extension of the range of critical elasticity.

[1] Gati et al., Sci. Adv. 2, e1601646 (2016)
[2] Zacharias et al., PRL 109, 176401 (2012)
[3] Agarmani et al., RSI 93, 113902 (2022)

TT 10.8 Mon 17:00 HSZ 204

Effect of uniaxial strain on the phononic and electronic excitations of Ta_2NiS_5 — •Mai Ye, Amir-Abbas Haghighirad, and Le Tacon Matthieu — Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany

Semiconductor Ta_2NiS_5 exhibits a structural transition from orthorhombic phase to monoclinic phase at 120 K, driven by acoustic instability [1]. Two Raman-active phonon modes, which have the same symmetry as the order parameter (B_{2g} symmetry), show continuous frequency softening on cooling from 300 K to 20 K. Moreover, a sharp exciton mode in the B_{2g} symmetry channel has been observed at 0.3 eV. We study the phonon modes and interband excitations of Ta_2NiS_5 under uniaxial strain at low temperature. With increasing tensive strain along crystallographic a axis, the frequency of the two B_{2g}-symmetry phonon modes and the band gap of this semiconductor both increase, with a 6.5% frequency increase of the lowest-energy B_{2g} phonon mode corresponding to a 4.1% increase of the gap size. On the contrary, the frequency change of the non-softening phonons is less than 1%. By analyzing the phonon intensity, we further find that the magnitude of the order parameter, and in turn the phase transition temperature, increases with the tensive strain. These experimental results demonstrate Ta_2NiS_5 as a suitable platform to explore the manipulation of lattice dynamics and electronic structure by applying uniaxial strain.

[1] Phys. Rev. B 104, 045102 (2021)

TT 10.9 Mon 17:15 HSZ 204

Magnetic anisotropy and low-energy spin dynamics in magnetic van der Waals compounds $Mn_2P_2S_6$ and $MnNiP_2S_6$ — •Joyal John Abraham[1,2], Yurii Senyk[1], Yuliia Shemerliuk[1], Sebastian Selter[1], Saicharan Aswartham[1], Bernd Büchner[1,3], Vladislav Kataev[1], and Alexey Alfonsov[1] — [1]Leibniz IFW Dresden, D-01069 — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01069 — [3]Institute for Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, D-01062

We report a comprehesive high-field electron spin resonance (ESR) study performed on single crystals of $Mn_2P_2S_6$ and $MnNiP_2S_6$ in the broad ranges of temperatures, frequencies and magnetic fields. Analysing the antiferromagnetic modes well below the ordering temperature T_N, we have found that the ground state, the order type and magnetic anisotropy (MA) change with increasing x in $(Mn_{1-x}Ni_x)_2P_2S_6$. In the case of $Mn_2P_2S_6$, an application of the linear spin wave theory enabled us to determine the anisotropy and exchange constants, important for a quantitative description of the ground state. A systematic increase of the g-factor and its anisotropy, measured at $T \gg T_N$, is observed with increasing Ni content, which, in turn, sheds light on the nature of MA in the ordered state. The investigation of the T-dependence of line shifts from the paramagnetic resonance position reveals already well above T_N the presence of the short range spin-spin correlations static on ESR time scale, which are more pronounced in $MnNiP_2S_6$.

TT 10.10 Mon 17:30 HSZ 204

Switching of magnetic anisotropy from out-of-plane to inplane in quasi-2D van der Waals $(Mn_{1-x}Ni_x)_2P_2S_6$ single crystals — •Yuliia Shemerliuk, Anja U. B. Wolter, Bernd Büchner, and Saicharan Aswartham — Institut für Festkörperforschung, Leibniz IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

In the recent years magnetic two-dimensional van der Waals materials are at the forefront of the research. Magnetism has been extensively investigated in the family of $TM_2P_2S_6$ (TM= Ni, Co, Fe, Mn & V). Transition metal TM substitution has been used as a technique to control magnetism in this family of compounds [1-3]. In this talk, we will present crystal growth by chemical vapor transport together with a thorough structural and magnetic characterization of the quasi-2D magnets $(Mn_{1-x}Ni_x)_2P_2S_6$ with x = 0, 0.3, 0.5, 0.7 & 1. As-grown crystals exhibit a layered morphology with weak van der Waals interlayer interactions parallel to the crystallographic ab plane of the monoclinic symmetry in the space group C2/m (No. 12). In this series, the two neighboring members $Mn_2P_2S_6$ and $Ni_2P_2S_6$ differ in magnetic atoms, magnetic easy axes, spin anisotropy, and nearest neighbor magnetic interactions. The magnetization measurements show an antiferromagnetic ground state for all grown crystals. The magnetic ordering temperature TN shows nonmonotonic behavior. The magnetic anisotropy switches from out-of-plane to in-plane as a function of composition.

TT 10.11 Mon 17:45 HSZ 204

Single crystal growth, structural and transport properties of the Mott insulator $BaCoS_2$ — •Haneen Abushammala, Teslin Thomas, Andreas Kreyssig, and Anna Böhmer — Institute for Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany.

The quasi-2D $BaCoS_2$ is a Mott insulator with a stripe-like antiferromagnetic ordering at T_N=290 K. Both chemical doping or hydrostatic pressure drive the system into a paramagnetic metallic phase. Interestingly, there is no structural transition at the metal-insulator transition of this phase, which offers ideal conditions to investigate the Mott transition in a model multiband system [1].

Nevertheless, $BaCoS_2$ remains little studied, and the interplay of electronic and structural features is still unclear. High-quality single crystals are needed to elucidate this issue. The synthesis of single-crystalline $BaCoS_2$ is challenging owing to its metastability, with a decomposition into Ba_2CoS_3, CoS and S below 850°C. The $BaCoS_2$ phase can only be obtained via quenching from high temperature. Moreover, $BaCoS_2$ melts incongruently, which calls for a flux growth method necessitating separation of the crystals from the flux by the end of the growth. We have successfully grown single crystals of pure and the hole-doped $BaCoS_2$ using a self-flux method with high-temperature flux separation and quench. The structural and anisotropic electrical transport properties are determined and discussed.

[1] H. Abushammala, B. Lenz, B. Baptiste, M. Casula, Y. Klein and A. Gauzzi, in preparation (2022).

TT 10.12 Mon 18:00 HSZ 204

Spin-orbit entangled crystal-field excitations in $5d^4$ $j = 0$ osmates — •Philipp Warzanowski[1], Marco Magnaterra[1], Philipp Stein[1], Quentin Faure[2], Christoph Sahle[2], Holger Schwab[1], Thomas Lorenz[1], Petra Becker[3], Ladislav Bohatý[3], Paul H. M. van Loosdrecht[1], and Markus Grüninger[1] — [1]Institute of Physics II, University of Cologne — [2]European Synchrotron Radiation Facility, Grenoble Cedex, France — [3]Sect. Crystallography, Institute of Geology and Mineralogy, University of Cologne

For strong spin-orbit coupling, the d^4 electron configuration may show a non-magnetic $j = 0$ ground state. In $5d^4$ iridates, magnetic behavior has been discussed controversially and finally it has been attributed to defects, while excitonic magnetism has been proposed for $4d^4$ ruthenates. We show that the $j = 0$ state is very well realized in the cubic antifluorite-type $5d^4$ osmates K_2OsCl_6 and K_2OsBr_6. The magnetic susceptibility exhibits van-Vleck type magnetism without a sizeable Curie-Weiss contribution. Employing resonant inelastic x-ray scattering (RIXS) and infrared spectroscopy as complementary techniques, we investigate the electronic excitations and determine the electronic parameters by comparison with local multiplet calculations. The cubic crystal-field splitting 10 Dq and the charge transfer energy are 15% smaller for the chlorine compound than for its bromide sister, whereas the intra-t_{2g} excitation energies are reduced by 4%. This allows us to quantify the influence of the e_g orbitals on the effective spin-orbit coupling for the t_{2g} orbitals.

TT 11: Spintronics, Spincalorics and Magnetotransport

Time: Monday 15:00–16:30 Location: HSZ 304

TT 11.1 Mon 15:00 HSZ 304

Van der Waals/non-van der Waals hybrids for superconducting spintronics — Roman Hartmann, Alfredo Spuri, Danilo Nikolic, Wolfgang Belzig, Elke Scheer, and •Angelo Di Bernardo — Universität Konstanz, Konstanz, Germany

The realization of Cooper pairs of electrons with parallel-aligned spins (i.e., spin-triplet pairs) has been demonstrated for a variety of three-dimensional (3D) superconductor/ferromagnet (S/F) heterostructures. Several studies have shown that using S/F system with a magnetically inhomogeneous F [1-2] it is possible to convertthe spin-singlet pairs of a conventional S into fully-polarized spin triplets - this has paved the way for superconducting spintronics. Van-der-Waals (vdW) heterostructures host a variety of unconventional phases, both superconducting and magnetic, which can be explored to realize two-dimensional (2D) superspintronic devices with novel functionalities and types of control compared to devices based on 3D S/F hybrids. The conversion of spin singlets into spin triplets across a 2D S/F vdW interface represents, however, the first step towards superconducting spintronics based on vdW hybrids. In this talk, I will show recent magnetotransport experiments obtained on F nanoflakes that are cleaved from 3D ionic F single crystals through a new approach. The unique properties of these nanoflakes are used for the fabrication of novel superspintronics devices, where the nanoflakes are coupled to conventional 2D vdW S materials.

[1] J. W. A. Robinson et al., Science 329, 59 (2010)
[2] A. Di Bernardo et al., Nat. Commun. 6, 8053 (2015)

TT 11.2 Mon 15:15 HSZ 304

Thermal transport in weakly coupled spin-$\frac{1}{2}$ Heisenberg ladders — •Anja Wenger, Christian Northe, and Ewelina Hankiewicz — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We investigate the weakly coupled spin-$\frac{1}{2}$ Heisenberg ladder in the low energy limit. As magnetic excitations significantly contribute to the thermal transport, we expose the ladder to a magnetic field and analyze the thermal conductivity and the specific heat capacity depending on the magnetization. Starting point is the spin-$\frac{1}{2}$ Heisenberg chain and its fermionic and bosonic description by conformal field theory. From coupling two spin chains and applying the (rescaled) bosonisation technique, a free theory for spin-ladders and its spectrum is obtained. Special interest lies on the conformal anomaly and the Tomonaga-Luttinger Liquid parameters. Introducing temperature to the theory gives access to the thermal transport properties.

TT 11.3 Mon 15:30 HSZ 304

Critical current control in ferromagnetic proximity junctions by magnetization and spin injection — •Lukas Kammermeier and Elke Scheer — Universität Konstanz, Konstanz, Germany

We exploit the inverse proximity effect of a ferromagnet on a superconductor to locally suppress the superconductivity in a thin wire and thereby create a Josephson junction.

We show that we can control the critical current I_c over a wider range by manipulating the magnetization state of the ferromagnet, possibly sensitive to single magnetic domains in proximity to the constriction. Additionally, the efficiency of spin injection by running a current from the spin-polarized ferromagnet into the junctions constriction will be presented.

TT 11.4 Mon 15:45 HSZ 304

On the connection between the chiral-induced spin selectivity effect and the chiro-optical activity: The case of an electron in a helix — •Solmar Varela[1], Gianaurelio Cuniberti[1], Rafael Gutierrez[1], Ernesto Medina[2], Vladimiro Mujica[3], and Jesus Ugalde[4] — [1]Chair of Materials Science and Nanotechnology, TU Dresden, Dresden — [2]Departamento de \'isica, Colegio de Ciencias e Ingenier\'ia, Universidad San Francisco de Quito, Ecuador — [3]School of Molecular Sciences, Arizona State University, USA — [4]Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU), Spain

We have obtained a connection between the chiro-optical activity and the spin-orbit interaction for a model system of an electron constrained to a helix, taking explicitly spin into account, in the presence of an electromagnetic field as a perturbation. Because of the chiral nature of the system, spatial inversion symmetry is broken, which in turn induces a connection between the electric and the magnetic responses of the system to the external electromagnetic field, that is absent in achiral systems. Despite the apparent simplicity of the model, it contains most of the relevant physics involved in this problem, and we have established a relationship between the optical activity response, via the Rosenfeld tensor and the spin polarization, defined as the average value of the Pauli spin-1/2 matrices. This relationship between the optical response and the CISS responses, can guide new efforts in the fields of reticular chemistry and material design for spintronics, and spin-selective chemistry.

TT 11.5 Mon 16:00 HSZ 304

Electron and spin-phonon interaction in DNA: A minimum analytical model — •Mayra Peralta[1], Solmar Varela[1], Vladimiro Mujica[2], Rafael Gutiérrez[1], Ernesto Medina[3], and Gianaurelio Cuniberti[1] — [1]Institute of Materials Science and Nanotechnology, Technische Universität Dresden, Dresden 01062, Germany — [2]School of Molecular Sciences, Arizona State University, TEMPE, AZ 85287 — [3]Departamento de Física, Colegio de Ciencias e Ingeniería, Universidad San Francisco de Quito, Diego de Robles y Vía Interoceánica, Quito, 170901, Ecuador

We analyze the influence of electron-phonon and spin-phonon interaction in a model for electron transfer(ET) in DNA in terms of the envelope function approach. We are specifically concerned with the effect of these interactions on the coherence of the ET process and how to model the interaction of DNA with phonon reservoirs of biological relevance. We assume that the electron bearing orbitals are half filled and derive the physics of the electron- and spin-phonon coupling in the vicinity in reciprocal space. In a first model for spinless electrons we find that at half filling, the acoustical modes are decoupled to ET at first order, while optical modes are predominant. The latter are associated with inter-strand vibrational modes in consistency with previous studies involving polaron models of ET. Coupling to acoustic modes depends on electron doping of DNA, while optical modes are always coupled within our model. When the spin is included, through the Spin-orbit coupling whose intensity is geometry dependent, we find that acoustical phonons become coupled independently of the doping.

TT 11.6 Mon 16:15 HSZ 304

Gate-tunable insulator-metal transition and weak antilocalization in two-dimensional tellurium — •Dorsa Fartab[1], José Guimarães[1,2], Marcus Schmidt[1], and Haijing Zhang[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews KY16 9SS, UK

Charge carrier density control is a key factor to modify the electronic functionality of materials. The ability to induce high charge carrier concentration into various two-dimensional materials has led to exotic phenomena such as insulator-metal transition and superconductivity. So far, different techniques have been used to achieve this. Meanwhile, electric double layer transistor (EDLT) is a highly promising platform as it can provide high charge carrier density of up to $10^{15} cm^{-2}$ in its channel material. This is two orders of magnitude larger than that in the conventional transistors as a result of using ionic liquids instead of common solid dielectrics. First, I will give a short overview on the EDLTs, then I will present our experimental results of ionic liquid gated two-dimensional tellurium (Te). Our results show the possibility of gate tuning insulator-metal phase transition and the gate and temperature-dependent weak antilocalization in p-type Te films. More interestingly, we have shown the ability of controlling the spin-orbit interaction in the material by changing the applied gate voltage.

TT 12: Topological Insulators (joint session MA/TT)

Time: Monday 15:00–17:15 Location: HSZ 403

TT 12.1 Mon 15:00 HSZ 403

Benchmark study of symmetry-adapted ML-DFT models for magnetically doped topological insulators — •Johannes Wasmer[1], Rubel Mozumder[1], Philipp Rüssmann[1,2], Ira Assent[1,3], and Stefan Blügel[1] — [1]Forschungszentrum Jülich, Germany — [2]University of Würzburg, Germany — [3]Aarhus University, Denmark

We present a benchmark study of surrogate models for impurities embedded into crystalline solids. Using the Korringa-Kohn-Rostoker Green Function method [1], we have built databases of several thousand calculations of single impurities (monomers) embedded into different elemental crystals, as well as magnetic transition metal impurity dimers embedded in the topological insulator Bi_2Te_3. We predict the converged monomer impurity electron potential and the isotropic exchange interaction of the impurity dimer in the classical Heisenberg model. From these surrogates, we intend to build transferable models for larger systems in the future, which will accelerate the convergence of our DFT codes. The study compares various recent E(3)-equivariant models such as ACE and MACE [2] in terms of performance and reproducible end-to-end workflows.

[1] P. Rüßmann et al., npj Comput Mater 7, 13 (2021)
[2] I. Batatia et al., arXiv:2206.07697 (2022)

TT 12.2 Mon 15:15 HSZ 403

High thorughput magnetic topological materials search II — •Iñigo Robredo[1,2], Yuanfeng Xu[3,4], Andrei Bernevig[2,3], Claudia Felser[1], Nicolas Regnault[3,6], Luis Elcoro[5], and Maia G. Vergniory[1,2] — [1]MPI CPFS Dresden — [2]DIPC — [3]Princeton University — [4]Zhejiang University — [5]Basque Country University — [6]Sorbonne Université

The development of topological quantum chemistry has proven to be a game changing tool for predicting topological phases in realistic materials, both non-magnetic and magnetic. Building on the work of previous studies, in this work we expand the family of magnetic insulators and semimetals with non-trivial topological properties. We analyzed 408 magnetic structures from the Bilbao Crystallographic Server magnetic database, whose crystal and magnetic structures have been experimentally reported. To take into account the localized nature of magnetic elements, we perform electronic structure calculations and topological diagnosis as a function of the Hubabrd U parameter. This results in a topological phase iagram for each material as a function of the Hubbard interaction potential. We provide full details of the materials, which can be readily grown to explore their new topological phenomena.

TT 12.3 Mon 15:30 HSZ 403

Manipulating topological feature of massive Dirac particle with scalar potential — •Sumit Ghosh[1,2], Yuriy Mokrousov[1,2], and Stefan Blügel[1] — [1]PGI-1, Forschungszentrum Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, Germany

Topology is one of the central aspect of modern spintronics. Different physical observables as well as transport properties that originates from the nontrivial topology of the system shows significant robustness against different external perturbation. Manipulating the topology of a system on the other hand is a highly non-trivial task since it requires tuning the internal degrees of freedom. In this presentation we are going to present an intrinsic mechanism to manipulate the topological feature and associated transport properties by using scalar potential. We systematically demonstrate how a scalar potential can invert the mass term of a massive Dirac particle which subsequently leads to the change of the topological index. We further demonstrate how this mechanism can be exploited to control the formation of edge states which can control the transport properties. This study thus provides a better understanding of the origin of the topological properties as well as a simple way to manipulate them. [https://arxiv.org/abs/2204.06412]

TT 12.4 Mon 15:45 HSZ 403

Mapping out the topological phase diagram of FeSn — Soumya Sankar[1], Ruizi Liu[2], Xuejian Gao[1], Qifang Li[3,4], JiaChang Zheng[1], Caiyun Chen[1], Chengping Zhang[1], Kun Qiang[2], Zi Yang Meng[3,4], Kam Tuen Law[1], Qiming Shao[1,2], and •Berthold Jäck[1] — [1]HKUST, Clear Water Bay, Kowloon, Hong Kong SAR — [2]HKUST, Department of Computer Science and Electrical Enginerring, Clear Water Bay, Kowloon, Hong Kong SAR — [3]Hong Kong University, Department of Physics, Pokfulam Road, Hong Kong SAR

— [4]University of Tokyo, Department of Physics, Hongo, Bunkyo City, Tokyo

Metallic kagome magnets exhibit a flat band and a Dirac point in their electronic structure and long-range magnetic order. The combination of these properties creates favourable conditions to search for strongly correlated and topological electronic states. The near-ideal kagome band structure of the inter metallic kagome series X1Y1 offers opportunities to study the interplay between strong electronic correlations, topology, and magnetism.

We have used molecular beam epitaxy and electronic transport measurements to study the interplay of magnetism and band topology in thin films of antiferromagnetic FeSn. We will present results from a magnetic field and temperature dependent study of the anomalous Hall effect. Combining these measurements with magnetic Monte-Carlo simulations and theoretical model calculations, we map out the topological phase diagram of FeSn over a large temperature range.

We acknowledge support by the GRC, and the Croucher Foundation.

15 min. break

TT 12.5 Mon 16:15 HSZ 403

Investigation of the magnetic topological insulator family (MnPn2Te4) (Pn2Te3) n, (Pn=Bi, Sb) by μSR and NMR — •Manaswini Sahoo[1,2], Anna Isaeva[1], Bernd Büchner[1], and Roberto De Renzi[2] — [1]Leibniz IFW Dresden, Dresden, Germany — [2]University of Parma,Parma, Italy

Time-reversal symmetry breaking in a topological insulator (TI) opens a surface gap and distinguishes chiral quantum states that could eventually be exploited in electrically controlled spintronic devices. The recent discovery of layered van der Waals materials opens a new approach to achieve this.(MnBi2Te4) (Bi2Te3) n is one of the first such examples, where the increasing number n of TI layers controls the magnetic dimensionality of the material. These compounds do display the quantum anomalous Hall effect, where spontaneous magnetization and spin-orbit coupling lead to a topologically non-trivial electronic structure. In the case of (MnBi2Te4) (Bi2Te3) n, Zero Field μSR shows more than one internal field at the muon site with the majority one decreasing in value when n is increased. The muon spin precessions display very fast relaxations of static inhomogeneous nature. Whereas in the sister compound MnSb2Te4, Zero Field μSR shows a broader distribution of magnetic field at the muon due to larger intermixing between Mn/Sb in the sample. Importantly, the weak Transverse Field shows a sharp magnetic transition at the same Tc, with a clear relaxation peak due to critical fluctuations, taking place in the whole volume of the material. This local information from μSR together with NMR is crucial to correctly interpret macroscopic magnetization data.

TT 12.6 Mon 16:30 HSZ 403

Magnetic dilution effect and topological phase transitions in antiferromagnet $Mn_{1-x}Pb_xBi_2Te_4$ — •Yueh-Ting Yao[1], Tiema Qian[2], Tay-Rong Chang[1,3,4], and Ni Ni[2] — [1]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [2]Department of Physics and Astronomy and California NanoSystems Institute, University of California, Los Angeles, California 90095, USA — [3]Center for Quantum Frontiers of Research and Technology (QFort), Tainan 701, Taiwan — [4]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan

The interplay between magnetism and topology have taken the central stage of modern condensed matter physics in the past three years. The fine control of magnetism and topology in a magnetic topological insulator is crucial for realizing various novel magnetic topological phases, such as axion insulator, magnetic Weyl semimetals, etc. In this work, we investigate the evolution of magnetism and band topology in $Mn_{1-x}Pb_xBi_2Te_4$ via angle resolved photoemission spectroscopy (ARPES), first-principles calculations, and electronic transports. We present the comprehensive phase diagram by controlling Pb content and magnetism in this alloy system. Moreover, we provide the first topological crystalline insulator with non-trivial glide mirror Chern number in MnBi2Te4-family materials, which is protected by nonsymmorphic symmetry arise from antiferromagnetic (AFM) configuration. Our work provides a fruitful platform with continuously tunable magnetism and topology for investigating emergent phenomena and pave a way towards potential new applications of nanoelectronics.

TT 12.7 Mon 16:45 HSZ 403

Thermal Hall Effect of Magnon-Phonon Hybrid Quasiparticles in a Fluctuating Heisenberg-Kitaev Antiferromagnet — •Robin R. Neumann[1], Alexander Mook[2], Jürgen Henk[1], and Ingrid Mertig[1] — [1]Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Johannes Gutenberg University, Mainz, Germany

Magnons, the quantized excitations of localized spins, and phonons, the quantized excitations of the lattice, are two types of quasiparticles that are responsible for heat transport in magnetic insulators. However, phonons by themselves do not contribute to the *transverse* heat current induced by a temperature gradient, i.e., the thermal Hall effect (THE). Magnons, on the other hand, may exhibit a Berry curvature, a magnetic field in reciprocal space, that leads to an intrinsic THE.

In this talk, I address the THE in a Heisenberg-Kitaev antiferromagnet subjected to a magnetic field. The applied field drives the system from a zigzag antiferromagnetic to a spin-flop state. The magnon-driven THE indicates the magnetic phase transition by a sign change at the critical field. Furthermore, when the magnetoelastic interaction is considered, the phonon and magnon bands hybridize and additional Berry curvature at the avoided crossings emerge. Depending on the strength of the spin-phonon coupling, this may lead to an overall reversal of the THE while the field-induced sign change at the critical field remains mostly robust. These results showcase that magnon-phonon hybridization can be pivotal for the interpretation of transport experiments.

TT 12.8 Mon 17:00 HSZ 403

Limitations of the Bulk-Boundary Correspondence in Topological Magnon Insulators due to Magnon-Magnon Interactions — •Jonas Habel[1], Johannes Knolle[1], Alexander Mook[2], and Josef Willsher[1] — [1]Technical University of Munich, Germany (Theory of Quantum Matter and Nanophysics) — [2]Johannes Gutenberg University Mainz, Germany

Magnon excitations in ordered quantum magnets can exhibit topological band structures characterized by non-zero Chern numbers. Such magnonic Chern insulators are widely believed to host protected chiral edge modes due to the bulk-boundary correspondence, in analogy to electronic Chern insulators. However, in contrast to electrons, magnons are bosons and can thus be subject to exotic number-nonconserving many-body interactions, enabling potentially strong spontaneous decays at zero temperature.

To assess their effect on the chiral edge magnons, we study a topological honeycomb-lattice ferromagnet with Dzyaloshinskii-Moriya interactions using many-body perturbation theory. We discover that non-harmonic terms of the spin-wave expansion may lead to severe lifetime reduction of edge modes and their delocalisation into the bulk. For sufficiently strong interactions, the spectral weight of the chiral edge magnons vanishes entirely. These findings indicate that topological magnon bands within the harmonic framework do not necessarily give rise to protected edge modes in the full spin theory, suggesting limitations of the bulk-boundary correspondence in this case.

TT 13: Focus Session: Physics Meets ML II – Understanding Machine Learning as Complex Interacting Systems (joint session DY/TT)

Machine-learning has recently entered and is now transforming many fields of science, enabling discoveries in a data-driven manner. As a scientific method, however, ML often lacks one defining feature: Explainability. We here seek discussions with pioneers in understanding, explaining, and improving machine learning methods from the point of view as a physical system of interacting elements. In fact, the history of approaching neuronal networks and problems of inference and learning as a problem of statistical physics has a long history, with a number of important discoveries early on. The close relation between spin glasses and neuronal networks are being currently exploited to address pressing questions, such as the remarkable generalization properties of neuronal networks despite their massive overparameterization and their behavior reminiscent of renormalization group transformations.

Organized by Sabine Andergassen (Tübingen) and Moritz Helias (Jülich)

Time: Monday 15:00–18:30 Location: ZEU 250

Invited Talk TT 13.1 Mon 15:00 ZEU 250
The challenge of structured disorder in statistical physics — •Marc Mezard — Bocconi University, Milano

Statistical physics offers many interesting tools to study machine learning. In most cases it needs to use a statistical ensemble of data. Most of the theoretical work has relied on unstructured data. Yet, the highly structured character of data used in training deep networks is a crucial ingredient of their performance. Modelling structured data, analyzing the learning and the generalization of deep networks trained on this data, are major challenges. This talk will describe several recent developments in this direction.

Invited Talk TT 13.2 Mon 15:30 ZEU 250
The emergence of concepts in shallow neural-networks — •Elena Agliari — Piazzale A. Moro 5, 00185 Roma

In the first part of the seminar I will introduce shallow neural-networks from a statistical-mechanics perspective, focusing on simple cases and on a naive scenario where information to be learnt is structureless. Then, inspired by biological information-processing, I will enrich the framework and make the network able to successfully and cheaply handle structured datasets. Results presented are both analytical and numerical.

Invited Talk TT 13.3 Mon 16:00 ZEU 250
Adaptive Kernel Approaches to Feature Learning in Deep Neural Networks — •Zohar Ringel — Racah Institute of Physics, Hebrew University in Jerusalem

Following the ever-increasing role of deep neural networks (DNNs) in our world, a better theoretical understanding of these complex artificial objects is desirable. Some progress in this direction has been seen lately in the realm of infinitely overparameterized DNNs. The outputs of such trained DNNs behave essentially as multivariate Gaussians governed by a certain covariance matrix called the kernel. While such infinite DNNs share many similarities with the finite ones used in practice, various important discrepancies exist. Most notably the fixed kernels of such DNNs stand in contrast to feature learning effects observed in finite DNNs. Such effects are crucial as they are the key to understanding how DNNs process data. To accommodate such effects within the Gaussian/kernel viewpoint, various ideas have been put forward. Here I will provide a short overview of those efforts and then discuss in some detail a general set of equations we developed for feature learning in fully trained/equilibrated DNNs. Interestingly, our approach shows that DNNs accommodate strong feature learning via mean-field effects while having decoupled layers and decoupled neurons within a layer. Furthermore, learning is achieved not by compression of information but rather by increasing neuron variance along label-relevant directions in function space.

TT 13.4 Mon 16:30 ZEU 250
Interpreting black-box ML with the help of physics — •Miriam Klopotek — University of Stuttgart, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany

Complexity is an unavoidable part of systems with emergent or even so-called intelligent capabilities. Ultimately, it stems from the many microscopic constituents with multiple possible states, which introduces a vast space of degrees of freedom. This is true both for many-body systems as well as modern machine learning (ML) systems. Today, the latter suffer notoriously from the 'black-box problem', i.e. they are inherently opaque. We argue that an engagement with physics can offer deep insights ultimately for a theory of operation and thus an interpretation, as well as powerful ways to assess their reliability and shortcomings. We show some results for a case study with beta-variational autoencoders (β-VAEs) [1], which we trained on data from a well-characterized model system of hard rods confined to 2D lattices [2].

[1] D. P. Kingma and M. Welling, ICLR 2014. D. J. Rezende, S. Mohamed, and D. Wierstra, ICML 2014, p. 1278-1286.
[2] P. Quiring, M. Klopotek and M. Oettel, Phys. Rev. E 100, 012707 (2019).

15 min. break

Invited Talk TT 13.5 Mon 17:00 ZEU 250
Analysing the dynamics of message passing algorithms — •Manfred Opper[1,2] and Burak Cakmak[1] — [1]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, 10587, Germany — [2]Centre for Systems Modelling and Quantitative Biomedicine, University of Birmingham, B15 2TT, United Kingdom

Message passing algorithms are deterministic methods which are designed for efficiently computing marginal statistics for probabilistic, Bayesian data models used in machine learning and statistics. Such algorithms have been developed in parallel within the machine learning and the statistical physics communities. They often provide highly accurate approximations at a much higher speed compared to exact Monte Carlo sampling. The fixed points of such algorithms can be analysed for high dimensional models (under the assumption of specific data distributions) using the replica method of statistical physics. In this talk we will focus on the dynamical properties of the algorithms. Applying dynamical functional techniques to the nonlinear dynamics, the degrees of freedom which interact via a random matrix can be decoupled in the limit of large systems resulting in exact stochastic single node dynamics. For general dynamical models, it is hard to further analyse this effective dynamics due to the occurence of memory terms. Surprisingly, for message passing algorithms memory terms are absent and exact results for convergence rates and stability can be derived for specific data distributions.

Invited Talk TT 13.6 Mon 17:30 ZEU 250
Deep Learning Theory Beyond the Kernel Limit — •Cengiz Pehlevan — Harvard University, USA

Deep learning has emerged as a successful paradigm for solving challenging machine learning and computational problems across a variety of domains. However, theoretical understanding of the training and generalization of modern deep learning methods lags behind current practice. I will give an overview of our recent results in this domain, including a new theory that we derived by applying dynamical field theory to deep learning dynamics. This theory gives insight into internal representations learned by the network under different learning rules.

TT 13.7 Mon 18:00 ZEU 250
Solving the Bethe–Salpeter equation with exponential con-

vergence — •Markus Wallerberger[1], Hiroshi Shinaoka[2], and Anna Kauch[1] — [1]TU Wien, Vienna, Austria — [2]Saitama University, Japan

The Bethe–Salpeter equation plays a crucial role in understanding the physics of correlated fermions, relating to optical excitations in solids as well as resonances in high-energy physics. Yet, it is notoriously difficult to control numerically, typically requiring an effort that scales polynomially with energy scales and accuracy. This puts many interesting systems out of computational reach.

Using the intermediate representation and sparse modeling for two-particle objects on the Matsubara axis, we develop an algorithm that solves the Bethe–Salpeter equation in $O(L^8)$ time with $O(L^4)$ memory, where L grows only logarithmically with inverse temperature, bandwidth, and desired accuracy. This opens the door for computations in hitherto inaccessible regimes. We benchmark the method on the Hubbard atom and on the multiorbital weak-coupling limit, where we observe the expected exponential convergence to the analytical results. We then showcase the method for a realistic impurity problem.

[1] M. Wallerberger et al., Phys. Rev. Research 3, 033168 (2021)

TT 13.8 Mon 18:15 ZEU 250

Making machines untangle the parquet equations — •Samuel Badr[1], Anna Kauch[1], Hiroshi Shinaoka[2], Karsten Held[1], and Markus Wallerberger[1] — [1]TU Wien, Vienna, Austria — [2]Saitama University, Saitama, Japan

Diagrammatic theories at the two-particle level are increasingly important in understanding the subtle interplay of phenomena occurring in strongly correlated electron systems. The parquet equations are a centerpiece of many such theories, since they are the simplest unbiased topological classification of two-particle diagrams. However, due to their eponymous interlocking structure, the parquet equations are vexingly difficult to solve, requiring prohibitive amounts of memory.

We tackle this problem using the recently developed, machine learning inspired, techniques: firstly, the overcomplete intermediate representation, a highly compressed model for two-particle objects which is guaranteed to converge exponentially; secondly, a sparse set of Matsubara frequencies tailored to the structure of the parquet equations. This allows us to perform convolutions and frequency shifts at no loss of accuracy.

We benchmark our solver for the Hubbard atom, where we reproduce analytic results, and then showcase the solver for more extended systems.

TT 14: Focus Session: Graphene Quantum Dots (joint session HL/TT)

Quantum dots have emerged as one of the contenders for a future quantum information processor. Bilayer graphene is now established as a material that allows high quality bi-polar Coulomb blockade measurement, time-dependent transport measurements and first relaxation time measurements. In contrast to the more conventional GaAs and Si-based systems, several exiting and unexpected observations in graphene have been explained by the peculiar graphene bandstructure, which is gate- tunable, the additional valley degree of freedom, and spin-valley coupling.

Organized by Klaus Ensslin

Time: Monday 15:00–17:45 Location: POT 361

Invited Talk TT 14.1 Mon 15:00 POT 361

Spin and valley lifetime in graphene quantum dots — •Guido Burkard — University of Konstanz, Germany

Graphene with its low nuclear spin density and weak spin-orbit coupling allows for long electron spin relaxation and coherence times. The spin and valley degrees of freedom of localized electrons can therefore be seen as potential embodiments of classical or quantum bits for computation. However, the formation of localized states in quantum dots requires some form of badgap engineering, and the mechanisms for spin and valley relaxation have not been completely understood so far. Bilayer graphene has an electrically controllable bandgap that allows for the formation of quantum dots. We present general theoretical considerations regarding the formation of quantum dots in graphene and report on recent progress in understanding the relevant physical mechanisms of spin and valley relaxation in electrostatically gated bilayer graphene quantum dots.

Invited Talk TT 14.2 Mon 15:30 POT 361

Microscopic modelling of electrostatically induced bilayer graphene quantum dots — •Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

Quantum nanostructures, e.g., quantum wires and quantum dots, are needed for applications in quantum information processing devices, such as transistors or qubits. In gapped bilayer graphene, one can confine charge carriers purely electrostatically, inducing smooth confinement potentials and thereby limiting edge-induced perturbances while allowing gate-defined control of the confined structure. In this talk, I will give an overview of our recent contributions toward the theoretical modelling of gate-defined bilayer graphene quantum dots, taking into account microscopic details of the material properties and the confinement. As an outlook, I will point towards current and future challenges in describing coupled bilayer graphene nanostructures, e.g., setups with multiple bilayer graphene quantum dots.

TT 14.3 Mon 16:00 POT 361

Valley relaxation in a single-electron bilayer graphene quantum dot — •Lin Wang and Guido Burkard — Department of Physics, University of Konstanz, D-78457, Germany

Bernal-stacked bilayer graphene (BLG) has a tunable gap controlled by an out-of-plane electric field. This makes BLG a possible candidate to form quantum dots (QDs) via quantum confinement. Spin-based qubits in BLG QDs have received great attention due to outstanding spin-coherence properties. Very recently, long spin relaxation times of a single-electron state in BLG QDs was reported [1,2]. In addition to spin, valley pseudospin is another degree of freedom in BLG. The two valleys experience opposite Berry curvatures and associated magnetic moments via an out-of-plane electric field. This provides a promising way to control valleys and further establish valley qubits. To assess the potential of valley qubits, the valley relaxation time is a crucial parameter since it directly limits the lifetime of encoded information. Here, we investigate the valley relaxation in a single-electron BLG QD due to intervalley coupling assisted by (i) 1/f charge noise and (ii) electron-phonon couplings arising from the deformation potential and bond-length change. Our calculation shows that valley relaxation time decreases with a power law dependence as a function of magnetic field, which is in a good agreement with very recent experiment.

References: [1]L. Banszerus, K. Hecker, S. Möller, E. Icking, K. Watanabe, T. Taniguchi, C. Volk and C. Stampfer, Nat. Commun. 13, 3637 (2022). [2] Lisa Maria Gächter et al., PRX Quantum 3, 020343 (2022).

30 min. break

Invited Talk TT 14.4 Mon 16:45 POT 361

Single-shot spin and valley Pauli blockade read-out in bilayer graphene quantum dots — •Chuyao Tong[1], Rebekka Garreis[1], Wister Wei Huang[1], Annika Kurzmann[1,2], Jocelyn Terle[1], Samuel Jele[1], Kenji Watanabe[3], Takashi Taniguchi[3], Thomas Ihn[1], and Klaus Ensslin[1] — [1]ETH Zurich, CH-8093 Zurich, Switzerland — [2]RWTH Aachen University, Aachen, 52074, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

In bilayer graphene quantum dots, apart from spins up and down, the additional valley degree of freedom K- and K+ gives rise to an unconventional single-dot two-carrier ground state: spin-triplet valley-singlet, altering the canonical even-odd double dot Pauli spin blockade picture. This ground state can be switched to a spin-singlet valley-triplet by a perpendicular magnetic field, allowing us to switch between valley-blockade at low, and spin-blockade at higher magnetic field for the two-carrier Pauli blockade (1,1) to (0,2). We employ charge sensing technology and perform single-shot Pauli blockade read-out at the two field regimes, probing characteristic relaxation times T1 between spin or valley -triplet and -singlet. The spin-T1 is measured to be up to 60ms, drastically decreasing with increasing inter-dot tunnel coupling and corroborating with recent experiments performed with single-dot Elzerman read-out. Moreover, we observe exceedingly long valley T1 longer than 500ms, robust with inter-dot tunnel coupling. These promisingly long spin- and valley T1 herald for long-living spin and valley bilayer graphene quantum dot qubits.

Invited Talk TT 14.5 Mon 17:15 POT 361

Particle-hole symmetry protects spin-valley blockade in graphene quantum dots — •Christian Volk[1,2], Luca Banszerus[1,2], Samuel Möller[1,2], Katrin Hecker[1,2], Eike Icking[1,2], Kenji Watanabe[3], Takashi Taniguchi[4], Fabian Hassler[5], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan — [5]JARA-Institute for Quantum Information, RWTH Aachen University

Particle-hole symmetry plays an important role for the characterization of topological phases in solid-state systems. Graphene is a prime example of a gapless particle-hole symmetric system. The intrinsic Kane-Mele spin-orbit coupling in graphene leads to a lifting of the spin-valley degeneracy and renders graphene a topological insulator in a quantum spin-Hall phase while preserving particle-hole symmetry.

Here, we show that the Kane-Mele spin-orbit gap leads to a lifting of the spin-valley degeneracy in bilayer graphene quantum dots, resulting in Kramer's doublets with different ordering for electron and hole states preserving particle-hole symmetry. We observe the creation of single electron-hole pairs with opposite quantum numbers and use the electron-hole symmetry to achieve a protected spin-valley blockade in electron-hole double quantum dots. The latter will allow spin-to-charge and valley-to-charge conversion, which is essential for the operation of spin and valley qubits.

TT 15: Quantum Transport and Quantum Hall Effects I (joint session HL/TT)

Time: Monday 15:00–17:15 Location: POT 251

TT 15.1 Mon 15:00 POT 251

Local Chern patches and networks of chiral modes in quantum Hall phases with spatial magnetic field profiles. — •Suraj Hegde and Tobias Meng — Institute of Theoretical Physics and Wurzburg-Dresden Cluster of Excellence ct.qmat, Technische Universitat Dresden, 01069 Dresden, Germany.

Transport experiments on curved Hall bars show a variety of non-trivial transport signatures. Motivated by these experiments, we develop a model that accounts for various features in multi-terminal Hall bar measurements and perform numerical simulations using KWANT. We model the effect of curvature of the sample through spatial variation of the magnetic field profile and find that it results in patches of quantum Hall phases characterised by different local Chern markers. We find that most of the transverse and longitudinal transport can be understood in terms of local Chern patches and an intricate interplay of chiral modes at the interface of different patches. We also show that the spatial magnetic field textures could provide a novel platform to engineer lattices formed by networks of chiral modes.

TT 15.2 Mon 15:15 POT 251

Effect of the external fields in high Chern number quantum anomalous Hall insulators — •Yuriko Baba[1,2], Francisco Domínguez-Adame[1], and Rafael A. Molina-Feŕandez[2] — [1]GISC, Departamento de Física de Materiales, Universidad Complutense, E–28040 Madrid, Spain — [2]Instituto de Estructura de la Materia, IEM-CSIC, E–28006 Madrid, Spain

Multilayer structures consisting of alternating magnetic and undoped topological insulator layers have been proved so far to be a convenient platform for creating a quantum Anomalous Hall state with a high Chern number [1]. However, in previous proposals, the Chern number can only be tuned by varying the doping concentration or the width of the magnetic topological insulator TI layers. This restricts the applications of the dissipationless chiral edge currents in electronics, since the number of conducting channels remains fixed. In this work, we propose a way of varying the Chern number at will by means of an external electric field applied along the stacking direction. The electric field generates the hybridization of the inverted bands, generating new topological channels. In this way, the number of Chern states can be tuned externally in the sample, without the need of modifying the number and width of the layers or the doping level. We showed that this effect can be uncovered by the variation of the transverse conductance as a function of the electric field at constant injection energy at the Fermi level. [2]

[1] Zhao, Y. F. et al., Nature, 588 (2020) 419
[2] arXiv:2208.03585

TT 15.3 Mon 15:30 POT 251

Novel thermo-electric transport channel in the conformal limit of tilted Weyl semimetals — Thorvald Ballestad[1], Alberto Cortijo[2], Maria Vozmediano[3], and •Alireza Qaiumzadeh[1] — [1]Center for Quantum Spintronics, Norwegian University of Science and Technology, Trondheim, Norway — [2]Universidad Autonoma de Madrid, Madrid, Spain — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

Recently, a new contribution to the Nernst current was proposed in 3D Dirac and Weyl semimetals, originated from quantum conformal anomaly [1,2]. In the present study, we analyze the effect of the tilt on the transverse thermo-electric coefficient of Weyl semimetals in the conformal limit, i.e., zero temperature and zero chemical potential. Using the Kubo formalism, we find a non-monotonic behavior of the thermoelectric conductivity as a function of the tilt perpendicular to the magnetic field, and a linear behavior when the tilt is aligned to the magnetic field. An "axial Nernst" current is generated in inversion symmetric materials when the tilt vector has a projection in the direction of the magnetic field. This analysis will help in the design and interpretation of thermo-electric transport experiments in recently discovered topological quantum materials [3].

[1] M. N. Chernodub et al, Phys. Rev. Lett. 120, 206601 (2018). [2] V. Arjona et al, Phys. Rev. B 99, 235123 (2019). [3] T. M Ballestad, A. Cortijo, M. A. H. Vozmediano, A. Qaiumzadeh, arXiv:2209.14331 (2022).

TT 15.4 Mon 15:45 POT 251

Selective scattering between counter-propagating edge states in a topological insulator — •Meng Hao[1,2], Li-Xian Wang[1,2], Fabian Schmitt[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Würzburg, Germany — [2]Physikalisches Institut (EP III) Würzburg University, Würzburg, Germany

The quantum Hall state, known by its dissipationless nature, comprises chiral edge states in a two-dimensional electron gas (2DEG). In the ordinary quantum Hall effect, all edge states propagate in the same direction, populated equally. Thus, they are immune to inter-edge-state scattering. In contrast, counter-propagating edge states, populated unequally, are naturally sensitive to the scattering process. However, a realization of this scenario so far was only possible by stacked layers of high-mobility 2DEGs, e.g., quantum wells or graphene. Here we realize the counter-propagating edge states in a three-dimensional topological insulator controlled by top and bottom gates. Surprisingly, the counter-propagating edge states prove to scatter into each other selectively. Our first attempt shows that this inter-edge-state scattering occurs exclusively between Landau levels with the same Landau index. We further propose a cross bar equipped with split-gates to determine the selection rule of scattering and scattering parameters unambiguously. Following this proposal, we will show some preliminary results and report our experimental advances.

30 min. break

TT 15.5 Mon 16:30 POT 251

Edge modes, Hall conductivity and topological features of a dice lattice: Fate of flat bands under strain — •Sayan Mondal and Saurabh Basu — Indian Institute of Technology Guwahati

We study the topological properties of a dice lattice, which has three atoms per unit cell (A, B, and C). In addition, the bands are systematically deformed via the introduction of anisotropy among the nearest neighbour (NN) hoppings in two distinct ways. In the first case, we apply the uniaxial strain, which alters the NN hoppings (between the sublattices A-B and B-C) along the direction of applied strain. While in the second case, we selectively tune the NN hopping between A and B sublattices which may be achieved by a controlled chemical pressure. The first case yields the Chern insulating lobes in the phase diagram with $C = \pm 2$ till a certain critical anisotropy, where the spectral gap vanishes. The quantized plateau in the anomalous Hall conductivity and the pair of chiral edge modes at each edge of a ribbon support the obtained values of the Chern numbers. Whereas, the second case (selective strain) shows distorted flat band in the dispersion spectrum, which alters the gap-closing condition as compared to the case of uniaxial strain. Also, the Chern insulating lobes in the phase diagram and the Hall conductivity have distinct features compared to the case above. However, in both cases, topological phase transitions take place which is demonstrated via the Chern number changing discontinuously from ± 2 to zero across the gap-closing transitions.

TT 15.6 Mon 16:45 POT 251

Structure-imposed electronic topology in graphene nanoribbons — •Florian Arnold[1], Tsai-Jung Liu[1], Agnieszka Kuc[2], and Thomas Heine[1,2,3] — [1]Technische Universität Dresden, Dresden, Germany — [2]HZDR, Leipzig, Germany — [3]Yonsei University, Seoul, Republic of Korea

Zigzag graphene nanoribbons (ZGNR) can be transformed into new structure types by removing terminal carbon atoms in a regular pattern. When a single atom is removed on each zigzag edge so-called cove-edged ZGNR (ZGNR-C) are created, while removing multiple atoms results in gulf-edged ZGNR (ZGNR-G). In our seminal work, we demonstrated the direct structure-electronic structure relation based on the structural parameters that unambiguously characterize ZGNR-C. This allowed to create a scheme that classifies their electronic state, i.e., if they are metallic, topological insulators or trivial semiconductors, and to find an empirical formula for the band gap of the semiconducting ribbons. Since then, we were able to expand this description to ZGNR-G systems where the chemical space of possible structures increases further due to the variable size of the gulf edges. With this, we give guidance to realize new graphene nanoribbon heterojunctions hosting topological states and investigate the transport properties of exemplary systems.

TT 15.7 Mon 17:00 POT 251

Massive and topological surface states in strained HgTe and evidence for parity anomaly — •Wouter Beugeling[1,2], Lixian Wang[1,2], David M. Mahler[1,2], Valentin L. Müller[1,2], Ewelina M. Hankiewicz[3], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Institute for Topological Insulators, Würzburg, Germany — [2]Physikalisches Institut (EP III), Würzburg University, Würzburg, Germany — [3]Institute for Theoretical Physics and Astrophysics (TP IV), Würzburg University, Würzburg, Germany

The idea that band inversion in a narrow-gap material can lead to Dirac-type surface states was noted by Volkov and Pankratov in the 1980's. Only about two decades later, it was realized that the surface states of topological insulators are the gapless Dirac states predicted by them. The massive Volkov-Pankratov states received much less attention. They are pulled from the bulk in a sufficiently large electric field and are topologically trivial. Until recently, direct evidence in the form of transport measurements was elusive.

From our magneto-transport experiments on a three-dimensional topological insulator heterostructure (strained HgTe), we demonstrate the coexistence of massless and massive Volkov-Pankratov states. The well-developed Hall quantization in the n- and the p-type regime is due to the topological surface state and the massive Volkov-Pankratov states, respectively, as confirmed by k·p theory. In a second series of experiments, we find a remarkable re-entrant quantum Hall effect in the p-type regime, which we can trace to spectral asymmetry, a salient manifestation of parity anomaly in a solid-state system.

TT 16: Poster: Transport

Time: Monday 15:00–18:00 Location: P2/OG4

TT 16.1 Mon 15:00 P2/OG4

Asymmetric and spatially resolved power dissipation in quantum transport — •Nico Leumer — Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Dissipation is a natural byproduct of quantum transport caused by various inelastic scattering events of electrons and their lost energy stimulates in turn the temperature profile of the underlying bulk material. Importantly though, electronic current may run only through a narrow part of the sample as, for instance, happens in the quantum Hall regime of graphene due to chiral edge channels (1); thus, dissipation has to be seen as a local quantity. The still rather recent invention of the Squid-on-tip technique in 2016 (2), paved the way to experimental access this challenge, where the temperature increases by merely a few hundred micro Kelvin on length scales of the order of nanometers.

Quantum point contacts (QPC's) are of particular interest in nanoscale transport, as electrons experience now a -perhaps energy dependent- transmission probability. On a hand waving level, QPC's increase the resistance electrons face from the sample locally, which is accompanied by areas of higher dissipation. In our recent project, we predict where and how much power is dissipated.

[1] A. Marguerite et al., Nature 575, 628 (2019)
[2] D. Halbertal et al., Nature 539, 407 (2016)

TT 16.2 Mon 15:00 P2/OG4

Resistive switching and peculiarities of conductivity of $TiTe_2$ point contacts — •Oksana Kvitnitskaya[1], Luminita Harnagea[2], Dmitri Efremov[3], Bernd Büchner[3,4], and Yurii Naidyuk[1] — [1]B.Verkin Institute for Low Temperature Physics and Engineering, NASU, Kharkiv, Ukraine — [2]Dep. of Physics, Indian Institute of Science Education and Research, Pune, Maharashtra, India — [3]Institute for Solid State Research, IFW Dresden, Dresden, Germany — [4]Institut für Festkörper- und Materialphysik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany

Ti-based dichalcogenides TiX_2 (X - S, Se, Te), display a variety of physical properties, depending on their lattice distortions, native defects, self-doping effects, intercalation, external pressure. They can exhibit semiconducting, semimetallic, CDW, and superconducting behavior, which together with their layered structure and unique properties upon exfoliation to monolayer limit, make them particularly interesting. Recently, we observed the resistive switching effect in $TiTe_2$ point-contacts (PCs). We attributed the effect to Se vacancy drift due to a high electric field in the PC core. Here we report the resistive switching in PCs with isoelectronic $TiTe_2$, where the ratio of the high resistance state to the low resistance state was so far up to several times, contrary to up to two orders of magnitude for $TiSe_2$. Additionally, we observed "camel-like" $dV/dI(V)$ spectra of $TiTe_2$ at helium temperature with two symmetric *vs* V=0 humps around +/-(200-300) mV, which vanished near 200 K.

TT 16.3 Mon 15:00 P2/OG4

Nonmonotonous Temperature Dependence of the Thermopower of Gold Atomic Contacts — Thomas Möller[1], •Marcel Strohmeier[1], Ruben Zerfass[1], Kim Nikolai Kirchberger[1], Danial Majidi[2], Juan Carlos Cuevas[3], Johannes Boneberg[1], Paul Leiderer[1], Wolfgang Belzig[1], and Elke Scheer[1] — [1]University of Konstanz, 78457 Konstanz, Germany — [2]Université Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 38042 Grenoble, France — [3]Universidad Autónoma de Madrid, E-28049 Madrid, Spain

We present measurements of the thermopower of atomic-size gold contacts realized by the mechanically controllable break junction (MCBJ) technique over a temperature range from 10 K to 295 K. While the conductance histograms confirm the quantum nature of the transport, we observe a non-monotonous temperature dependence of the ensemble-averaged thermopower (taking into account contacts between 1 and 20 $G_0 = 2e^2/h$) with a minimum of -2 μV/K at about 150 K. Our observations at low and high temperature are compatible with values reported in the literature [1-5], but the non-monotonous behavior in between disagrees with the expected linear increase of the thermopower for quantum coherent conductors described by the Landauer formula. We discuss several possible mechanisms, that may be at the origin of the deviation, such as phonon contributions or an energy-dependent transmission function. Both aspects can be addressed experimentally by analyzing current-voltage characteristics. We present here results obtained for Au and for Cu atomic contacts.

TT 16.4 Mon 15:00 P2/OG4

Analyzing vibrational instabilities arising from non-conservative current-induced forces in nanosystems with a semi-classical approach — •Robin L. Grether, Samuel Rudge, and Michael Thoss — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Deutschland

Understanding the electric properties of nanosystems such as molecular junctions is a crucial task for modern physics. For molecular junctions, these properties are often governed by an electronic-vibrational coupling, which can lead to an instability of the junction in some cases.

We provide an in-depth analysis of the vibrational instabilities caused by non-conservative current-induced forces in a molecular junction using a semi-classical approach that exploits the time-scale separation between the fast electronic dynamics and the much slower vibrational dynamics. In particular, we use a Born-Markov master equation for the electronic degrees of freedom in combination with a semi-classical Langevin equation for the vibrational dynamics [1]. Within this framework, we study the dynamics of a junction composed of two electronic levels and two harmonic vibrational modes [2] for various parameters.

[1] W. Dou *et al.*, J. Chem. Phys. **145**, 054102 (2016)
[2] J.-T. Lü *et al.*, Phys. Rev. B **85**, 245444 (2012)

TT 16.5 Mon 15:00 P2/OG4

Full counting statistics of electron transport through periodically driven quantum dots analysed with factorial cumulants — •Johann Zöllner, Eric Kleinherbers, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg

The electron transport through quantum dots is a stochastic process. Factorial cumulants of full counting statistics can be used to analyse current and current fluctuations of electrons [1]. We present methods to calculate factorial cumulants for periodically driven systems. This makes it possible to investigate effects in which a periodic drive and noise both take part. An example for such an effect is stochastic resonance, which has already been observed in quantum dots [2]. We will explain the meaning of factorial cumulants for stochastic resonance.

[1] P. Stegmann, B. Sothmann, A. Hucht, J. König, Phys. Rev. B 92, 155413 (2015)
[2] T. Wagner, P. Talkner, J. C. Bayer, E. P. Rugeramigabo, P. Hänggi, R. J. Haug, Nat. Phys. 15, 330(2019)

TT 16.6 Mon 15:00 P2/OG4

Rational design of halide perovskite-based quantum dots using ab-inotio many body techniques — •Manaswita Kar, Benjamin Lenz, and Michele Casula — IMPMC, Sorbonne Université-CNRS, Jussieu, 75005 Paris, France

Quantum dots (QDs) have attracted increasing attention as next generation functional materials, because of their unique size dependent colour tunability, due to quantum-confinement effect. However, the cost of production of these QDs is very high, thereby limiting their large scale industrial applications. Halide perovskite-based QDs provide single photon emission at room temperature and can be manufactured comparatively easily. These perovskites have a complex structural form and bears a large compositional space. As a result of this, only a limited number of these perovskite QDs have been tested so far. Here, we aim to identify the most promising perovskite based QDs for coherent photon emission applications by characterising their optical properties from theoretical simulations. Towards this aim, we employ the many body Green's function (GW) and Bethe-Salpeter equation (BSE) techniques to study the excited state properties of the QDs, which are known to be not well captured by standard ground state methods, such as Density Functional Theory (DFT). From this study, we finally envision find the best halide perovskite based quantum dot, that is both structurally and thermodynamically stable and can be manufactured for large scale commercial applications.

TT 16.7 Mon 15:00 P2/OG4

Device and contact engineering of MoS_2 nanotubes and nanoribbons — •Konstantin D. Schneider[1], Robin T. K. Schock[1], Jonathan Neuwald[1], Matthias Kronseder[1], Luka Pirker[2], 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, Institute Jožef Stefan, 1000 Ljubljana, Slovenia

Even though low-temperature transport measurements of a MoS_2 nanotube have already demonstrated Coulomb blockade at 300 mK,[1] Fermi level pinning near the conduction band at the metal-MoS_2 interface requires reactive low-work function metals, which then damage the MoS_2. Recently, bismuth[2] was shown to drastically reduce contact resistances in planar MoS_2.

Here, we present millikelvin transport measurements on MoS_2 nanotubes and nanoribbons with bismuth contacts.[3] Our nanotubes are grown via a chemical transport reaction, yielding diameters down to 7 nm and lengths up to several millimeters. Nanotubes were either suspended or placed on hexagonal boron nitride (hBN) in order to reduce disorder from the SiO_2 substrate. The resulting devices show Coulomb blockade, with a rich set of features. Contacts are transparent, and the temperature dependence hints at single level transport.

[1] S. Reinhardt *et al.*, Phys. Stat. Sol. RRL **13**, 1900251 (2019)
[2] P. C. Shen *et al.*, Nature 593, **211** (2021)
[3] R. T. K. Schock *et al.* arXiv:2209.15515

TT 16.8 Mon 15:00 P2/OG4

Weak localization in semiconductor heterostructures with strong spin orbit interaction — •Simon Feyrer, Jaydean Schmidt, Michael Prager, Dominique Bougeard, and Christoph Strunk — Institute of Experimental and Applied Physics, University of Regensburg, Germany

We present measurements of weak localization (WL) and weak anti-localization (WAL) performed on quasi-1D wires patterned into an InAs based quantum well. Due to the confinement of the electrons along the wires, the D'yakonov-Perel spin relaxation is expected to be suppressed resulting in WL instead of WAL. As consequence of the spin orbit interaction anisotropy, the amplitude of the WL is sensitive to the direction of an applied in-plane magnetic field and provides an estimate of the ratio between the Rashba and Dresselhaus spin orbit coefficient [1,2].

By fitting the measured WAL and WL-curves, the highest spin relaxation rate was extracted for the wires orientated along the $[01\bar{1}]$ crystal axis. A clear suppression of spin relaxation was observed along the [001] wire direction.

[1] T. Nishimura et al., Phys. Rev. B **103**, 094412 (2021)
[2] A. Sasaki et al., Nat. Nanotechnol. **9**, 703 (2014)

TT 16.9 Mon 15:00 P2/OG4

Revealing the role of Klein tunneling in Aharanov-Bohm graphene rings — •Ching-Hung Chiu and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan City, Taiwan

Graphene, the ideal testbed of relativistic quantum mechanics, have been widely used to explore not only the exotic transport properties of Dirac fermions but also to confirm classic quantum-mechanical phenomena such as the Aharanov-Bohm effect. Motivated by a recent experiment [1], here we perform quantum transport simulations in the ballistic limit at zero temperature, considering an Aharanov-Bohm ring made of graphene with the same sample and gate geometry as the experiment. Preliminary properties from our simulations such as the gate and magnetic field dependence of the two-terminal conductance are rather consistent with the experiment, confirming their claim of the observed Aharanov-Bohm effect. To probe the effect of Klein tunneling, however, we propose a modified design using a local gate that makes pn interfaces perpendicular to the arm of the ring, different from the experiment. Based on our new design, we show that Klein tunneling may sharpen the Aharanov-Bohm oscillation frequency due to the screening of the transverse modes.

[1] J. Dauber et al., arXiv:2008.02556v3

TT 16.10 Mon 15:00 P2/OG4

Transport properties of pn junctions in 2D materials: Graphene vs MoS_2 — •Yu-Ting Xiao and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Graphene and monolayer MoS_2 both belong to the family of 2D materials. The former is known as a Dirac semimetal where electrons behave like relativistic Dirac fermions due to the gapless energy band linear in momentum, while the latter shows typical semiconducting behaviors due to the gapped energy band quadratic in momentum, with which electrons behave as standard Schrödinger fermions. In terms of transport, Dirac and Schrödinger electrons exhibit distinct behaviors, among which the so-called Klein tunneling [1] is perhaps one of the best known. To further identify their difference in transport properties, here we perform quantum transport simulations for pn junctions in various 2D systems, including graphene, MoS_2, and other toy models for 2D semiconductors. Our results identify transport properties that are unique to Dirac fermions as well as those that do not significantly differ from the two.

[1] M. Katsnelson, K. Novoselov, and A. Geim, Nat. Phys. 2, 620 (2006)

TT 16.11 Mon 15:00 P2/OG4

Quantum transport simulation for graphene devices with sawtooth-shaped n-p-n junctions — •Zhe-Bin Hsu and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Graphene, a gapless two-dimensional semimetal made of carbon atoms arranged in a honeycomb lattice, is an ideal platform for studying electron optics both experimentally and theoretically. Because of its lack of energy gap, n- and p-type carriers in graphene can be easily tuned simply by electrical gating. Typical graphene n-p-n junctions are created by local gates of rectangular shapes that exhibit Fabry-Pérot interference of electron waves in the clean limit. A recent experiment [1] realized a Dirac fermion reflector of graphene using sawtooth-shaped npn junctions, reporting not only the suppressed Fabry-Pérot interference but also resistance enhancement. Motivated by this experiment, we perform quantum transport simulations for graphene considering similar gate and sample geometries. Good consistency between our simulation and the experiment [1] will be shown. Further tests on other shaped top gates are performed in order to find the optimal gate geometry for best enhanced resistance. Our work shows that sawtooth-shaped graphene n-p-n junctions cannot work as a field-effect transistor (FET), even though the transmission can be reduced by a certain amount.

[1] S. Morikawa et al., Semicond. Sci. Technol. 32, 045010 (2017)

TT 16.12 Mon 15:00 P2/OG4

Electron correlation and confinement effects in quasi-one-dimensional quantum wires at high-density — Ankush Girdhar[1], Vinod Ashokan[1], Neil Drummond[2], •Klaus Morawetz[3,4], and Kare Narain Pathak[5] — [1]Department of Physics, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar (Punjab), 144 011, India — [2]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom — [3]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [4]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [5]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India

The correlation energy, pair-correlation function, static structure factor, and momentum density of ferromagnetic quasi-one-dimensional quantum wires are calculated using the quantum Monte Carlo (QMC) method for various wire widths b and density parameters r_s. The peak in the static structure factor at $k = 2k_F$ grows as the wire width decreases. The Tomonaga-Luttinger liquid parameter K_ρ is found to increase by about 10% between wire widths $b = 0.01$ and $b = 0.5$. The ground-state properties of finite thickness wires is compared to the first-order random phase approximation (RPA), which is exact in the high-density limit. Analytical expressions for the static structure factor and correlation energy are derived.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] Phys. Rev. B 101 (2020) 075130
[4] Phys. Rev. B 104 (2021) 035149
[5] Phys. Rev. B 105 (2022) 115140

TT 16.13 Mon 15:00 P2/OG4

Ground state properties of electron-electron biwire systems — Rajesh O. Sharma[1], Neil Drummond[2], Vinod Ashokan[1], Kare Narain Pathak[3], and •Klaus Morawetz[4,5] — [1]Department of Physics, Dr. B.R. Ambedkar National Institute of Technology, Jalandhar (Punjab), 144 011, India — [2]Department of Physics, Lancaster University, Lancaster LA1 4YB, United Kingdom — [3]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [4]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [5]International Institute of Physics-UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

Variational Monte Carlo (VMC) method is used to study the ground-state properties of a parallel infinitely-thin electron-electron quantum biwire system. The ground-state energy, the correlation energy, the interaction energy, the pair-correlation function (PCF), the static structure factor (SSF), and the momentum distribution (MD) function is calculated. As two parallel wires approach each other, inter-wire correlations increase while intra-wire correlations decrease. The SSF shows a peak at $2k_F$ at higher densities. A second peak starts to appear at $4k_F$ when $r_s = 2$ and $d = 0.2$ a.u. For lower densities, the first peak completely disappears and the height of the second peak keeps increasing with r_s and d. The behaviour of the PCF and SSF show that the electron-electron biwire system under goes into a quasi-Wigner crystalline state at densities higher compared to the case of a single wire.

[1] Eur. Phys. J. B 91 (2018) 29
[2] Phys. Rev. B 97 (2018) 155147
[3] Phys. Rev. B 101 (2020) 075130
[4]Phys. Rev. B 104 (2021) 035149]

TT 16.14 Mon 15:00 P2/OG4

Integrating coplanar resonators and carbon nanotubes for microwave optomechanics — Akong Loh, Fabian Stadler, •Furkan Özyigit, Nicole Kellner, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

The optomechanical coupling of a carbon nanotube and a superconducting coplanar microwave resonator has been achieved [1,2] in our previous work. The carbon nanotube acts as a quantum dot, responding to gate voltages in a highly nonlinear way. This can be used to enhance the optomechanical coupling strength by several orders of magnitude. Recent work has focused on improving the electronic properties of the microwave resonators, to maximize quality factors in presence of the nanotube coupling electrodes. Currently, we redevelop insertion of carbon nanotubes as the mechanical counterpart. Here, we give an overview of recent improvements and ongoing measurements on this fascinating optomechanical system: at proper optimization, it can have figures of merit close to several interesting parameter regimes, as, e.g., strong optomechanical coupling (with hybridization of vibrons and photons) and the quantum coherent limit (where manipulation is faster than thermal decoherence).

[1] S. Blien *et al.*, Nat. Comm. **11**, 1636 (2020)
[2] N. Hüttner *et al.*, in preparation.

TT 16.15 Mon 15:00 P2/OG4

Description of defective graphene by means of the Dirac equation coupled to curvature and torsion — •Enkeleta Berisha and Nikodem Szpak — Fakultät für Physik, Universität Duisburg-Essen, Duisburg, Germany

The continuum theory of lattice defects (dislocations and disclinations) offers a practical description of the electron transport at the mesoscale at which the microscopic (ab initio) models become too complex. It can be linked to the geometrical concepts of curvature and torsion whithin the Riemann-Cartan geometry. In General Relativity there is an ongoing discussion about the equivalence of these two objects. In solid state physics both objects have concrete interpretations in terms of disclinations and dislocations. The application to a two-dimensional system can shed new light on this problem. We focus on graphene whose electron dynamics is described by the Dirac equation which exhibits such defects. This leads to the coupling of the effective Dirac equation to curvature and torsion, thus opening the possibility of mapping these objects onto each other. We study particular lattice configurations and interpret them in terms of curvature or torsion. Moreover, we compare the quantum current flows with the semiclassical trajectories in the effective Riemann-Cartan geometry.

TT 16.16 Mon 15:00 P2/OG4

Strain-induced pseudo-Landau levels in semimetals from dimensional reduction — •Fabian Köhler and Matthias Vojta — Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

Non-uniform strain applied to graphene's honeycomb lattice can induce pseudo-Landau levels in the single-particle spectrum. We generalize this procedure to d-dimensional hyperdiamond-lattices and solve the corresponding continuum theory. The unstrained tight-binding Hamiltonian has semimetallic bandstructure with a (d-2)-dimensional nodal manifold, which transforms into a series of relativistic Landau levels under suitable strain. We show that a mechanism of dimensional reduction is at play here that goes beyond the conventional minimal coupling framework. This mechanism generates two-dimensional Landau-level problems with identical level spacing at each point of the nodal manifold.

TT 16.17 Mon 15:00 P2/OG4

Semi-classical vibrational dynamics in molecular junctions: Anharmonic potentials and non-linear couplings — •Martin Mäck, Samuel Rudge, and Michael Thoss — Physikalisches Institut, Universität Freiburg

Non-conservative current-induced forces can lead to vibrational instabilities in molecular junctions, even at low bias voltages [1]. A common approach is to treat the vibrational dynamics semi-classically as influenced by quantum mechanical electronic degrees of freedom. Within these treatments, the vibrational modes are often assumed to be harmonic and linearly coupled to the electronic degrees of freedom. However, at the onset of vibrational instabilities, such harmonic potentials might no longer realistically describe the dynamics.

In this contribution, we use a recently developed hierachical equations of motion (HEOM) approach [2] to semi-classical Langevin dynamics [3] to study systems for which the introduction of anharmonic potentials and non-linear electron-vibrational coupling might play an important role for the vibrational dynamics of the system.

[1] J.T. Lü, M. Brandbyge, and P. Hedegård, Nano Lett. 2010, 10, 5, 1657
[2] C. Schinabeck, A. Erpenbeck, R. Härtle, and M. Thoss, Phys. Rev. B 94, 201407
[3] S. L. Rudge, Y. Ke, and M. Thoss, arXiv: 2211.14215

TT 16.18 Mon 15:00 P2/OG4

Solving non-interacting open bosonic systems — •Steven Kim and Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University

Open quantum systems that interact with their Markovian environment are described by a Lindblad master equation. We study non-interacting bosonic systems that are subject to single photon loss. The corresponding Liouvillian superoperator is at most of quadratic order in ladder operators. An analysis of the eigenvalues can give insight into possible instabilites as well as phase transitions. Especially the latter has gained growing interest for PT-symmetric systems. The difficulty in solving such systems for its eigenmodes lies in preserving the canonical commutation relation, which is why the standard way of diagonalization is not possible. In this work, we propose a new method to obtain the diagonalized form of any non-interacting bosonic system using symplectic transformations. We are able to diagonalize a general complex matrix, while maintaining the symplectic form that encodes the commutation relations of the bosonic ladder operators. We show that non-Hermitian Hamiltonians naturally appear while solving the Lindblad master equation and that the eigenmodes can be obtained by solving a reduced system. Including counting fields into the Lindbladian makes the efficient calculation of the cumulant generating functions of arbitrary observables possible.

TT 17: Topology: Quantum Hall Systems

Time: Monday 16:45–18:45 Location: HSZ 304

TT 17.1 Mon 16:45 HSZ 304

Quantum Hall effect in the 2d topological insulator HgTe in pulsed magnetic fields of up to 65 T — •Christopher Fuchs[1,2], Tobias Kiessling[1,2], Saquib Shamim[1,2], Lena Fürst[1,2], Hartmut Buhmann[1,2], and Laurens W. Molenkamp[1,2] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]Institute for Topological Insulators, Würzburg, Germany

HgTe quantum wells are a two-dimensional topological insulator with highest electron mobilities as large as $1 \cdot 10^6\,\mathrm{cm}^2/\mathrm{Vs}$. As a result of this outstanding sample quality, the material shows a well-resolved electron-type as well as hole-type quantum Hall effect, which has been studied extensively at lowest temperatures and in fields of up to 16 T. Here, we present an extension of this parameter space all the way to 65 T using pulsed magnetic fields. The high field behavior of the electron-type quantum Hall effect is studied, revealing that it forms a smooth continuation of the low field (< 20 T) behavior. For example, a characteristic breakdown of the quantum Hall effect, which occurs at the filling factor $\nu = 1/2$, is observed at > 50 T for corresponding carrier densities. In addition, a general circuit, wiring and analysis scheme for measurements of the quantum Hall effect within a few milliseconds (a magnetic field pulse lasts only around 100 ms) is presented, along with design rules for gated samples. The presented method is universal and can be applied to any other gated semiconductor/2d sample for transport studies in pulsed magnetic fields.

TT 17.2 Mon 17:00 HSZ 304

Robustness of the topological quantization of the Hall conductivity for correlated lattice electrons at finite temperatures — Anton Markov[1], •Georg Rohringer[2], and Alexey Rubtsov[1] — [1]Moscow, Russia — [2]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany

Electrons on a two-dimensional lattice which is exposed to a strong uniform magnetic field show intriguing physical phenomena. The spectrum of such systems exhibits a complex (multi)band structure known as Hofstadter's butterfly. For fillings at which the system is a band insulator, one observes a quantized integer-valued Hall conductivity σ_{xy} corresponding to a topological invariant, the first Chern number C_1 . This is robust against many-body interactions as long as no changes in the gap structure occur. Strictly speaking, this stability holds only at zero temperatures T , while for $T > 0$ correlation effects have to be taken into account. In our paper, we address this question by presenting a dynamical mean-field theory (DMFT) study of the Hubbard model in a uniform magnetic field. The inclusion of local correlations at finite temperature leads to (i) a shrinking of the integer plateaus of σ_{xy} as a function of the chemical potential and (ii) eventually to a deviation from these integer values. We demonstrate that these effects can be related to a correlation-driven narrowing and filling of the band gap, respectively.

Invited Talk TT 17.3 Mon 17:15 HSZ 304

Noise signatures of anyon statistics and Andreev scattering in the $\nu = 1/3$ fractional quantum Hall regime — •Anne Anthore, Pierre Glidic, Olivier Maillet, Colin Piquard, Abdel Aassime, and Frédéric Pierre — U Paris Cité, U Paris-Saclay, CNRS, C2N, Palaiseau (France)

Anyons are exotic quasiparticles which can carry a fractional charge of an electron and with an exchange statistics inbetween that of fermions and bosons. These properties were revealed using quantum point contacts (QPC) in the fractional quantum Hall regime[1,2].

In this talk, I will report further noise investigation of anyon physics. Sourcing e/3 anyons at a first QPC, noise measured on a downstream "analyzer" QPC reveals different mechanisms. Setting the analyser to allow e/3 tunneling charges, we reproduce the negative cross-correlations previously observed[2], indicative of a non-trivial anyon exchange phase[3]. When 1 e charges tunnel across the analyser, the braid phase is predicted to be trivial. Our observation of negative cross-correlations points on a scattering mechanism akin to Andreev reflection at Normal/Superconductor interfaces, as suggested in[4].

Remarkably, in both cases, electrical conduction across the analyzer conserves neither the nature nor the number of quasiparticles, rending the beam-splitter analogy of a QPC lapsed.

[1] L. Saminadayar et al., PRL 79, 2526 (1997)
[2] H. Bartolomei et al., Science 368, 173 (2020)
[3] B. Rosenow et al., PRL 116, 156802 (2016)
[4] C. L. Kane and M. P. A. Fisher, PRB 67, 045307 (2003)

TT 17.4 Mon 17:45 HSZ 304

Topological properties of a two-dimensional non-symmorphic wallpaper group lattice — •Miguel Ángel Jiménez Herrera[1] and Dario Bercioux[1,2] — [1]Donostia International Physics Center, 20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

We investigate the topological spectral properties of a two-dimensional electronic lattice belonging to a non-symmorphic wallpaper group: the herringbone lattice. We induce the topological phase either by applying an external magnetic field perpendicular to the plane of the lattice, and by enabling spin-orbit coupling of Kane-Mele type. On the one hand, when applying a magnetic field, the bands of the lattice rearrange into Landau levels. The phase diagram of the system shows a fractal disposition of the band gaps, known as the Hofstadter butterfly. Each gap is characterized by a non-zero Chern number whose distribution follows the Diophantine equation. On the other hand, we study the effects of enabling spin-orbit coupling in the lattice. We study both bulk and ribbon geometry, to reveal the helical states appearing at the edges of the ribbon, arising from the topological properties of the bulk.

TT 17.5 Mon 18:00 HSZ 304

Hofstadter butterflies in hyperbolic space — •Alexander Stegmaier[1], Lavi Upreti[4], Ronny Thomale[1], and Igor Boettcher[2,3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, University of Alberta, Edmonton, Alberta T6G 2E1, Canada — [3]Theoretical Physics Institute, University of Alberta, Edmonton, Alberta T6G 2E1, Canada — [4]Department of Physics, University of Konstanz, 78464 Konstanz, Germany

Hofstadter's Butterfly is the spectrum of a charged particle moving in a tight binding lattice under a constant magnetic field. Beyond its well-known fractal-shaped spectrum, this model is also relevant as a prototypical topological Chern insulator.

In light of recent interest in the physics of lattices in hyperbolic space, we re-consider the problem of Hofstadter's butterfly in {p,q} lattices. They tile the hyperbolic plane, a 2D space with constant negative curvature, with regular p-gons, q of which meet at each vertex. We develop methods to calculate the bulk spectra of a hyperbolic tight-binding system and apply them to uncover the features of Hofstadter's Butterflies in hyperbolic space. We find that the move to negatively curved space destroys the spectra's fractality, but preserves features of the spectral gaps, depending on the type of tiling {p,q}.

TT 17.6 Mon 18:15 HSZ 304

Observation and applications of non-Hermitian topology in a multi-terminal quantum Hall device — •Kyrylo Ochkan[1], Viktor Könye[1], Anastasiia Chyzhykova[1,2], Jan Budich[3], Jeroen van den Brink[1], Cosma Fulga[1], and Joseph Kyrylo[1] — [1]IFW Dresden, Deutschland — [2]Taras Shevchenko National University of Kyiv, Ukraine — [3]TU Dresden, Deutschland

One of the simplest examples of non-Hermitian topology is encountered in the Hatano-Nelson (HN) model, a one-dimensional chain where the hopping in one direction is larger than in the opposite direction. We present here the first experimental observation of non-Hermitian topology in a quantum condensed-matter system. The measurements are done in a multi-terminal quantum Hall device etched in a high mobility GaAs/AlGaAs two-dimensional electron gas ring. The conductance matrix that connects the currents flowing from the active contacts to the ground with the voltage of the active contacts is topologically equivalent to the HN Hamiltonian.

In our device, we directly measure and evidence the non-Hermitian skin effect. We also compute for our experimental device two topological invariants that are found to be more robust than the Chern number. We finally use the unique properties of our system and continuously tune the system configuration between open and periodic boundary conditions.

In this talk, we present the latest developments with regard to the application of the devices with these topological properties.

TT 17.7 Mon 18:30 HSZ 304

Dirac Landau levels on a pseudosphere — •Maximilian Fürst[1], Denis Kochan[1,2], Cosimo Gorini[3], and Klaus Richter[1] — [1]Universität Regensburg, 93053 Regensburg, Deutschland — [2]Slovak Academy of Sciences, 84511 Bratislava, Slovakia — [3]Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Topological insulator nanowires host Dirac-like surface states with strongly suppressed backscattering [1]. As suggested in Ref. [2], surfaces with conical singularity could host Quantum Hall states which lead to an intrinsic angular momentum quantization of an electronic fluid which is put on the tip of the singularity. Topological insulators might be a good platform to examine this experimentally. However, they host surface states with Dirac-like dispersion instead of Schrödinger-like which is assumed in Ref. [2]. This raises the question if such effect may also be observed in those systems. A first step towards the answer is to choose an appropriate surface and calculate the Dirac Landau levels on it. We choose the pseudosphere which has a conical singularity and allows for analytical solution of the emerging eigenvalue equations. The spectrum and the eigenstates are computed for a constant magnetic field which is aligned perpendicularly to the surface. We further use the tight-binding package *Kwant* [3] to verify our analytically gained results numerically (see Ref. [4]).

[1] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011)
[2] T. Can *et al.*, Phys. Rev. Lett. **117**, 266803 (2016)
[3] C. W. Groth *et al.*, New J. Phys. **16**, 063065 (2014)
[4] R. Kozlovsky *et al.*, Phys. Rev. Lett. **124**, 126804 (2020)

TT 18: Nano- and Optomechanics

Time: Monday 17:15–18:30 Location: HSZ 201

TT 18.1 Mon 17:15 HSZ 201

Microwave optomechanics of the transversal carbon nanotube vibration — •Akong Loh, Fabian Stadler, Furkan Özyigit, Nicole Kellner, Niklas Hüttner, and Andreas K. Hüttel — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Recently, optomechanical coupling of a carbon nanotube and a coplanar microwave resonator has been achieved[1,2]. In this case, the nanotube acts as a mechanical resonator as well as a quantum dot. The coupling is enhanced by several order of magnitude by via the nonlinearity of Coulomb blockade. This novel optomechanical system presents several interesting features. For optimized paramters, e.g., strong optomechanical coupling (with hybridization of vibrons and photons) and the quantum coherent limit (where manipulation is faster than thermal decoherence) could be reached. Significant improvements of our microwave resonators have recently been achieved. Ongoing work aims to optimize the mechanical resonator, via improving the nanotube growth and the transfer of the nanotubes onto the resonator chip, as well as the cryogenic millikelvin setup for the measurements.

[1] S. Blien *et al.*, Nat. Comm. 11, 1636 (2020)
[2] N. Hüttner *et al.*, in preparation.

TT 18.2 Mon 17:30 HSZ 201

Squeezed mechanical states in nano-electromechanical systems — •Korbinian Rubenbauer[1,2,3], Thomas Luschmann[1,2,3], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayrische Akademie der Wissenschaften, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technologies, Munich, Germany

The generation of nonclassical quantum states in a mechanical system such as squeezed states is not only an essential milestone for quantum-enhanced sensing of ultra-small forces and accelerations, but will also enhance our understanding of the foundations of quantum theory. Optomechanical systems coupling a mechanical displacement to a microwave resonator represent one way to implement protocols resulting in squeezed mechanical states and their readout. Here, we experimentally explore a scheme for the generation and detection of squeezed mechanical states using microwave control and spectroscopy of a nanoelectromechanical system. In detail, we investigate a system based on a nanomechanical string resonator inductively coupled via a SQUID to a superconducting microwave resonator. Within this presentation, we discuss the challenges regarding the experimental implementation and the required parameter regime, and present preliminary experimental data.

TT 18.3 Mon 17:45 HSZ 201

Nanowire deflection detection based on a coupled mechanical oscillator — Maneesha Sharma, Aniruddha Satyadharma Prasad, Norbert H. Freitag, Bernd Büchner, and •Thomas Mühl — Leibniz Institute for Solid State and Materials Research IFW Dresden, 01069 Dresden, Germany

The field of nanowire (NW) technology represents an exciting and steadily growing research area with applications in ultra-sensitive mass and force sensing. Existing detection methods for NW deflection and oscillation include optical and field emission approaches. However, they are challenging for detecting small diameter NWs because of heating produced by the laser beam and the impact of the high electric field. Alternatively, the deflection of a NW can be detected indirectly by co-resonantly coupling the NW to a cantilever and measuring it using a scanning probe microscope. Here, we prove experimentally that co-resonantly coupled devices are sensitive to small force derivatives in a similar way as standalone NWs do. We detect force derivatives as small as 10^{-9} N/m with a bandwidth of 1 Hz at room temperature. The detection technique presented in this work verifies a major step in boosting NW-based force and mass sensing.

TT 18.4 Mon 18:00 HSZ 201

Symmetry breaking in a parametrically modulated quantum oscillator — •Daniel Boness[1], Mark Dykman[2], and Wolfgang Belzig[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Department of Physics and Astronomy, Michigan State University, East Lansing, Michigan 48824, USA

A weakly damped nonlinear oscillator modulated close to twice its eigenfrequency has two stable states, which have the same vibration amplitudes but opposite phases. The states are equally populated due to classical or quantum fluctuations.

An extra force at half the modulation frequency lifts the symmetry of the states, generally. We study how the symmetry breaking occurs in the quantum regime.

As we show, a significant change of the state populations can take place already for a weak extra force. The mechanism is the force-induced change of the rates of interstate switching. The change is exponential in the ratio of the force amplitude to the appropriately scaled quantum length. It is large even where the effect of the force on the mean-field oscillator dynamics is small.

TT 18.5 Mon 18:15 HSZ 201

Quantum friction between metals in the hydrodynamic — •Kunmin Wu, Thomas Schmidt, and Maria Belén Farias — Faculty of Science, Technology and Medicine, 162 A, avenue de la Faïencerie, L-1511 Luxembourg

In this work, we study the phenomenon of quantum friction in a system consisting on a moving atom at a constant speed parallel to a metallic slab. We use a hydrodynamic model to describe the degrees of freedom of a clean metal without internal dissipation. The moving and polarizable atom is modeled as a two-level system with a unique (l = 0) ground state and a three-fold degenerate (l = 1) excited state. We show that a quantum frictional force is present even in the absence of intrinsic damping in the metal, but that there is a velocity threshold giving rise to such a force. In particular, to have non-vanishing friction demands that the atom must move at a velocity larger than the effective speed of sound in the material. We provide analytical arguments to show that this result holds at all orders in perturbation theory. Besides, we also explore how the spatial dispersion, which is determined by the sound speed in the hydrodynamic regime, affects the friction. Our numerical results show that the spatial dispersion has less effect on the friction when the speed of atom is much higher than the sound speed.

TT 19: Focus Session: New Perspectives for Adiabatic Demagnetization Refrigeration in the Kelvin and sub-Kelvin Range (joint session TT/MA)

Efficient cooling into the Kelvin and sub-Kelvin range is a long-standing challenge relevant to both fundamental research and future quantum technologies. The standard cooling cycle based on vapor compression exploits expensive and rare helium. Low-temperature physicists world-wide are presently looking for cheaper and accessible alternatives, not to mention the need of compact cooling technology for desktop quantum technology, or special requirements for applications such as space missions and scanning tunneling microscopes. One of the key candidates is adiabatic demagnetization refrigeration (ADR). ADR is based on magnetic solids with a huge magnetocaloric effect and requires no helium. Even if paramagnetic salts are known and used for ADR applications for almost a century, there is an ongoing quest for materials with better magnetocaloric and mechanical properties, thermal conductivity, and vacuum compatibility. In this symposium, new fundamental ideas and the recent successful design and characterization of quantum materials for improved ADR will be highlighted. These materials exploit collective phenomena in correlated electron systems, such as the concept of geometrically frustrated magnetism to push the entropy to low temperatures, as well as heavy-fermion, and quantum-critical states.

Organizers: Andreas Honecker (CY Cergy Paris Université) and Jürgen Schnack (Universität Bielefeld)

Time: Tuesday 9:30–13:15 Location: HSZ 03

Invited Talk TT 19.1 Tue 9:30 HSZ 03

Self-cooling molecular spin quantum processors — •Marco Evangelisti[1], Fernando Luis[1], Elias Palacios[1], David Aguilà[2], and Guillem Aromí[2] — [1]INMA, CSIC & Universidad de Zaragoza, Spain — [2]Dept. Química Inorgànica, Universidad de Barcelona, Spain

Cryogenic refrigeration is crucial for a wide range of emerging applications in the field of quantum technologies. Indeed, thermal energy must be minimized to avoid the excitation of vibrational motions that could disturb quantum operations. Synthetic chemistry provides a sophisticated methodology for the design and synthesis of materials displaying a wide variety of properties. Molecular materials are capable of excellent and unique characteristics that can be exploited either for caloric cooling[1] or spin-based quantum computing[2]. However, these features are not yet being implemented as such to act together within the same material, that is, at the molecular scale. Here, we show that a spin qubit (or qudit) can be brought into proximity with a spin centre that acts as a cooler. To this end, we make use of rare-earth-based asymmetric molecular dimers. A chemically engineered structural asymmetry introduces different coordination environments for each metal ion, operating similarly as for molecular quantum gates reported by some of us[3]. This strategy allows selecting individually both constituent ions, leading to e.g. the direct observation of the cooling of a single Er(III) ion qubit, or a Tm(III) electronuclear spin qudit, driven chiefly by the demagnetization of a single Gd(III) ion located within the same molecule.

[1] Dalton Trans. 39, 4672 (2010)
[2] Nat. Chem. 11, 301 (2019)
[3] Phys. Rev. Lett. 107, 117203 (2011)

Invited Talk TT 19.2 Tue 10:00 HSZ 03

Triangular rare-earth borates for milli-Kelvin adiabatic demagnetization refrigeration — •Philipp Gegenwart — Experi-

mental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

Adiabatic demagnetization refrigeration (ADR) is a classical cooling technique with renewed recent attention as alternative to costly and elaborate ^{3}He/^{4}He dilution refrigeration. Established water containing ADR salts suffer from chemical instability which requires delicate treatment to avoid degradation and ensure good thermal contact. Water-free $KBaYb(BO_3)_2$ is an excellent alternative with high entropy density that allows ADR to below 20 mK [1]. Sintered pellets with silver powder admixture to ensure good thermal coupling are easy to manufacture, inexpensive and long-term stable even upon heating up to 700°C, enabling also ultra-high vacuum applications. $KBaYb(BO_3)_2$ belongs to a family of rare-earth-based borates with triangular arrangement of magnetic moments. We discuss the impact of geometrical frustration and structural randomness on its low-temperature properties and demonstrate the enormous tunability of cooling power and operating temperature by chemical substitution.

[1] Y. Tokiwa, S. Bachus, K. Kavita, A. Jesche, A.A. Tsirlin, and P. Gegenwart, Commun. Mater. 2 (2021) 42.

Invited Talk TT 19.3 Tue 10:30 HSZ 03

A millikelvin scanning tunnelling microscope in ultra-high vacuum with adiabatic demagnetisation refrigeration — •Ruslan Temirov — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — University of Cologne, Institute of Physics II, Cologne, Germany

Scanning tunnelling microscopes (STMs) operating in ultra-high vacuum (UHV) and low-temperature conditions are used widely for imaging and precise manipulation of surface nanostructures. A growing interest in studies of quantum-coherent phenomena in such nanostructures stimulates the development of STMs that operate at very low millikelvin temperatures. This contribution presents the design of a first-ever UHV STM cooled by adiabatic demagnetisation refrigeration (ADR) to below 30 mK. The use of ADR makes the STM design modular and helps it to reach a remarkable degree of mechanical stability. Tunnelling spectra collected on an atomically clean superconducting Al(100) surface reveal that the electronic temperature of the tunnelling junction is less than 80 mK. The inelastic electron tunnelling spectroscopy of an individual electron spin performed in magnetic fields of up to 8 Tesla validates the STM capabilities for quantum nanoscience research.

15 min. break

Invited Talk TT 19.4 Tue 11:15 HSZ 03

ADR cryostats in low temperature physics and their applications — •Doreen Wernicke — Entropy GmbH, Gmunder Str. 37a, 81379 München

Entropy GmbH is a company founded in 2010 in Munich, Germany, specializing in the development and manufacture of low temperature cryostats. All Entropy cryostats are based on closed-cycle pre-cooling to temperatures below 3K. Further cooling stages such as ADR units, Joule-Thomson stages, and dilution refrigerators including electronics and software are proprietary developments. The modular design of all cryostats offers the possibility of adaptation to many different experiments and applications. One of Entropy's most common products are the ADR cryostats. The presentation will explain the principle of ADR cooling and features such as base temperature and holding time at operating temperature. Applications for low temperature device operation such as various types of superconducting detectors (TES, MKIDs, SQUIDs, SNSPDs) and Qubit characterization will be presented to demonstrate the performance and limitations of adiabatic demagnetization refrigeration.

Invited Talk TT 19.5 Tue 11:45 HSZ 03

Frustrated dipolar materials for low-temperature magnetic refrigeration — •Mike Zhitomirsky — Institute of Interdisciplinary Research, CEA-Grenoble, France

Low-temperature refrigeration is crucial for emergent quantum-information technologies and other scientific applications that outstretch from space telescopes to medicine. This growing demand fuels an interest in alternative low-temperature techniques including the adiabatic demagnetization refrigeration. The existing ADR technologies for the sub-Kelvin range utilize dilute paramagnetic salts of Cr and Fe magnetic ions, which have limited efficiency at higher temperatures. I shall discuss general directions of the ongoing search of prospective refrigerant materials by exploring collective effects in systems of interacting magnetic moments as opposed to noninteracting moments in paramagnetic salts. Specifically, I focus on geometrically frustrated magnets with a residual ground-state degeneracy as well as on dipolar magnets. I present new experimental and theoretical results obtained recently in Grenoble for two dipolar materials: $Yb_3Ga_5O_{12}$, which is a spin-1/2 dipolar ferromagnet on a hyper-Kagome lattice, and $GdLiF_4$, which exhibits a hidden magnetic frustration. The striking properties of the latter material including a fractional magnetization plateau demonstrate importance of new magnetocaloric materials not only for applied but also for basic research in magnetism.

TT 19.6 Tue 12:15 HSZ 03

ADR based sub-Kelvin cryostats for applied quantum technologies — •Pau Jorba[1], Felix Rucker[1], Steffen Säubert[1], Alexander Regnat[1], Jan Spallek[1], and Christian Pfleiderer[2] — [1]kiutra GmbH, Flößergasse 2, D-81369 München, Germany — [2]Physik-Department, Technische Universität München, D-85748 Garching, Germany

In view of the increasing demand for the cooling of quantum electronic devices, the development of scalable cooling solutions that provide low temperatures independent of rare helium-3 will be mandatory for the adoption and commercial use of next-generation quantum technologies. We present novel ADR based sub-Kelvin cryostats[1] specifically developed for the characterization and operation of quantum devices. We address how known challenges of ADR systems such as limited hold time and magnetic stray fields can be overcome. Specifically, we describe how continuous sub-Kelvin cooling and wide-range temperature control can be achieved by combining multiple ADR units and mechanical thermal switches. We also present a novel sample loader mechanism[2] that allows taking advantage of the solid-state nature of ADR and to cool samples from room temperature to 100 mK in less than 3 hours.

[1] Regnat et al. (2018) Cryogen-free cooling apparatus (EP 3163222). European Patent Office.
[2] Spallek et al. (2022) System and method for inserting a sample into a chamber (EP 3632560). European Patent Office.

TT 19.7 Tue 12:30 HSZ 03

ADR below the ordering temperature in triangular $KBaGd(BO_3)_2$ — •Noah Winterhalter-Stocker[1], Alexander Bellon[1], Fabian Hirschberger[1], Sebastian Bachus[1], Sebastian Erdmann[1], Alexander Tsirlin[1,2], Yoshifumi Tokiwa[1,3], Anton Jesche[1], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86159 Augsburg, Germany — [2]Felix Bloch Institute for Solid-State Physics, Leipzig University, D-04103 Leipzig, Germany — [3]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195, Japan

Compared to the triangular ADR magnet $KBaYb(BO_3)_2$ [1] the isotructural sister compound $KBaGd(BO_3)_2$ with spin 7/2 moments has a three times enhanced magnetic entropy density of 192 $mJK^{-1}cm^{-3}$. We report a low-temperature magnetic and thermodynamic investigation of polycrystalline $KBaGd(BO_3)_2$ down to 50 mK. Specific heat indicates an antiferromagnetic phase transition at 263 mK, strongly broadened due to randomness and frustration, that becomes suppressed beyond 0.5 T. Further increase of magnetic field shifts the available entropy of R log 8 towards high temperatures. Interestingly, ADR of a pellet utilizing the same setup as used in [1] reveals a minimal temperature if $T_{\min}$=122 mK that is more than twice below T_N along with a hold time of more than 8 hours. The combination of minimal temperature and entropy density in $KBaGd(BO_3)_2$ is outstanding among known ADR materials.

[1] Y. Tokiwa *et al.*, Communications Materials **2.1**, 1-6 (2021)

TT 19.8 Tue 12:45 HSZ 03

Magnetocaloric properties of $(RE)_3Ga_5O_{12}$ (RE=Tb, Gd, Nd, Dy) — Markus Kleinhans[1], Klaus Eibensteiner[1,2], Jon Leiner[1], •Christoph Resch[1], Lukas Worch[1], Marc Wilde[1], Jan Spallek[1,2], Alexander Regnat[1,2], and Christian Pfleiderer[1] — [1]Physik Department, Technical University Munich, D-85748 Garching, Germany — [2]kiutra GmbH, Rupert-Mayer-Str. 44, D-81379 Munich, Germany

We report the characteristic magnetic properties of several members of the rare earth garnet family, $Gd_3Ga_5O_{12}$ (GGG), $Dy_3Ga_5O_{12}$ (DGG), $Tb_3Ga_5O_{12}$ (TGG), and Nd_3Ga5O_{12} (NGG), and compare their relative potential utility for magnetocaloric cooling, including their minimal adiabatic demagnetization refrigeration (ADR) temperatures and relative cooling parameters. A main objective of this work was to find potential improvements over the magnetocaloric properties of GGG for use in low temperature ADR cryostats. Using Tb^{+3} and Dy^{+3} in the RE-site oers, in principle, a higher saturation magnetization and Nd^{+3} gives a lower de Gennes factor and therefore potentially low transition temperature. Our results show that $Dy_3Ga_5O_{12}$ yields an optimal relative cooling parameter (RCP) at low applied fields and a low transition temperature, which would allow for the design of more efficient ADR cryostats.

[1] M. Kleinhans et al., arXiv/2204.01752; Phys. Rev. Appl. in press (2022).

TT 19.9 Tue 13:00 HSZ 03

Study of the large rotational magnetocaloric effect in Ni(en)(H_2O)$_4$$SO_4$·2$H_2O$ — •Róbert Tarasenko, Petro Danylchenko, Erik Čižmár, Vladimír Tkáč, Alexander Feher, Alžbeta Orendáčová, and Martin Orendáč — Institute of Physics, Faculty of Science, Pavol Jozef Šafárik University, Park Angelinum 9, 041 54 Košice, Slovakia

The title compound Ni(en)(H_2O)$_4$$SO_4$·2$H_2O$ (en = ethylenediamine) has been identified as a spin-1 paramagnet with the nonmagnetic ground state introduced by the easy-plane anisotropy $D/k_B = 11.6$ K with $E/D = 0.1$ and negligible exchange interactions $J \approx 0$. We present an experimental study of the rotational magnetocaloric effect (MCE) in single crystals at temperatures above 2 K, associated with adiabatic crystal rotation between the easy plane and hard axis in magnetic fields up to 7 T. The experimental observations are completed with *ab* initio calculations of the anisotropy parameters. Theoretical simulations of the rotational MCE in the $S = 1$ paramagnet were performed and the simulations were compared with experimental data. A large rotational magnetic entropy change ≈16.9 $\mathrm{Jkg^{-1}K^{-1}}$ has been achieved in 7 T. The adiabatic rotation of the crystal in 7 T starting at the initial temperature of 4.2 K leads to the cooling of the sample down to 0.34 K, which suggests the application of this material in low-temperatures cooling. Our simulations show that $S = 1$ Ni(II)-based systems with easy-plane anisotropy can have better rotational magnetocaloric properties than costly materials containing rare-earth elements.

Supported by project No. APVV-18-0197.

TT 20: Superconductivity: Tunnelling and Josephson Junctions

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

TT 20.1 Tue 9:30 HSZ 103

Calorimetry of a phase slip in a Josephson junction — Efe Gümüs[1], Danial Majidi[1], Danilo Nikolic[2], Patrick Raif[2], Bayan Karimi[3], Joonas Peltonen[3], Elke Scheer[2], Jukka Pekola[3], Hervé Courtois[1], Wolfgang Belzig[2], and •Clemens Winkelmann[1] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, Grenoble, France — [2]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [3]Centre of Excellence, Department of Applied Physics, Aalto University School of Science, Aalto, Finland

Josephson junctions are a central element in superconducting quantum technology; in these devices, irreversibility arises from abrupt slips of the quantum phase difference across the junction. This phase slip is often visualized as the tunnelling of a flux quantum in the transverse direction to the superconducting weak link, which produces dissipation. Here we detect the instantaneous heat release caused by a phase slip in a Josephson junction, signalled by an abrupt increase in the local electronic temperature in the weak link and subsequent relaxation back to equilibrium. Beyond the advance in experimental quantum thermodynamics of observing heat in an elementary quantum process, our approach could allow experimentally investigating the ubiquity of dissipation in quantum devices, particularly in superconducting quantum sensors and qubits.

TT 20.2 Tue 9:45 HSZ 103

Measurement of two coupled Bloch oscillators based on Al/AlO_x/Al-Josephson junctions — •Fabian Kaap and Sergey Lotkhov — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Deutschland Braunschweig

We investigate a system of two coupled Bloch oscillators based on $\sim 50 \times 50\,\mathrm{nm}^2$ Josephson junctions, where one oscillator is a flux tunable SQUID and one is a single junction, respectively. To suppress the quantum oscillations of charge and enable the occurrence of coherent Bloch oscillations, the leads include high ohmic microstrips made from oxidized titanium. Between the resistors and junctions, we design the connection via a capacitively coupled pair of high-kinetic-inductance meanders of granular aluminum. When only the single junction is actively driven by an external bias current I_{B1} the Coulomb blockade of this junction can be tuned by the flux through the passive, non-driven SQUID. If additionally a current I_{B2} is applied through the SQUID we observe synchronisation effects in the IV-curves of both Bloch oscillators when the currents coincide, $I_{\mathrm{B1}} \approx I_{\mathrm{B2}}$. We address experimental issues, such as electron overheating in the leads, the presence of higher harmonics at low bias currents and the onset of Zener tunneling.

TT 20.3 Tue 10:00 HSZ 103

Phase-dependent transport in thermally driven superconducting single-electron transistors — Alexander G. Bauer and •Björn Sothmann — Theoretische Physik, Universität Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

We investigate thermally driven transport of heat and charge in a superconducting single-electron transistor by means of a real-time diagrammatic transport theory. Our theoretical approach allows us to account for strong Coulomb interactions and arbitrary nonequilibrium conditions while performing a systematic expansion in the tunnel coupling. We find that a temperature bias across the system gives rise to finite heat and charge currents close to the particle-hole symmetric point which depend both on the gate voltage as well as on the phase difference between the superconducting reservoirs. The finite thermoelectric effect arises due to level renormalization from virtual tunneling processes. Furthermore, we find that the phase bias can give rise to finite charge currents even in the presence of an inversion-symmetric temperature bias.

TT 20.4 Tue 10:15 HSZ 103

Josephson nanojunctions fabricated by He focused ion beam irradiation — •Edward Goldobin[1], Max Karrer[1], Christoph Schmid[1], Katja Wurster[1], Ramón Manzorro[2,3], Javier Pablo-Navarro[2,3], Cesar Magen[2,3], Reinhold Kleiner[1], and Dieter Koelle[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain — [3]Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, Spain

We use a focused He ion beam (He-FIB) for the nanofabrication of Josephson junctions (JJs) and more complex devices based on $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films [1]. Using an optimum He-FIB irradiation dose, we “write” Josephson barriers across YBCO microbridges. Such JJs have RCSJ-like I–V characteristics, and the dependence of the critical current vs. magnetic field resembles a Fraunhofer pattern. Using higher irradiation doses, we induce insulating regions that can be used for nanopatterning of various circuits, i.e., patterning of SQUID loops, constriction JJs (cJJs), etc.

Investigations of the irradiated regions by scanning transmission electron microscopy (STEM) provide information on the modification of the crystalline structure of YBCO on the atomic scale. STEM analysis reveals the amorphization thresholds for irradiation of 1D and 2D patterns (depending on the beam size), and provides insights into the current resolution limits for the fabricaton of YBCO cJJs.

[1] B. Müller et al., Phys. Rev. Applied **11**, 044082 (2019)

TT 20.5 Tue 10:30 HSZ 103

Theory of scanned Josephson tunneling spectroscopy in cuprates — •Peayush Choubey[1] and Peter Hirschfeld[2] — [1]Department of Physics, Indian Institute of Technology Roorkee, Roorkee 247667, India — [2]Department of Physics, University of Florida, Gainesville, Florida 32611, USA

The scanned Josephson tunneling spectroscopy (SJTS) is a direct local probe of superconducting gap order parameter. To the best of our knowledge, SJTS studies have been limited to the cases where superconducting sample and superconducting tip, both, have the same gap symmetry- either s-wave or d-wave. One might assume that in an s-to-d SJTS study of cuprates the critical current would vanish everywhere, as naively expected for planar junctions. We show here that this is not the case. Employing first-principles Wannier functions for $Bi_2Sr_2CaCu_2O_8$, we develop a scheme to compute Josephson critical current and quasiparticle tunneling current measured by SJTS with sub-angstrom resolution. We demonstrate that the critical current due to tunneling between an s-wave tip and a superconducting cuprate sample has largest magnitude above O sites and it vanishes above Cu sites as a direct consequence of the d-wave gap symmetry in cuprates. Moreover, we predict various signatures of pair density waves in underdoped cuprates that can be tested in future SJTS studies.

TT 20.6 Tue 10:45 HSZ 103

Critical temperature of superconductor-ferromagnetic bilayers with helimagnetic metals — •Danilo Nikolic, Subrata Chakraborty, Alfredo Spuri, Elke Scheer, Angelo Di Bernardo, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Motivated by recent experiments on the proximity effect in superconductor-ferromagnet structures with the helimagnetic ordering of magnetization in the latter, we present a systematic theoretical study of the critical temperature of such systems. By employing the quasiclassical Usadel approach [1], we account for two different configurations of magnetization in the ferromagnet and investigate their impact on the critical temperature (T_c) of the superconductor. Besides recovering the known results for the case of uniform magnetization [2], we find a nontrivial behavior of T_c in the case of spiral magnetization. Our theory suggests that this can be attributed to the emergence of long-range spin-triplet correlations generated in the ferromagnet [3]. Finally, our model predicts that the presence of spiral magnetization can reduce the critical temperature in the experimentally relevant range of parameters. This effect is the subject of ongoing experiments.

[1] A. I. Buzdin, Rev. Mod. Phys. **77**, 935 (2005)
[2] Z. Radović *et al.*, Phys. Rev. B **44**, 759 (1991);
Ya. V. Fominov *et al.*, Phys. Rev B **66**, 014507 (2002)
[3] A. F. Volkov *et al.*, Phys. Rev. B **73**, 104412 (2006)

TT 20.7 Tue 11:00 HSZ 103

Equal-spin Cooper pair injection in superconducting spintronics devices — •Matthias Eschrig[1] and Xavier Montiel[2] — [1]Institute of Physics, University of Greifswald, Germany — [2]Department of Materials Science & Metallurgy, University of Cambridge, UK

In a number of recent experiments unusual behavior was observed in ferromagnet/ferromagnet/superconductor devices when a precession of the magnetization was induced by ferromagnetic resonance. By using a non-equilibrium Usadel Green function formalism, we solve for spin-resolved distribution functions and demonstrate that the spin injection process in superconductors is governed by the inverse proximity effect in the superconducting layer. We find that equal-spin Cooper pairs, which are produced by the two misaligned ferromagnetic layers, transport spin inside the S layer. This then results in an increase of the injected spin current below the superconducting critical temperature. Our calculations provide the first evidence of the essential role of equal-spin Cooper pairs on spin-transport properties of S/F devices and pave new avenues for the design of superconducting spintronics devices.

15 min. break

TT 20.8 Tue 11:30 HSZ 103

Vortex phase transitions in frustrated two-dimensional semiconductor-superconductor Josephson junction arrays — •Simon Reinhardt[1], Christian Baumgartner[1], Sergei Gronin[2], Geoffrey C. Gardner[2], Tyler Lindemann[2], Michael J. Manfra[2], Tatyana I. Baturina[1], Nicola Paradiso[1], and Christoph Strunk[1] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Purdue University, West Lafayette, Indiana 47907, USA

We study two-dimensional Josephson junction arrays in hybrid aluminum/InGaAs/InAs semiconductor-superconductor heterostructures. Using a cold resonator technique, we measure both the inductive response as well as the DC transport properties of the array. A perpendicular magnetic field induces highly ordered vortex configurations for integer and fractional values of the frustration parameter. In the vicinity of the matching fields we observe pronounced dip-to-peak transitions of the differential resistance as a function of current bias, which have previously been interpreted as signatures of a non-equilibrium vortex Mott transition [1]. The scaling behaviour of the differential conductance in our array of ballistic SNS junctions is compared with previous results on diffusive Josephson junction arrays.

[1] N. Poccia et al., Science **349**, 1202 (2015)

TT 20.9 Tue 11:45 HSZ 103

Engineering the speedup of quantum tunneling in Josephson systems via dissipation — •Dominik Maile[1], Joachim Ankerhold[1], Sabine Andergassen[2], Wolfgang Belzig[3], and Gianluca Rastelli[4] — [1]Institut für Komplexe Quantensysteme, Universität Ulm — [2]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen — [3]Fachbereich Physik, Universität Konstanz — [4]INO-CNR BEC Center and Dipartimento di Fisica, Università di Trento

We theoretically investigate the escape rate occurring via quantum tunneling in a system affected by tailored dissipation [1]. Specifically, we study the environmental assisted quantum tunneling of the superconducting phase in a current-biased Josephson junction. We consider Ohmic resistors inducing dissipation both in the phase and in the charge of the quantum circuit. We find that the charge dissipation leads to an enhancement of the quantum escape rate. This effect appears already in the low Ohmic regime and also occurs in the presence of phase dissipation that favors localization. Inserting realistic circuit parameters, we address the question of its experimental observability and discuss suitable parameter spaces for the observation of the enhanced rate.

[1] D.Maile *et al.*, PRB 106, 045408 (2022)

TT 20.10 Tue 12:00 HSZ 103

Complete magnetic control over the superconducting thermoelectric effect — •Jabir Ali Ouassou[1], César González-Ruano[2], Diego Caso[2], Farkhad G. Aliev[2], and Jacob Linder[1] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [2]Departamento Física de la Materia Condensada C-III, INC and IFIMAC, Universidad Autónoma de Madrid, Madrid 28049, Spain

Giant thermoelectric effects are known to arise at the interface between a superconductor and strongly polarized ferromagnet, and this enables the construction of efficient thermoelectric generators. We predict that the thermopower of such generators can be completely controlled by a magnetic input signal: not only can the thermopower be toggled on and off by rotating a magnet, but even the sign of the thermopower can be reversed. This *in situ* control diverges from conventional thermoelectrics, where the thermopower is usually fixed by the device design.

TT 20.11 Tue 12:15 HSZ 103

Quantum phases in a frustrated sawtooth chain of Josephson junctions — •Benedikt J.P. Pernack, Mikhail V. Fistul, and Ilya M. Eremin — Ruhr-Universität Bochum, Bochum Germany

We present a theoretical study of quantum phases occurring in a frustrated sawtooth chain of small Josephson junctions. In the model the frustration f arises due to the Josephson couplings having alternating signs (0 and π Josephson junctions) in a single lattice cell. At the critical value of $f = 3/4$ such a system displays a phase transition from the ordered state into the frustrated one with a highly degenerate ground state characterized by penetration of topological (anti)vortices [1]. Introducing additional capacitances to the ground, we derive an effective Ising quantum spins model with a long-range interaction between well separated vortices/antivortices, and obtain various collective quantum phases and quantum phase transitions between them.

[1] A. Andreanov and M. V. Fistul, J. Phys. A: Math. Theor. 52, 105101 (2019)

TT 20.12 Tue 12:30 HSZ 103

Low-energy model for superconducting quantum dot systems — •Vladislav Pokorný[1] and Martin Žonda[2] — [1]FZU - Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic

We present a method to extract the Andreev bound state energies of a single-level quantum dot connected to superconducting leads from the imaginary-time results of quantum Monte-Carlo method without the use of analytic continuation techniques like maximum entropy method. We describe the system using the superconducting impurity Anderson model and show that for low energies it maps on an atomic-like model. The parameters of this model can be extracted from the self-energy calculated in imaginary-frequency domain using the hybridization-expansion quantum Monte Carlo method. We compare the results to zero-temperature numerical renormalization group data to show the limits of usability of the low-energy model.

TT 20.13 Tue 12:45 HSZ 103

Tracking current path in multi-terminal graphene Josephson junctions — •Devang Parmar — Institute for Quantum Materials and Technologies (IQMT), Karlsruhe institute of Technology, 76021 Karlsruhe, Germany.

Multiterminal Josephson junctions have been predicted to be platforms to observe various exotic phenomena such as new topological phases of matter [1], correlated states [2-5] or the so-called Andreev molecules [6,7]. In order to control the electronic properties of these complex devices, it is important to comprehend and track the supercurrent flow with respect to their geometries and superconducting lead peculiarities.

Here, we investigated the supercurrent in multi-terminal superconductor-graphene-superconductor (SGS) junctions. Together with magnetic interferometry experiments in these multiterminal graphene devices, we clearly observe that the contact transparencies can be very different from one lead to the other which mainly drives the entire transport properties in SGS. Our work provides insights of the supercurrent flow in multiterminal Josephson junctions and paves the way for further investigations in more complex multiterminal devices.

[1] R. P. Riwar et al., Nat Commun 7, 11167 (2016)
[2] A. Freyn et al., Phys. Rev. Lett. 106, 257005 (2011)
[3] A. H. Pfeffer et al., Phys. Rev. B 90, 075401 (2014)
[4] R. Mélin et al., Phys. Rev. B 100, 035450 (2019)
[5] K.-F. Huang et al., arXiv preprint arXiv:2008.03419 (2020)
[6] Z. Su et al., Nat. Commun. 8, 585 (2017)
[7] J.-D. Pillet et al., Nano Lett. 19, 7138 (2019)

TT 21: Correlated Electrons: Electronic Structure Calculations

Time: Tuesday 9:30–11:45 Location: HSZ 201

TT 21.1 Tue 9:30 HSZ 201

Revealing electronic correlations in YNi_2B_2C using photoemission spectroscopy — •Aki Pulkkinen[1], Geoffroy Kremer[2], Vladimir Strocov[3], Frank Weber[4], Ján Minár[1], and Claude Monney[5] — [1]New Technologies-Research Center, University of West Bohemia, Pilsen, Czech Republic — [2]Département Physique de la Matière et des Matériaux, Institut Jean Lamour, Université de Lorraine/CNRS, France — [3]Paul Scherrer Institut, Swiss Light Source, Villigen, Switzerland — [4]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe, Germany — [5]Département de Physique and Fribourg Center for Nanomaterials, Université de Fribourg, Fribourg, Switzerland

YNi_2B_2C is an intermetallic borocarbide superconductor with a complex electronic band structure that has a very strong Ni character near the Fermi energy. We present density functional theory (DFT) and one-step model of photoemission results for YNi_2B_2C and compare them to experimental soft x-ray angle resolved photoemission spectroscopy (SX-ARPES) measurements. We show that moderate electron correlations have to be included, using dynamical mean field theory (DFT+DMFT) applied to the Ni d-states, to reach the best agreement between the experimental and theoretical SX-ARPES spectra. The one-step model calculations allow us to identify the effect of DFT+DMFT on the energy bands observed in the SX-ARPES measurements.

TT 21.2 Tue 9:45 HSZ 201

Distortion and pressure induced phase transitions in double perovskite La_2CoTiO_6 — •Sromona Nandi[1], Ashis K. Nandy[2], and Rudra Sekhar Manna[1] — [1]Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517619, AP, India — [2]School of Physical Sciences, National Institute of Science Education and Research, An OCC of Homi Bhabha National Institute, Jatni-752050, India

We study the density-functional theory spin-polarized electronic structure calculations for a double perovskite La_2CoTiO_6 where the magnetic moment comes from the Co^{2+} as Ti is in 4^+ state. Due to the rotation and volume mismatch between the TiO_6 and CoO_6 octahedra (∠Co-O-Ti is 151–153°), the system is distorted at ambient pressure. The Co-moments align antiferromagnetically at low temperature and show an insulating transport property with a band gap of 1 eV, consistent with the experiment [1]. With the removal of distortion, i.e., ideal undistorted structure (∠Co-O-Ti is 180°) shows a metallic behavior. Such metallic state can also be achieved with the application of hydrostatic pressure on the distorted structure accompanied by the quenching of Co-moment in the metallic phase which can be understood by the shifting of the exchange splitting of the Co $3d$ orbitals at the Fermi level. In addition, atomic projected density of states analysis of the Co sublattices shows an interesting half-metallic like intermediate state which could be interesting for spintronics applications.

[1] K. L. Holman *et al.*, J. Solid State Chem. **180**, 75 (2007)

TT 21.3 Tue 10:00 HSZ 201

Oxygen vacancies at the origin of pinned moments in oxide interfaces: the example of tetragonal $CuO/SrTiO_3$ — •Benjamin Bacq-Labreuil[1], Benjamin Lenz[2], and Silke Biermann[3] — [1]Institut Quantique, Université de Sherbrooke, Sherbrooke, Canada — [2]Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, Sorbonne Université, Paris, France — [3]Centre de Physique Théorique, Ecole Polytechnique, Palaiseau, France

Obtaining an accurate theoretical description of the emergent phenomena in oxide heterostructures is a major challenge. Recently, intriguing paramagnetic spin and pinned orbital moments have been discovered by x-ray magnetic circular dichroïsm measurements at the Cu $L_{2,3}$-edge of a tetragonal $CuO/SrTiO_3$ heterostructure. Using first principles calculations, we propose a scenario that explains both types of moments [1], based on the formation of oxygen vacancies in the TiO_2 interface layer. We show the emergence of a paramagnetic 2D electron gas hosted in the interface CuO layer. It is invisible at the Ti $L_{2,3}$-edge since the valence of the Ti atoms remains unchanged. Strong structural distortions breaking both the local and global fourfold rotation C_4 symmetries at the interface lead to the in-plane pinning of the Cu orbital moment close to the vacancy. Our results, and in particular the pinning of the orbital moment, may have implications for other systems, especially monoxide/dioxide interfaces with similar metal-oxygen bond length and weak spin-orbit coupling.

[1] B. Bacq-Labreuil, et al, arXiv:2210.15084 (2022).

TT 21.4 Tue 10:15 HSZ 201

New superexchange paths due to synergetic breathing and hopping in corner-sharing cuprates — •Nikolay A. Bogdanov[1], Giovanni Li Manni[1], Sandeep Sharma[1,2], Olle Gunnarsson[1], and Ali Alavi[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Chemistry, University of Colorado Boulder, Boulder, CO, USA — [3]University Chemical Laboratory, Cambridge, UK

We present *ab initio* quantum chemistry calculations of the nearest-neighbour superexchange antiferromagnetic spin coupling J for two cuprates, Sr_2CuO_3 and La_2CuO_4. Good agreement with experimental estimates is obtained for both systems. We also find that J increases substantially as the distance between Cu and apical O is increased.

Analysis of the correlated wavefunctions together with extended superexchange models shows that there is an important synergetic effect of the Coulomb interaction and the O–Cu hopping. When an extra electron hops into Cu $3d$ orbital, Coulomb interaction leads to the orbital breathing (expansion), which on its turn reinforces electron hopping. This correlated breathing-enhanced hopping mechanism is a new ingredient in superexchange models. Our analysis shows that suppression of the described mechanism leads to a drastic reduction in the antiferromagnetic coupling, indicating that it is of primary importance in generating the strong interactions.

TT 21.5 Tue 10:30 HSZ 201

DFT with corrections for an efficient and accurate description of strong electron correlations in NiO — •Julian Gebhardt[1,2]

and Christian Elsässer[1,2,3] — [1]Fraunhofer IWM, 79108 Freiburg — [2]Cluster of Excellence livMatS, University of Freiburg — [3]Freiburg Materials Research Center, University of Freiburg

An efficient and accurate description of the electronic structure of a strongly correlated oxide like NiO has been notoriously difficult. Here, we study the capabilities and limitations of two frequently employed correction schemes, a DFT+U on-site correction and a DFT+1/2 self-energy correction. While both methods individually are unable to provide satisfactory results, in combination they provide a very good description of all relevant physical quantities. Since both methods cope with different shortcomings of common DFT methods (using local-density or generalized-gradient approximations), their combination is not mutually dependent and remains broadly applicable. The combined approach retains the computational efficiency of DFT calculations while providing significantly improved predictive power.

TT 21.6 Tue 10:45 HSZ 201

$LaVO_3$: A true Kugel-Khomskii system — •Xuejing Zhang[1], Erik Koch[1,2], and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA High-Performance Computing, 52062 Aachen, Germany

Almost 50 years ago, Kugel' and Khomskii (KK) showed in a classic paper that, in strongly correlated materials, orbital ordering can arise from pure superexchange interactions [1]. It can, however, also result from the crystal-field splitting via a lattice distortion, i.e., from electron-lattice coupling. Despite the intensive search, it has been hard to find an undisputed realization of a KK system. We identify that the t_{2g}^2 perovskite $LaVO_3$, in its orthorhombic phase, is a rare case of a system hosting an orbital-ordering KK phase transition rather than being controlled by the Coulomb-enhanced crystal-field splitting [2]. We find that, as a consequence of this, the magnetic transition is close to (and even above) the superexchange driven orbital-ordering transition, whereas typically magnetism arises at much lower temperatures than orbital ordering. To explore the effects of crystal-field splitting and filling, we compare to YVO_3 and t_{2g}^1 titanates. In all these materials the crystal field is sufficiently large to suppress the KK phase transition [3].

[1] K. I. Kugel' and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)]
[2] X. J. Zhang, E. Koch, E. Pavarini, Phys. Rev. B **106**, 115110 (2022)
[3] X. J. Zhang, E. Koch, E. Pavarini, Phys. Rev. B **102**, 035113 (2020)

TT 21.7 Tue 11:00 HSZ 201

Orbital-selective metal-insulator transitions in the presence of strong magnetic fluctuations — •Evgeny Stepanov — CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Orbital-selective phenomena that can be realised in materials attract enormous interest. A prominent example is an orbital-selective Mott phase, where itinerant and localised electrons live in different orbitals of the same material. Since its theoretical prediction, the orbital-selective Mott transition has been intensively studied by the state-of-the-art theoretical methods that are based on local approximations to electronic correlations, namely the dynamical mean-field theory and the slave-spin approach. Nevertheless, the existence of the orbital-selective Mott phase in realistic materials is still heavily debated and has not yet been realised experimentally.

In this talk, I will show that consistently taking into account non-local magnetic fluctuations completely changes the physical picture in the Hubbard-Kanamori model, where the orbital-selective Mott transition was predicted in the framework of the local theories. I will show that upon lowering temperature the considered system undergoes the Néel transition to an ordered antiferromagnetic phase before it experiences the orbital-selective Mott transition. Importantly, the former occurs simultaneously for all orbitals, which eliminates the orbital selectivity from the metal-insulator transition. The possibility to realise an orbital selective Néel transition will also be discussed.

TT 21.8 Tue 11:15 HSZ 201

Quantum chemical study on cobalt(II) in honeycomb lattices based on multi-configurational approaches — •Thorben Petersen and Liviu Hozoi — Leibniz IFW Dresden, 01069 Dresden, Germany

Quantum Spin Liquids (QSLs) are fascinating materials that display quantum entanglement and host unconventional fractionated excitations. While QSL behavior was found in Cu(II) $3d^9$ cuprates, $4d^5$ $RuCl_3$, $5d^5$ iridates and triangular-lattice $4f^{13}$ oxides, we here explore $3d^7$ Co(II) compounds such as $Na_2Co_2TeO_6$, which form spin-orbit-entangled $J_{\rm eff} = 1/2$ pseudo-spin moments at Co(II) sites that potentially realize Kitaev-magnetism. In this study, we apply multi-configurational quantum-chemistry methods like CASSCF and beyond to model the $t_{2g}^5\,e_g^2$ magnetic sites in these honeycomb oxides by carefully designing an embedded cluster model to represent the extended bulk lattice. With this, we quantify the extent of the $3d$-site multiplet structure and spin-orbit coupling associated with the $^4T_{2\rm g}$ ground state term. Moreover, our model will be validated against experimental magnetization data and first impressions on the $3d^7$-$3d^7$ intersite couplings will be given.

TT 21.9 Tue 11:30 HSZ 201

Calculation of atomic forces for correlated materials, preliminary results — •Dorota Gotfryd[1], Robinson Outerovitch[1], Marc Torrent[1], Ambroise van Roekeghem[2], and Bernard Amadon[1] — [1]CEA, DAM, DIF 91297 Arpajon CEDEX, France — [2]CEA, LITEN 38054 Grenoble, France

Atomic forces are crucial ingredientis for phonon spectra or molecular dynamics calculations. Within Abinit package, one can currently perform such calculations for weakly or strongly correlated systems, obtaining forces via density functional theory (DFT) or DFT + U methods, correspondingly.

We are working on extending the existing implementation of atomic forces in Abinit to DFT+DMFT (dynamical mean-field theory). Such application would allow for the calculation of forces close to metal/Mott insulator transition where the details of electronic correlations matter and DFT + U approximation is often insufficient for capturing the physics.

We derive the atomic forces for DFT + DMFT as functional derivatives of the free energy functional over the atomic positions and transform them to the projector-augmented wave (PAW) approximation of DFT using Wannier functions as correlated orbitals. We show that the DFT and DFT + DMFT versions of the forces differ by just two terms in the PAW language and we discuss the details of the implementation.

TT 22: Nonequilibrium Quantum Many-Body Systems I (joint session TT/DY)

Time: Tuesday 9:30–13:15 Location: HSZ 204

TT 22.1 Tue 9:30 HSZ 204

Ultrafast dynamics of quantum many-body systems including dynamical screening and strong coupling — •Michael Bonitz[1], Jan-Philip Joost[1], Hannes Ohldag[1], Erik Schroedter[1], and Iva Brezinova[2] — [1]CAU Kiel, Institute for Theoretical Physics and Astrophysics — [2]TU Wien, Institute of Applied Physics, Vienna, Austria

Dynamical screening is a key property of charged many-particle systems. Its theoretical description is based on the GW approximation that is extensively applied for ground-state and equilibrium situations. The main limitation of the GW approximation is the neglect of strong electronic correlation effects. Here we derive the nonequilibrium dynamically screened ladder (DSL) approximation that self-consistently includes, in addition to the GW diagrams, also particle-particle and particle-hole T-matrix diagrams. Our DSL approach is formulated within the G1-G2 scheme [1,2] that is linear in time, in contrast to the cubic scaling of standard Nonequilibrium Green functions simulations. The price to pay for this speedup is the need to store the two-particle Green function. This can be avoided with a recently developed quantum fluctuations approach [3].

[1] N. Schluenzen et al., Phys. Rev. Lett. 124, 076601 (2020)
[2] J.-P. Joost al., Phys. Rev. B 105, 165155 (2022)
[3] E. Schroedter et al., Cond. Mat. Phys. 25 , 23401 (2022)

TT 22.2 Tue 9:45 HSZ 204

Spectral response of a charge density wave insulator to periodic driving — •Alexander Osterkorn, Constantin Meyer, and Salvatore Manmana — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

Periodically driven quantum many-body systems host unconventional behavior not realized at equilibrium. Here we address in detail the emergence of a cosine-like band in the gap region of the non-equilibrium single-particle spectral function of strongly interacting spinless fermions on a chain in the charge density wave phase [1]. We compare the dynamics of the periodically driven system to the quench dynamics with an effective Floquet Hamiltonian and discuss the role of doublon excitations in both cases. This is investigated using both matrix product state based time evolution techniques as well as time-dependent Hartree-Fock. [1] arXiv:2205.09557

TT 22.3 Tue 10:00 HSZ 204

Floquet engineering in tilted lattices — •Melissa Will[1], Pablo Sala[2,3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Department of Physics and Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, California 91125, USA — [3]Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, California 91125, USA

Quantum many-body systems out of equilibrium can exhibit very rich and exciting phenomena. A particularly important question is whether and how a quantum system thermalizes under unitary evolution. In this context three classes of systems have been identified: ergodic, localized and an intermediate regime exhibiting so called quantum many-body scars. In this talk we discuss whether a time-periodic, local drive can induce thermalization of a localized system. We consider interacting hard-core bosons in an one dimensional, tilted system with periodic driving. We find that the system becomes ergodic for resonant driving frequencies. In contrast, if the tilt is not close to a multiple of driving frequency, the system stays localized. This observation can theoretically be understood by deriving an effective Hamiltonian using a Magnus expansion. Using large scale numerical methods, we explore entanglement entropy and imbalance over time. Our theoretical predictions are in good agreement with numerics.

TT 22.4 Tue 10:15 HSZ 204

Photoinduced spinful excitons in Hubbard systems with magnetic superstructures — Constantin Meyer and •Salvatore R. Manmana — Institute for Theoretical Physics, Göttingen University, Friedrich-Hund-Platz 1, 37077 Göttingen

The possibility to form excitons in photo-illuminated correlated materials is central from fundamental and application oriented perspectives. We show how the interplay of electron-electron interactions and a magnetic superstructure leads to the formation of a peculiar spinful exciton, which can be detected in the nonequilibrium spectral function and the time-dependent optical conductivity. We study these quantities by using matrix product states (MPS) following an electron-hole excitation in a class of one-dimensional Hubbard models with on-site interactions and alternating local magnetic fields, which realize correlated band insulators. An excitation in only one specific spin direction leads to an additional band in the gap region of the spectral function only in the opposite spin direction, and to an additional peak in the optical conductivity. We discuss implications for experimental studies in correlated insulator systems.

TT 22.5 Tue 10:30 HSZ 204

Photoinduced pairing states of excitonic insulators — •Satoshi Ejima — DLR Quantencomputing-Initiative, Hamburg, Germany

Applying the time-dependent density-matrix renormalization group technique, we explore photoinduced pairing states in the half-filled extended Falicov-Kimball model (EFKM) in one dimension, both with and without internal SU(2) symmetry. In the time-dependent photoemission spectra simulated with the optimal pump pulse parameters, an extra band appears above the Fermi energy after pulse irradiation, implying a photoinduced metallization. Even in the absence of the SU(2) structure, the electron-electron pair correlations can also be enhanced during the pump, while they decrease over time after pulse irradiation. This suggests a possible photoexcited metallization of Ta_2NiSe_5, a strong candidate for an excitonic insulator material, for which the EFKM is considered to be the minimal theoretical model. Computing the time-dependent photoemission spectra with the parameter set for this material, i.e., in the EFKM without SU(2) symmetry, we demonstrate the photoinduced insulator-to-metal transition, in accord with recent findings in time- and angle-resolved photoemission spectroscopy experiments on Ta_2NiSe_5.

[1] S. Ejima, F. Lange, H. Fehske, Phys. Rev. B **105**, 245126 (2022)

15 min. break

Invited Talk TT 22.6 Tue 11:00 HSZ 204

Higgs spectroscopy of superconductors in nonequilibrium — •Dirk Manske — Max-Planck-Institut für Festkörperforschung

Higgs spectroscopy is a new and emergent field [1-3] that allows to classify and determine the superconducting order parameter by means of ultra-fast optical spectroscopy. There are two important ways to activate the Higgs mode in superconductors, namely a single-cycle *quench* or an adiabatic, multicycle *drive* pulse, which I will discuss in detail. Furthermore, I will review and report on the latest progress on Higgs spectroscopy, in particular on the role of the third-harmonic-generation (THG) [4-6] and the possible IR-activation of the Higgs mode by impurities or external dc current [7,8]. I also provide new predictions for time-resolved ARPES experiments in which, after a quench, a continuum of Higgs mode is observable and a phase information of the superconducting gap function would be possible to extract [9]. Finally, I show that the Higgs mode may shed some light on the 25-years-old A1g-puzzle in equilibrium Raman scattering on high-T_c cuprates [10].

[1] Nat. Commun. 11, 287 (2020)
[2] Phys. Rev. B 101, 184519 (2020)
[3] Nat. Commun. 11, 1793 (2020)
[4] Phys. Rev. B 104, 174508 (2021)
[5] Nature Commun., accepted (2022)
[6] Nature Commun., submitted (2022)
[7] Phys. Rev. B 101, 220507 (2020)
[8] Phys. Rev. B 104, 134504 (2021)
[9] Phys. Rev. B 101, 224510 (2020)
[10] Phys. Rev. Lett. 127, 197001 (2021)

TT 22.7 Tue 11:30 HSZ 204

Periodically driven spin-1/2 XXZ antiferromagnetic chains — •Aslam Parvej, Imke Schneider, and Sebastian Eggert — Technische Universität Kaiserslautern, Kaiserslautern, Germany

Time-periodically driven quantum systems are of great interest due to the possibility of unconventional states of matter and Floquet engineering. The interplay of many-body interactions and time-periodic manipulations facilitate new phenomena in the steady state. We analyze the Floquet steady states of finite spin-1/2 XXZ antiferromagnetic chains with periodically driven anisotropy parameter at frequencies below the band width, so that resonances are in principle possible. We use a numerical real-time approach with an adiabatic time evolution protocol by ramping up the driving amplitude of the external periodic drive to prepare a non-equilibrium Floquet steady state. Parametric resonances are expected when the driving frequencies are equal to twice the energy gaps in a finite system. However, the observed resonance absorption of energy and heating is surprisingly weak in our system even for large driving amplitude. This changes if a square wave is used for driving.

TT 22.8 Tue 11:45 HSZ 204

Controllable effects of the mass term in time-periodic driven sine-Gordon models. — •Dimo Claude[1], Simon Jäger[1], Christoph Dauer[1], Piotr Chudzinski[2], Imke Schneider[1], and Sebastian Eggert[1] — [1]Physics Department and Research Center OPTIMAS, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany. — [2]Institute of Fundamental Technological Research, Polish Academy of Science, 02-106 Warszawa, Poland.

Recently, the full Floquet solution of a Luttinger Liquid with periodically modulated interactions has been derived and resonant wavevectors have been identified. There, the quantum state can only be stabilized when damping mechanisms of the one-dimensional systems are included. In our work, we investigate the time-periodic Luttinger Liquid under a non-linear perturbation which originates from the Sine-Gordon potential. This term provides interactions among the different modes of the Luttinger Liquid and can potentially confine the parametrically amplified modes. We investigate this model up to fourth order of the phase field using a mean-field approach. The resulting effective model is quadratic in the field operators while the non-linearity remains, due to the explicit dependence of the frequencies on the time-dependent quantum state. Using a self-consistency relation between the number of density wave excitations and the systems' energy, we discuss the formation of a non-equilibrium steady state and study its stability.

TT 22.9 Tue 12:00 HSZ 204

Influence of phononic dissipation on impact ionization processes in a photodriven Mott insulator — •Paolo Gazzaneo, Tommaso Maria Mazzocchi, Jan Lotze, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

It has been suggested that in strongly correlated materials, highly photoexcited charge carriers could use their extra energy to excite additional carriers across the Mott gap via impact ionization [1,2]. However, the influence of electron-phonon scattering on photocurrent and impact ionization in Mott photovoltaic setups is still an open question.

We address this issue in a nonequilibrium steady state study on the occurrence of impact ionization in a simplified model of a Mott photovoltaic device in presence of acoustic phonons [3], consisting of a Mott-insulating layer coupled to two wide-band fermion leads.

For a small hybridization to the leads, we obtain a peak in the photocurrent as a function of the driving frequency which can be associated with impact ionization processes, while for larger hybridizations we find a suppression of impact ionization with respect to direct photovoltaic excitations. The effect of acoustic phonons produces a slight enhancement of the photocurrent for small driving frequencies and a suppression at frequencies around the main peak at all considered hybridization strengths.

[1] E. Manousakis, Phys. Rev. B 82, 125109 (2010)
[2] J. E. Coulter et al., Phys. Rev. B 90, 165142 (2014)
[3] Gazzaneo et al., Phys. Rev. B 106, 195140 (2022)

TT 22.10 Tue 12:15 HSZ 204

Correlated Mott insulators in strong electric fields: Role of phonons in heat dissipation — •Tommaso Maria Mazzocchi, Paolo Gazzaneo, Jan Lotze, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz, Austria

Mott-insulating models can undergo an insulator-to-metal transition when subject to a constant bias voltage [1], which makes them suitable to describe the resistive switch observed in correlated insulators [2]. Nonequilibrium state-of-the-art techniques rely on the coupling to fermion baths to dissipate the field-induced excess energy [1,3]. However, a realistic description of heat-exchange requires the inclusion of phonons. In [4] we study a single-band Hubbard model in a static electric field coupled to electron and acoustic phonon baths. The nonequilibrium steady-state is addressed via the dynamical mean-field theory using the auxiliary master equation approach as impurity solver. Phonons are included via the Migdal approximation. Using both the electron and phonon baths the steady-state current is slightly enhanced by phonons for field strengths close to half of the gap and suppressed at the gap resonance. With phonons alone, dissipation can occur only at the resonances and the current at the metallic phase is suppressed by almost one order of magnitude.

[1] C. Aron, Phys. Rev. B 86, 085127 (2012)
[2] E. Janod et al., Adv. Funct. Mater. 25, 6277 (2015)
[3] Y. Murakami et al., Phys. Rev. B 98, 075102 (2018)
[4] T.M. Mazzocchi et al., Phys. Rev. B 106, 125123 (2022)

TT 22.11 Tue 12:30 HSZ 204

Correlated Mott insulators and photovoltaics out of equilibrium: phonons and heat dissipation — •Enrico Arrigoni, Tommaso Mazzocchi, Paolo Gazzaneo, Daniel Werner, and Jan Lotze — Institute of Theoretical and Computational Physics, Graz University of Technology, 8010 Graz Austria

I will present recent results for correlated Mott systems in a nonequilibrium driven steady state. Results are obtained via nonequilibrium Dynamical Mean Field Theory with an impurity solver based upon a combination of Keldysh Green's functions and Lindblad formalism for open quantum systems [1]. Recent improvements based upon a Configuration Interaction treatment of the many body Lindblad equation allow for an efficient solution of the impurity problem deep in the Kondo regime [2].

In particular, I will discuss the interplay of strong correlation and Joule dissipation by phonons near the Mott dielectric breakdown [3] and in photoexcitation induced transport across a Mott insulating gap [4].

[1] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013)
A. Dorda et al., Phys. Rev. B 89 165105 (2014)
A. Dorda et al., Phys. Rev. B 92, 125145 (2015)
[2] D. Werner et al., arXiv:2210.09623 (2022)
[3] T. Mazzocchi at al., Phys. Rev. B 106, 125123 (2022)
[4] M. Sorantin et al., Phys. Rev. B 97, 115113 (2018)
P. Gazzaneo et al. Phys. Rev. B 106, 195140 (2022)

TT 22.12 Tue 12:45 HSZ 204

Photoinduced prethermal order parameter dynamics in the two-dimensional large-N Hubbard-Heisenberg model — •Alexander Osterkorn and Stefan Kehrein — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany

We study the microscopic dynamics of competing ordered phases in a two-dimensional correlated electron model [1], which is driven with a pulsed electric field of finite duration. In order to go beyond a mean-field treatment of the electronic interactions we adopt a large-N generalization of the Hubbard model and combine it with the semiclassical fermionic truncated Wigner approximation as a time evolution method. This allows us to calculate dephasing corrections to the mean-field dynamics and to obtain stationary states, which we interpret as prethermal order. We use this framework to simulate the light-induced transition between two competing phases (bond density wave and staggered flux) and find that the post-pulse stationary state order parameter values are not determined alone by the amount of absorbed energy but depend explicitly on the driving frequency and field direction. While the transition between the two prethermal phases takes place at similar total energies in the low- and high-frequency regimes, we identify an intermediate frequency regime for which it occurs with minimal heating [2].

[1] Phys. Rev. B 39, 11538 (1989)
[2] arXiv:2205.06620

TT 22.13 Tue 13:00 HSZ 204

Observation of magnon bound states in the long-range, anisotropic Heisenberg model — Florian Kranzl[1], •Stefan Birnkammer[2], Manoj Joshi[1], Alvise Bastianello[2], Rainer Blatt[1], Michael Knap[2], and Christian Roos[1] — [1]Universität Innsbruck, Innsbruck, Austria — [2]Technische Universität München, Garching, Germany

Over the recent years coherent, time-periodic modulation has been established as a versatile tool for realizing novel Hamiltonians. Using this approach, known as Floquet engineering, we experimentally realize a long-ranged, anisotropic Heisenberg model with tunable interactions in a trapped ion quantum simulator. We demonstrate that the spectrum of the model contains not only single magnon excitations but also composite magnon bound states. For the experimentally realized long-range interactions, the group velocity of magnons is unbounded. Nonetheless, for sufficiently strong interactions we observe bound states of these unconventional magnons which possess a non-diverging group velocity. By measuring the configurational mutual information between two disjoint intervals, we demonstrate the implications of the bound state formation on the entanglement dynamics of the system. Our observations provide key insights into the peculiar role of composite excitations in the non-equilibrium dynamics of quantum many-body systems.

TT 23: Kagome Systems

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

TT 23.1 Tue 9:30 HSZ 304

Broadband optical investigations of the CDW state in Kagome metals AV_3Sb_5 (A = K, Rb, Cs) — •E. Uykur[1,2], M. Wenzel[1], B.R. Ortiz[3,4], S.D. Wilson[4], S. Winnerl[2], M. Dressel[1], and A. A. Tsirlin[5] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569, Stuttgart, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Inst. Ion Beam Phys. & Mat. Res., 01328 Dresden, Germany — [3]Materials Department and California Nanosystems Institute,University of California Santa Barbara, Santa Barbara, CA, 93106, United States — [4]Materials Department, University of California Santa Barbara, Santa Barbara, CA, 93106, United States — [5]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

We present a broadband optical study of non-magnetic Kagome metals AV_3Sb_5 (A = K, Rb, Cs) down to 10 K. Different contributions to the optical spectra have been discussed and compared with the DFT calculations in normal and charge density wave (CDW) states. Spectra reflect the response of the 2D Dirac fermions and are frequency-independent in a broad energy range. Low energies are governed by the itinerant and localized charge carriers that show a spectral weight redistribution below the CDW transition. Our results show that the CDW gaps evolve systematically between the siblings (K<Cs<Rb) in line with their transition temperatures. We further use the experimental spectral weight to gauge the effect of electronic correlations and find it increasing with reducing the size of A.

TT 23.2 Tue 9:45 HSZ 304

Complex charge order in the AV_3Sb_5 kagome metals — •Morten Christensen[1], Turan Birol[2], Brian Andersen[1], and Rafael Fernandes[3] — [1]Niels Bohr Institute, University of Copenhagen — [2]Department of Chemical Engineering and Materials Science, University of Minnesota — [3]School of Physics and Astronomy, University of Minnesota

The kagome lattice, consisting of an array of corner-sharing triangles, offers a rich platform to study the behavior of correlated electrons. In kagome metals, the electronic band structure exhibits Dirac points, flat bands, and van Hove singularities - features which promote the role of electronic correlations. A family of recently discovered kagome metals, AV_3Sb_5 (A=K, Rb, Cs), provides a realization of these features. These materials exhibit an enigmatic superconducting order, which emerges from a three-dimensional charge-density wave (CDW) phase. While the precise nature of the CDW phase is still unknown, there are indications of both time-reversal symmetry breaking and nematicity inside the charge-ordered phase. Starting from from the low-energy electronic states near the van Hove singularities, we construct a phenomenological model to describe the CDW phase. The order parameters of this model are either real, corresponding to bond distortions, or imaginary, corresponding to loop-currents. These CDW orders can coexist or compete which results in a rich landscape of subsidiary orders, including various types of multipolar magnetic orders. These have unique experimental signatures which can aid in pinpointing the precise nature of the CDW phase observed in experiments.

TT 23.3 Tue 10:00 HSZ 304

Investigation of the charge density wave in single crystal CsV_3Sb_5 under hydrostatic pressure — •Fabian Stier[1], Tobias Ritschel[1], Marein Rahn[1], Chandra Shekhar[2], Claudia Felser[2], and Jochen Geck[1] — [1]IFMP, TU Dresden, Germany — [2]MPI CPfS, Dresden, Germany

The topological Z_2 kagome materials AV_3Sb_5 (A = K, Rb, Cs) show a nontrivial electronic topology, exhibit superconductivity (SC) and a charge-density-wave (CDW) order. CsV_3Sb_5 shows a CDW below 90K with a 2x2x4 superstructure, which changes around 60K to a 2x2x2 superstructure. To investigate the interplay of CDW-order and SC we performed single crystal x-ray diffraction under hydrostatic pressure, with Argon as a pressure medium, up to 2 GPa and 20K. In this pressure range the SC shows two distinct domes, where Tc is enhanced and shows two maxima. The 2x2x2 CDW at low temperatues persists under pressure up to the first extremum of $T_c \sim 0.7$ GPa, where for a short pressure range both, the CDW and a new emerging incommensurate CDW coexists. While the first CDW quickly vanishes, the incommensurate CDW persists up to pressures where the SC shows another extremum in T_c. Above this pressure, $\sim$ 1.5GPa, no CDW could be detected. An accurate knowledge of these structural modifications will be essential to explain the relationship of topology and superconductivity in this class of materials.

TT 23.4 Tue 10:15 HSZ 304

Indication of a strong coupling charge density wave in CsV_3Sb_5 — •Leander Peis[1,2,3], Ge He[1,4], and Rudolf Hackl[1,2,3] — [1]Walther Meissner Institut, Bayerische Akademie der Wissenschaften, Garching 85748, Germany — [2]Technische Universität München, Garching 85748, Germany — [3]IFW Dresden, Dresden 01062, Germany — [4]University College Cork, Cork, Ireland

A prominent example for studying the interplay of electronic correlations and non-trivial topology is the material class of AV_3Sb_5 (A=K,Rb,Cs), displaying unconventional charge order in the range of 100 K and superconductivity at temperatures below 2.5 K. Here, we present a polarization-dependent Raman scattering study of the Kagome metal CsV_3Sb_5, focusing on the charge density wave (CDW). We resolve several signatures of strong-coupling between the lattice and the electronic system. First, the energy of the A_{1g} Γ-point phonon exhibits a discontinuity at the phase transition temperature T_{CDW} = 95 K. Second, the magnitude and symmetry dependence of the observed CDW energy gap 2Δ suggest strong coupling and a substantial anisotropy. Third, the observed A_{1g} amplitude mode depends weaker on temperature than expected and displays an asymmetric Fano-type line shape, particularly around 70 K. We interpret this deviation in terms of strong coupling between the phonon-like amplitude mode and the electronic continuum. To the best of our knowledge such an asymmetry of an amplitude mode has not been observed before.

TT 23.5 Tue 10:30 HSZ 304

X-ray diffraction on the charge-density wave in the Kagome superconductor RbV_3Sb_5 — •Sabreen Hammouda[1], Yu-Hui Liang[2], Po-Chun Chang[2], Carsten Paulmann[3], Yishui Zhou[1], Adrian Merrit[1], Pikesh Pal[1], Rahaf Yaseen[1], Hongxiong Liu[4], Youguo Shi[4], Chao-Hung Du[2], and Yixi Su[1] — [1]JCNS-MLZ, Forschungszentrum Jülich, 85748 Garching, Germany — [2]Dept. of Phys., Tamkang University, Tamsui 251, Taiwan — [3]DESY, 22607 Hamburg, Germany — [4]IOP, CAS, Beijing 100190, China

The newly discovered Kagome superconductors AV_3Sb_5 (A=K, Rb or Cs), in which non-trivial band topology, charge-density wave (CDW), and superconductivity are intertwined, have attracted tremendous interests. Despite extensive recent investigations via X-ray diffraction (XRD) and other complementary local probe techniques, it remains a major challenge to gain a consistent picture of the CDW modulation across different AV_3Sb_5 samples. In this talk, we will present our recent single-crystal XRD investigations (in-house and synchrotron) of the CDW modulations over a wide temperature range in the less-studied RbV_3Sb_5. A unique CDW modulation of the 2x2x2 type can be confirmed for RbV_3Sb_5 below T_{CDW} = 102 K, and no evidence for CDW fluctuations above T_{CDW} could be found. Our detailed temperature dependence measurements of the CDW superstructure reflections indicate a second-order phase transition with a 2D Ising character. A comparison to other AV_3Sb_5 compounds and possible implications on the understanding of the nature of the CDW in these Kagome superconductors will be given.

TT 23.6 Tue 10:45 HSZ 304

$\mathbb{Z}_2$ topological insulator and Hubbard interactions on the Kagome lattice — Irakli Titvinidze[1], •Julian Legendre[2,3], Maarten Grothus[1], Bernhard Irsigler[1], Karyn Le Hur[2], and Walter Hofstetter[1] — [1]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]CPHT, CNRS, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [3]Department of Physics and Materials Science, University of Luxembourg, 1511 Luxembourg, Luxembourg

The study of topological phase transitions has been a very active field of research since the 80's; in recent decades topological insulators have been one of the major foci in this field. Understanding the role of the interactions in such systems is also currently is major challenge for the scientific community. In this talk, I will present a study of a time-reversal invariant topological model, with Hubbard interactions, on the Kagome lattice. The topological model contains intrinsic and Rashba spin-orbit coupling terms and position-dependent onsite energies. Relying on several analytical methods, I will show how the $\mathbb{Z}_2$ topological phase, resulting from the flux term, is tuned by varying the amplitude(s) of on-site energy terms and/or of the Rashba spin-orbit coupling term, at filling $n = 2/3$. Then, we will study the effect of Hubbard interactions on the topological properties for a specific on-site energy configuration and at vanishing Rashba spin-orbit coupling. We will use perturbation theory in the large Hubbard amplitude U limit and a mean-field method for smaller U. I will compare these analytical results with numerical results obtained by our collaborators.

TT 23.7 Tue 11:00 HSZ 304

Temperature-dependent pump-probe spectroscopy of the magetic Kagome metal Fe_3Sn_2 — •M. G. Faria[1], Q. Wang[2], H. C. Lei[2], A. Pashkin[1], S. Winnerl[1], M. Helm[1,3], and E. Uykur[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Department of Physics and Beijing Key Laboratory of Opto-electronic Functional Materials & Micro-nano Devices, Renmin University of China, 100872 Beijing, China — [3]Institute for Applied Physics, Technische Universität Dresden, 01069 Dresden, Germany

In this study, we present optical pump-probe measurements on a magnetic Kagome metal, Fe_3Sn_2, under different temperatures down to 10 K. The obtained spectra can be fitted with a double exponential decay, indicating that the system has two distinct relaxation processes. Additionally, some unexpected and pronounced oscillations are dominating the spectra, giving evidence of a strong electron-phonon coupling in Fe_3Sn_2, at least in this ultra-fast regime. The frequency of this coupled phonon is determined to be around 2.5 THz. Finally, we will discuss the temperature and pump fluence dependence of the observed phonon coupling and the distinct relaxation dynamics in this material.

15 min. break

TT 23.8 Tue 11:30 HSZ 304

Complex magnetic orders and the emergent topological Hall effect in the kagome metal $ErMn_6Sn_6$ — •Yishui Zhou[1], Changjiang Yi[2], Dmitry Khalyavin[3], Fabio Orlandi[3], Pascal Manuel[3], Sabreen Hammouda[1], Adrian Merritt[1], Claudia Felser[2], Thomas Brückel[4], and Yixi Su[1] — [1]JCNS-MLZ, Forschungszentrum Jülich GmbH, Garching, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]ISIS Neutron & Muon Facility, STFC, Rutherford Appleton Laboratory, Didcot, UK — [4]JCNS-2 & PGI-4, Forschungszentrum Jülich GmbH, Jülich, Germany

Following the discovery of a quantum-limit magnetic Chern phase in $TbMn_6Sn_6$, the magnetic topological metal series RMn_6Sn_6 (R=Gd-Yb, and Y, Lu, etc.), that possesses an ideal Kagome lattice of Mn, has emerged as a new platform to explore exotic states and novel functionalities. We have recently carried out the growth of high-quality single crystals of the magnetic Kagome metal $ErMn_6Sn_6$, and the physical properties characterizations via the magnetic susceptibility, heat capacity, and Hall conductivity measurements. We have also undertaken comprehensive neutron diffraction experiments on both single-crystal and powder samples at the WISH diffractometer at ISIS. Our study has clearly hinted a fascinating interplay between topologically non-trivial electronic band structures, magnetism and electronic correlations in $ErMn_6Sn_6$.

TT 23.9 Tue 11:45 HSZ 304

Thermodynamics of the spin-half square Kagome lattice antiferromagnet — •Jürgen Schnack[1], Oleg Derzhko[2], and Johannes Richter[3] — [1]Fakultät für Physik, Universität Bielefeld, D-33501 Bielefeld, Germany — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 79011 Lviv, Ukraine — [3]Institut für Physik, Universität Magdeburg, D-39016 Magdeburg & Max-Planck-Institut für Physik Komplexer Systeme, D-01187 Dresden, Germany

Over the last decade, the interest in the spin-1/2 Heisenberg antiferromagnet (HAF) on the square Kagome lattice has been growing as a model system of quantum magnetism with a quantum paramagnetic ground state, flat-band physics near the saturation field, and quantum scars. Here, we present large-scale numerical investigations of the specific heat, the entropy, as well as the susceptibility by means of the finite-temperature Lanczos method for system sizes of N = 18, ..., 54. We find that the specific heat exhibits a low-temperature shoulder below the major maximum which can be attributed to low-lying singlet excitations filling the singlet-triplet gap, which is significantly larger than the singlet-singlet gap. For the susceptibility the singlet-triplet gap leads to an exponentially activated low-temperature behavior. The maximum of the susceptibility is found at a pretty low temperature T/J = 0.146 (for N = 42). We find a striking similarity of our data with the corresponding ones for the Kagome HAF down to very low temperatures.

TT 23.10 Tue 12:00 HSZ 304

Asymmetric melting of the 1/3-plateau for the Kagome lattice antiferromagnet — •Henrik Schlüter[1], Jürgen Schnack[1], and Johannes Richter[2] — [1]Bielefeld University, Bielefeld, Germany — [2]University of Magdeburg and MPIPKS Dresden, Germany

The Kagome lattice Heisenberg antiferromagnet (KHAF) is a rich source of unconventional physics not only regarding its spin-liquid ground state but also with respect to its behavior at non-zero field and temperature.

Here we investigate the phenomenon of the asymmetric melting of the magnetization plateau at 1/3 of the saturation magnetization, see Refs.[1, 2]. We explain the effect by discussing the energy diagram and the density of states constructed from finite-temperature Lanczos data for KHAF with up to 48 sites [3].

[1] J. Schnack, J. Schulenburg, J. Richter, Phys. Rev. B 98, 094423 (2018)
[2] Takahiro Misawa, Yuichi Motoyama, and Youhei Yamaji, Phys. Rev. B 102, 094419 (2020)
[3] H. Schlüter, F. Gayk, H.-J. Schmidt, A. Honecker, J. Schnack, Z. Naturforsch. A 76, 823 (2021)

TT 23.11 Tue 12:15 HSZ 304

Classical and quantum frustrated models of planar X-Y spins on the Kagome lattice: anisotropic magnetic patterns — •Oliver Neyenhuys, Mikhail Fistul, and Ilya Eremin — Ruhr Universität Bochum

We present a theoretical study of various highly anisotropic magnetic patterns occurring in the geometrically frustrated model of planar X-Y spins on the Kagome two-dimensional lattice. Frustration is introduced by a specific spatial arrangement of both ferromagnetic and anti-ferromagnetic bonds between adjacent magnetic moments on the lattice vertices. At the critical value of frustration f = 3/4 such a system displays the phase transition from an ordered ferromagnetic state to frustrated regime featuring a highly degenerate ground state in which topological (anti)vortices penetrate each cell. Taking into account a generous amount of topological constraints, the thermal fluctuations and the quantum tunneling induced transitions between these vortices/anti-vortices, we derive an effective Ising spin Hamiltonian on the corresponding hexagonal lattice, in which a strong long-range interaction between a well separated (anti)vortices occurs. By making use of the mean field analysis and direct numerical diagonalization of the Hamiltonian we characterize various classical and quantum phases and phase transitions between them for large and small Kagome lattices. Experimental observation of such magnetic patterns with coherent networks of superconducting qubits will be discussed.

TT 23.12 Tue 12:30 HSZ 304

Magnon-phonon coupling in the Kagome-lattice antiferromagnet Mn_3Ge — •Aleksandr Sukhanov, Nikita Andriushin, Anton Kulbakov, and Dmytro Inosov — Institut für Festkörper- und Materialphysik, Technische Universität Dresden, D-01069 Dresden

Magnons and phonons, which are quanta of spin excitations and crystal-lattice vibrations in ordered materials, respectively, can be strongly coupled together when their dispersion relations intersect in reciprocal space. This results in hybridised collective spin-lattice excitations, also known as magnetoelastic (ME) modes.

The metallic hexagonal compound Mn_3Ge is characterized by a noncollinear spin order due to the geometric frustration of the Kagome lattice formed by Mn ions. Our earlier studies showed that Mn_3Ge belongs to a rare class of materials that possess very strong ME coupling. The ME effect is manifested in the large negative thermal expansion of the material and high-pressure tuning of its remarkable anomalous Hall effect. Most intriguing is a previous observation that the noncollinear spin structure of Mn_3Ge can be driven into a collinear ferromagnetic state under a hydrostatic pressure of ∼5 GPa. This, in turn, provides hints on how the magnetic structure is linked to the unconventional electron transport phenomena in this material.

In this talk, we will discuss the results of our recent single-crystal inelastic neutron and x-ray scattering spectroscopy measurements of Mn_3Ge. We were able to clearly resolve momenta and energy of the ME hybridization. The experimental results are supported with the first-principle lattice dynamics calculations.

TT 23.13 Tue 12:45 HSZ 304

Raman scattering study of magnetism in the Kagome materials Fe_3Sn_2 and $Co_3Sn_2S_2$ — •Rudi Hackl[1,2,3], Ge He[4], and Leander Peis[1,2,3] — [1]Walther-Meissner-Institut, 85748 Garching, Germany — [2]Technische Universität München, 85748 Garching, Germany — [3]IFW Dresden, Dresden 01062, Germany — [4]University College Cork, Cork, Ireland

Fe_3Sn_2 and $Co_3Sn_2S_2$ have triangularly coordinated layers of $3d$ transition metal ions sitting on a Kagome network. Both compounds have Dirac and Weyl nodes in the band structure. Fe_3Sn_2 is ferromagnetic below 670 K, and the spins start to reorient from perpendicular to parallel to the Kagome layer below 150 K. This reorientation was first observed by Mössbauer spectroscopy but has in general little influence on other observables such as thermal expansion or magnetization. In our Raman study we find an anomaly of the line width and the energy of the lowest A_{1g} phonon where the Sn atoms vibrate perpendicular to the Fe plane. We interpret the anomaly in terms of an enhanced spin-phonon coupling below approximately 150 K. $Co_3Sn_2S_2$ starts ordering antiferromagnetically below 175 K and turns into a ferromagnet in the low-temperature limit. Here, the spins are first in plane and the order is nearly frustrated. Below 100 K the spins point along the c-axis and are parallel. The A_{1g} phonon couples strongly to a continuum as highlighted by the asymmetric Fano-type line shape. The asymmetry is maximal close to the magnetic transition. We argue that small changes of the lattice have an effect on the magnetism.

TT 24: Quantum Dots: Transport (joint session HL/TT)

Time: Tuesday 9:30–12:15 Location: POT 151

TT 24.1 Tue 9:30 POT 151

Contact formation analysis of nickel to SiGeOI to form Nickel-Germano-silicide using Flash lamp annealing — •Muhammad Moazzam Khan[1], Slawomir Prucnal[1], and Yordan M. Georgiev[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, D-01328 Dresden, Germany — [2]Institute of Electronics at the Bulgarian Academy of Sciences, 72, Tzarigradsko chaussee blvd, 1784-Sofia, Bulgaria

In CMOS technology, parasitic source/drain (S/D) resistance becomes more crucial in determining the overall device performance as the device dimensions get smaller. The contact resistance dominates this parasitic S/D resistance to a great extent, which limits the drive current. In order to have minimal impact on electrical performance, the contact should have linear Current-Voltage characteristics and negligible resistance in comparison to the device resistance. When replacing silicon with silicon-germanium as a channel material in future devices, it is necessary to investigate the contact formation mechanism in order to develop suitable contacts for energy-efficient devices. In this work, we are investigating metal semiconductor contact formation on SiGeOI using flash lamp annealing and studying their properties using structural and electrical characterization.

TT 24.2 Tue 9:45 POT 151

Predicting charge density maps in 2D nanostructures with machine learning techniques — •Amanda Teodora Preda[1,2,3], Calin Andrei Pantis-Simut[1,2,3], Nicolae Filipoiu[2,3], Lucian Ion[2], Andrei Manolescu[4], and George Alexandru Nemnes[1,2,3] — [1]Research Institute of the University of Bucharest (ICUB), Sos. Panduri 90, Bucharest, Romania — [2]University of Bucharest, Faculty of Physics, 077125 Magurele-Ilfov, Romania — [3]Horia Hulubei National Institute for Physics and Nuclear Engineering, 077126 Magurele-Ilfov, Romania — [4]Department of Engineering, Reykjavik University, Menntavegur 1, IS-102 Reykjavik, Iceland

Machine learning (ML) models have the potential to significantly improve and assist the design process of nanodevices that require precise control of the quantum states.

For 2D nanoelectronic structures, charge and spin densities are relevant observables and are also suited for ML techniques which employ image processing. The model systems that we considered are two dimensional quantum dots with multiple electrons and random confinement potentials. With convolutional neural networks, we built a ML model to predict whether a configuration displays singlet-triplet transitions in the ground state. For image translation problems, we used models based on conditional generative adversarial networks in order to predict the charge density distribution for arbitrary interacting systems taking as input either the non-interacting cases or just the shape of the confining potential.

TT 24.3 Tue 10:00 POT 151

Mesoscopic transport properties of individually prepared GaN-nanowire field-effect transistors — •Hannes Hergert[1,2], Matthias T. Elm[1,2,3], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Giessen, Germany — [2]Center for Materials Research, Giessen, Germany — [3]Institute of Physical Chemistry, Giessen, Germany

In order to keep the optimization of transistors within Moore's law new material systems as well as new transistor concepts such as GaN-nanowire field effect transistors (NW-FET) are needed. In this work we characterize the electrical transport properties of single NW-FET. Furthermore, we are able to obtain a deeper understanding of the mesoscopic transport processes. Unintentionally doped GaN-nanowires were fabricated using molecular-beam-epitaxy and device fabrication was performed by a combination of different lithographic methods and atomic layer deposition. After an annealing process the nanowire's resistance shows an ohmic behaviour. Electrical transport measurements were performed between 2 and 280 K. The investigated NW-FET exhibits a transfer characteristic identical to those of classical field-effect transistors. We show that the electrical transport is dominated by two transport processes: a transport within a metal-like impurity band at low temperatures and a hopping process at higher temperatures. Furthermore we were able to identify universal conductance fluctuations at temperatures below 140 K, which arise from the shift of the Fermi level when applying a topgate voltage.

TT 24.4 Tue 10:15 POT 151

Multi-Channel Kondo Effect in Few-Electron Quantum Dots — •Olfa Dani[1], Johannes C. Bayer[1], Timo Wagner[1], Gertrud Zwicknagl[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, Germany

The Kondo effect is a many particle entangled system, that involves the interaction between a localized spin in the quantum dot and free electrons in the electron reservoirs. This entanglement can be calculated using simplifying assumptions concerning the electronic structure of the quantum dot.

In this work we investigate a quantum dot device formed electrostatically in a two-dimensional electron gas using top-gates. A quantum point contact is used as a sensitive charge detector to detect single-electrons tunneling through the system. This enables us to know the exact number of electrons in the quantum dot (Ne). By changing the applied gate voltage, we are able to control Ne.

A Zero-bias anomaly is observed for a strong coupling to the leads and possible symmetrical tunnel barriers. This Kondo resonance appears for successive Ne showing a deviation from the conjectured odd-even behavior. The Kondo resonance is strongest for Ne=9 and displays a particle-hole symmetry for Ne =7,..,11. It is absent for Ne =6 and Ne = 12. These observations indicate the influence of the shell structure [1] of the electronic states in the quantum dot where orbital degeneracy is present.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64, 701-736 (2001).

TT 24.5 Tue 10:30 POT 151

Highly Conductive Silicon Nanowires by Modulation-Doping via Aluminum-Induced Acceptor States in an SiO2-shell — •Daniel Hiller[1], Ingmar Ratschinski[1], Soundarya Nagarajan[2], Jens Trommer[2], Thomas Mikolajick[2,3], and Dirk König[4] — [1]Institute of Applied Physics, TU Bergakademie Freiberg, Germany — [2]Nanoelectronic Materials Laboratory gGmbH, Dresden, Germany — [3]Institute of Semiconductors and Microsystems, TU Dresden, Germany — [4]Integrated Materials Design Lab, ANU, Canberra, Australia

Silicon nanowires (Si NWs) enable maximum gate control over the source-drain current when configured in a gate-all-around FET-architecture. However, Si NWs with few nm in diameter suffer from severe difficulties with efficient impurity doping due to a multitude of physical and technological problems (diffusion, dielectric and quantum confinement, statistics of small numbers, etc.). Here, we present a novel doping concept for Si NWs comparable to the modulation doping approach of III-V semiconductors. Based on results from density functional theory (DFT) calculations, we use Al-doped SiO2 shells around the Si NWs, which contain unoccupied Al-induced acceptor states that are energetically located below the Si valence band edge. These states can capture electrons from the Si, creating free holes as majority charge carriers [1-5]. In this presentation, recent results from the experimental realization of this concept on Si NWs are shown. We demonstrate that modulation doping using SiO2:Al-shells allows for several orders of magnitude lower resistances when compared to undoped SiO2-shells. [1] D. König et al., Sci. Rep. 7, 46703 (2017)

30 min. break

TT 24.6 Tue 11:15 POT 151

Carrier dynamics in quantum-dot tunnel- injection structures: microscopic theory and experiment — •Michael Lorke[1], Igor Khanonkin[2], Stephan Michael[1], Johann Peter Reithmaier[3], Gadi Eisenstein[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Otto-Hahn-Allee 1, Bremen, 28359, Germany — [2]Electrical Engineering Department and Russel Berrie Nanotechnology Institute, Technion, Haifa, 32000, Israel — [3]Technische Physik, Institute of Nanostructure Technologies and Analytics, Center of Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Kassel, 34132, Germany

Among the challenges for the next generation of semiconductor lasers is the enhancement of their modulation speed to satisfy the need for higher data transfer rates. For this purpose, tunnel injection lasers are an appealing concept, as they promise improved modulation rates and better temperature stability. Moreover, they eliminate a major detri- mental effect of quantum dot lasers, which is the gain nonlinearity caused by hot carriers. It is shown in this work how the aforementioned improvements depend on the design of tunnel-injection devices. We perform a theory-experiment comparison on scattering times in tunnel injection devices to highlight the importance of alignment between the injector well and the quantum dot ensemble. It is shown how differences in the coupling to the injector quantum well caused by the alignment lead to scattering times into the quantum dot ensemble that vary by an order of magnitude.

TT 24.7 Tue 11:30 POT 151

Electron transport through a quantum dot in controlled heat bath environment — •Hatef Ghannadi maragheh, Johannes C. Bayer, and Rolf J. Haug — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany

For optimizing any device, amongst them semiconductor-based qubit, one has to understand the effects of the environment on them. In this sort of devices, not just quantum states of the channel but also the state of the particles is affected [1-3]. The device consists of split-gate quantum dot in a GaAs/AlGaAs heterostructure. The temperature of the measurement ranged from 49.9 mK to 800 mK.

There have been several works on explaining how electron transport through the quantum dot system would behave for different temperatures [4-5]. As the temperature changes, the Fermi distribution of the lead*s changes. This influenced the conductivity of the dot since in the presence of the bias voltage the transport window gets altered. Besides, depending on the presence of energy levels in the transfer window, the conductivity is manipulated by changing the temperature. For low temperatures, due to the local density of states and coupling of the barrier gates to the leads, fluctuations start to emerge.

[1]*K. C. Nowack et al, Science 318, 1430-1433 (2007)
[2]*Pioro-Ladrière, et al, Nature Physics 4, 776*779 (2008)
[3]*Jan K Kühne, et al, physica status solidi (b) 256(6) (2019)
[4]*E. B. Foxman, et al, Phys. Rev. B 47, 10020(R) (1993)
[5]*O. Dani, et al, Communications Physics 5 (1), 1-7 (2022)

TT 24.8 Tue 11:45 POT 151

Manipulation of temporal correlations in single-electron tunneling — •Johannes C. Bayer, Adrian Schmidt, Timo Wagner, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Precisely timed single-particle operations are of critical importance for quantum technologies operating at fixed clock cycles. A detailed understanding of the interplay between an external drive and the response of the single-particle source is essential for achieving and improving the accuracy in the time domain. We here demonstrate a high level of control over the time domain of a driven single electron transistor (SET). Using a gate defined quantum dot connected to a highly sensitive charge detector [1] allows detecting electrons tunneling into and out of the SET in real-time [2, 3]. The tunneling rates of such devices are controllable by gate voltages. We drive the SET by modulating gate voltages periodically in time and use time-dependent tunneling rates [2] and waiting time distributions [4] to analyze the impact of the driving parameters on temporal correlations in the tunneling times.

[1] J. C. Bayer, T. Wagner, E. P. Rugeramigabo and R. J. Haug, Ann. Phys. 531, 1800393 (2019)
[2] T. Wagner, P. Talkner, J. C. Bayer, E. P. Rugeramigabo, P. Hänggi and R. J. Haug, Nat. Phys. 15, 330-334 (2019)
[3] R. Hussein, S. Kohler, J. C. Bayer, T. Wagner and R. J. Haug, Phys. Rev. Lett. 125, 206801 (2020)
[4] F. Brange, A. Schmidt, J. C. Bayer, T.Wagner, C. Flindt and R. J. Haug, Sci. Adv. 7, eabe0793 (2021)

TT 24.9 Tue 12:00 POT 151

Scalable integrated readout electronics for semiconductor quantum dots — •Jonas Bühler[1], Arun Ashok[1], Lammert Duipmans[1], Patrick Vliex[1], Christian Grewing[1], André Zambanini[1], and Stefan Van Waasen[1,2] — [1]Central Institute of Engineering, Electronics and Analytics, Electronics Systems (ZEA-2) Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]Faculty of Engineering, Communication Systems, University Duisburg-Essen, 47057 Duisburg, Germany

Quantum computing is one of the promising candidates to overcome the limitations of *classical* computing, e.g. von Neumann architecture. Nowadays much progress has been made on the implementation of scalable qubits. This work focuses on semiconductor qubits, which need operating temperatures near 0 K. Room temperature electronics for control and readout, which are limiting the bandwidth and the scalability due to parasitic elements and heat conduction, are still widely used. Some progress has been made to integrate the qubit control and readout in the direct vicinity of the qubit at cryogenic temperatures. Especially readout electronics still have a limited scalability because of circuit size and power consumption. This work tries to overcome those limitations by comparing different readout architectures and implement a multiplexed and integrated readout circuit with lower area and power consumption. This integrated circuit in a 22nm FD-SOI technology will be placed on top of scalable quantum computing architectures and therefore might be a crucial step on the way to a multi-million qubit quantum computer.

TT 25: Molecular Electronics and Photonics (joint session TT/CPP)

Time: Tuesday 12:00–13:00 Location: HSZ 201

TT 25.1 Tue 12:00 HSZ 201

Single photon emitters in hBN via ultra-low energy helium ion implantation — •Renu Rani[1], Mihn Bui[1,2], Chenfeng Lu[1,2], Bilal Malik[1,2], Felix Junge[3], Thorsten Brazda[1], Detlev Grützmacher[1,2], Hans Höfsäss[3], and Beata Kardynał[1,2] — [1]Peter Grünberg Institut-9, Forschungszentrum Jülich, Jülich — [2]Department of Physics, RWTH Aachen, Aachen — [3]II. Institute of Physics, University of Göttingen, 37077 Göttingen

A discovery of quantum emitters in hexagonal boron nitride (hBN) has recently incited immense interest for quantum technologies. It offers a platform for fundamental science but is also of interest for applications in quantum photonics owing to its robust single photon emission at room temperature. Recent studies have suggested that these SPEs are associated with intrinsic defects, which led to efforts to engineer the SPE in hBN by various methods such as plasma treatment, annealing, laser, e-beam and ion irradiation methods. Despite these efforts, the origin of single photon emission and the correlation of emission with particular defects still need to be scrutinized. Here we use ultralow energy ion implantation to introduce defects in hBN. We show that helium ions with energies as low as 50 eV are extremely efficient in introducing single photon emitters in hBN. We also show that low temperature annealing increases the density of the emitters. We consider the possible defects that helium ions at the implantation energy can generate in hBN and use statistical data on single photon emitters to discuss the possible origin of the emission. Finally, we discuss the viability of creating emitters in pre-selected locations.

TT 25.2 Tue 12:15 HSZ 201

Mechanosensitive single-molecule junctions — •Fabian Pauly — University of Augsburg, Augsburg, Germany

Quantum interference of electron waves passing through a single-molecule junction provides a powerful way to influence its electrical properties. By distorting a molecule, showing a destructive quantum interference, small changes of electrode distance can lead to huge changes of electrical conductance. This mechanosensitivity is a desirable feature for highly sensitive stress sensors. Here, I will discuss recent combined experimental and theoretical studies of mechanosensitive molecular wires based on paracyclophanes and porphyrins [1-4]. Experimental findings are interpreted in terms of quantum interference effects between molecular frontier orbitals by theoretical calculations based on density functional theory and the Landauer scattering formalism.

[1] D. Stefani et al., Nano Lett. 18, 5981 (2018)
[2] K. Reznikova et al., J. Am. Chem. Soc. 143, 13944 (2021)
[3] W. M. Schosser et al., Nanoscale 14, 984 (2022)
[4] C. Hsu et al., Chem. Sci. 13, 8017 (2022)

TT 25.3 Tue 12:30 HSZ 201

Designing mechanosensitive molecules: A genetic algorithm-based approach — •Matthias Blaschke and Fabian Pauly — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

Single molecules can be used as miniaturized functional electronic components, when connected to metallic electrodes. Mechanosensitivity describes a change of conductance for a certain change of electrode separation and is a desirable feature for applications such as ultrasensitive stress sensors [1-4]. We combine methods of artificial intelligence with high-level simulations based on electronic structure theory to design optimized mechanosensitive molecules from predefined building blocks. In this way we overcome time-consuming, inefficient trial and error cycles in molecular design. We unveil the black-box machinery usually connected to methods of artificial intelligence by presenting all important evolutionary processes. In addition, we identify general features that characterize well-performing molecules. Our genetic algorithm provides a systematic and powerful way to search chemical space and to identify the most promising molecular candidates.

[1] D. Stefani et al., Nano Lett. 18, 5981 (2018)
[2] K. Reznikova et al., J. Am. Chem. Soc. 143, 13944 (2021)
[3] W. M. Schosser et al., Nanoscale 14, 984 (2022)
[4] C. Hsu et al., Chem. Sci. 13, 8017 (2022)

TT 25.4 Tue 12:45 HSZ 201

Towards cavity-mediated molecule-molecule coupling — •André Pscherer[1], Jahangir Nobakht[1], Tobias Utikal[1], Stephan Götzinger[2,1,3], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Department of Physics, Friedrich- Alexander University Erlangen-Nürnberg (FAU), Erlangen, Germany — [3]Graduate School in Advanced Optical Technologies (SAOT), Friedrich-Alexander University Erlangen-Nürnberg, Erlangen, Germany

We recently demonstrated that a single molecule coupled to a Fabry-Pérot cavity reacts nonlinearly to light at the single-photon level. This was shown in four-wave mixing, optical switching and photon number sorting experiments [1]. We aim to exploit this level of control to couple two molecules to each other via the cavity mode and to explore two-photon transitions that become possible in such a system. We gain access to the excited state population through spectrally tailored cavity mirrors which transmit red-shifted fluorescence. In this contribution, we will report on our progress, challenges, and intermediate results.

[1] A. Pscherer et al., Phys. Rev. Lett. **127**, 133603 (2021)

TT 26: Members' Assembly

Topics: Status report on current meeting, Elections, Miscellaneous, Outlook 2024

Time: Tuesday 14:00–15:30 Location: HSZ 304

All members of the Low Temperature Physics Division are invited to participate.

TT 27: Focus Session: Unconventional Transport Phenomena in Low-Dimensional Superconducting Heterostructures

The investigation of new superconducting systems and effects is key to the development of superconducting electronics and quantum technologies. Recent studies have demonstrated that systems of low dimensionality in particular offer enormous possibilities for the realization of unconventional superconducting phases and quantum states. An effect hosted by low-dimensional superconducting systems is the supercurrent diode effect. The supercurrent diode effect was experimentally observed in 2020 and has since then been intensively investigated worldwide. The effect has been seen in a variety of low-dimensionality hybrid systems, such as two-dimensional van der Waals heterostructures, in magnetic proximity systems as well superlattices. The origin of the effect, however, is still under debate and several explanations have been proposed for its underlying mechanism including lack of inversion symmetry, spin-orbit coupling and screening effects. This Focus session will bring together the most recent developments in the field of superconducting effects in low-dimensionality systems and update the community on their physics and perspective applications, with particular attention to recent results related to the supercurrent diode effect.

Organizers: Wolfgang Belzig and Angelo Di Bernardo (Universität Konstanz)

Time: Wednesday 9:30–13:00 Location: HSZ 03

Invited Talk TT 27.1 Wed 9:30 HSZ 03

Superconducting diode effect in Rashba superlattice — •Teruo Ono — Kyoto University, Japan

The diode effect is fundamental to electronic devices and is widely used in rectifiers and AC-DC converters. However, conventional diodes have an energy loss due to finite resistance. We found the superconducting diode effect (SDE) in Nb/V/Ta superlattices with a polar structure, which is the ultimate diode effect exhibiting a superconducting state in one direction and a normal state in the other [1-3]. SDE can be considered as the nonreciprocity of the critical current for the metal-superconductor transition. We also found the reverse effect, i.e., the nonreciprocal critical magnetic field under the application of the supercurrent [4]. We also found that the polarity of the superconducting diode shows a sign reversal as a magnetic field is increased, which can be considered as the crossover and phase transitions of the finite-momentum pairing states predicted theoretically [5]. SDE in Nb/V/Ta superlattices needs an application of an external magnetic field to break the time reversal symmetry, which is a disadvantage in applications. We recently succeeded in demonstrating SDE in a zero-field by introducing ferromagnetic layers in superlattices [6]. The polarity of the SDE is controlled by the magnetization direction of the ferromagnetic layer, leading to development of novel non-volatile memories and logic circuits with ultralow power consumption.

[1] J. Magn. Soc. Japan 43, 17 (2019)
[2] Nature 584, 373 (2020)
[3] Jpn. J. Appl. Phys. 60, 060902 (2021)
[4] Appl. Phys. Express 14, 073003 (2021)
[5] Phys. Rev. Lett. 128, 037001 (2022)
[6] Nat. Nanotechnol. 17, 823 (2022)

Invited Talk TT 27.2 Wed 10:00 HSZ 03

Quasiparticle-based and Cooper-pair based superconducting diodes — •Maria Spies[1], Stefan Ilić[2], Sebastián Bergeret[2], Francesco Giazotto[1], and Elia Strambini[1] — [1]NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, I-56127 Pisa, Italy — [2]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSICUPV/ EHU, E-20018 Donostia-San Sebastián, Spain

Diodes are key elements for electronics, optics, and detection. Their evolution towards low dissipation electronics has lead to the hybridization with superconductors (S) and the realization of non-reciprocal transport of both quasiparticles and Cooper pairs. That occurs when both spatial inversion and time-reversal symmetries are broken.

Here, we review both effects comparing their efficiencies and basic principles. The quasi-particle diode is a superconducting tunnel junction with zero conductance in only one direction. The directionselective propagation of the charge has been obtained through the broken electron-hole symmetry induced by the spin selection of a ferromagnetic tunnel barrier made of a EuS thin film separating a superconducting Al and a normal metal Cu layer. It achieves a large rectification of up to 40%.

On the other hand, supercurrent diodes made with hybrid S/spinorbit/ S Josephson Junctions or with two-dimensional Rashba superconductors have been demonstrated to show zero resistance in only one direction. We describe the equation of the supercurrent diode effect in a generic formalism that may inspire novel devices based on helical magnetism induced in conventional superconductors.

Invited Talk TT 27.3 Wed 10:30 HSZ 03

Non-reciprocal superconductivity and the field free Josephson diode — •Mazhar Ali — TU Delft, Delft, Netherlands

Nonreciprocal transport is incredibly important in technology; for example, asymmetry in the current-voltage response in semiconductor junctions has been the cornerstone of computing technology for half a century. The diode effect is a very basic demonstration of nonreciprocity. Nonreciprocal superconductivity, however, proved elusive, and only in 2020 was the superconducting diode effect (superconducting in one direction while normal conducting in the other) discovered for the first time in a bulk alloy of V/Nb/Ta. By breaking both inversion and time reversal symmetry (using an applied magnetic field), a difference in the critical superconducting current (I) for positive vs negative voltages (V) was seen. Recently, we demonstrated a Josephson diode (JD), created in a quantum material Josephson junction (QMJJ, a junction made up of two superconductors separated by a barrier comprised of a quantum material). A diodic effect was seen without an applied magnetic field; a puzzling result for theoretical physicists but an important advance for potential technological application. Using an inversion symmetry breaking heterostructure of $NbSe_2/Nb_3Br_2/NbSe_2$, half-wave rectification of a square-wave excitation was achieved with low switching current density, high rectification ratio, and high robustness. Future directions for optimizations and novel explorations, as well as a broader impact of using other quantum materials will be discussed.

15 min. break

TT 27.4 Wed 11:15 HSZ 03

Investigating the mechanism behind the Josephson Diode Effect in $NiTe_2$/superconductor Devices — •Emily C. McFarlane[1], Jonas A. Krieger[1], Mihir Date[1], Banabir Pal[1], Procopios C. Constantinou[2], Vladimir N. Strocov[2], Stuart S. P. Parkin[1], and Niels B. M. Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland

The Josephson diode - recently realized in NiTe2/superconductor devices in the presence of an external magnetic field [1] - has many potential uses in new superconducting memory and logic devices. These $NiTe_2$/Ti/Nb devices are the first Josephson diodes where the Josephson diode effect (JDE) was concluded to arise from finite momentum Cooper pairing. However, the role of the Ti layer directly at the $NiTe_2$ interface is not yet fully understood. Ti-doped $NiTe_2$ is seen to be superconducting [2], so here we investigate the possibility of intrinsic superconductivity at the $NiTe_2$/Ti interface by investigating its electronic structure with angle-resolved photoelectron spectroscopy. In isostructural $PdTe_2$, a van Hove singularity (vHS) near the Fermi level was linked to intrinsic superconductivity [3]. We find a similar vHS in the vicinity of the Fermi level in the electronic structure of $NiTe_2$, which can be shifted in energy at the interface due to a doping effect by aluminium.

[1] B. Pal *et al.*, Nat. Phys. 18, 1228 (2022)
[2] B. S. de Lima *et al.*, Solid State Commun. 283, 27 (2018)
[3] Kyoo Kim *et al.*, Phys. Rev. B 97, 165102 (2018)

TT 27.5 Wed 11:30 HSZ 03

Reversal of the AC and DC supercurrent diode effect in ballistic Josephson junctions — Andreas Costa[1], Christian Baumgartner[1], Simon Reinhardt[1], Sergei Gronin[2], Geoffrey C. Gardner[2], Tyler Lindemann[2], Michael J. Manfra[2], Denis Kochan[1], Jaroslav Fabian[1], •Nicola Paradiso[1], and Christoph Strunk[1] — [1]University of Regensburg — [2]Purdue University

Recent experiments [1,2] have demonstrated that the supercurrent diode effect (SDE), –i.e., a nonreciprocal supercurrent– can be obtained by applying a Zeeman field in the presence of spin-orbit coupling. The effect consists in a finite difference ΔI_c between positive I_c^+ and negative $|I_c^-|$ critical current (DC SDE), and an asymmetry in the Josephson inductance as a function of current (AC SDE). In this work, we show that, at high in-plane fields, the AC and DC SDE both change sign. Based on a minimal and analytical model, we clearly identify the origin of this sign change in terms of a 0-π-like transition –an effect predicted in the literature [3] but so far never experimentally observed. Thanks to our inductance measurements we can directly link the AC SDE reversal to the modification of the CPR induced by the Zeeman field. Our results illustrate the power of the Josephson inductance as a probe of phase transitions in unconventional superconductors.

[1] Ando *et al.*, Nature **584**, 373 (2020)
[2] Baumgartner *et al.*, Nature Nano. **17**, 39, (2022)
[3] Yokoyama *et al.*, Phys. Rev. B **89**, 195407 (2014)

TT 27.6 Wed 11:45 HSZ 03

Theoretical study of the supercurrent diode effect in 2DEG Josephson junctions — •Andreas Costa[1], Denis Kochan[1,2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]Slovak Academy of Sciences, Slovakia

Superconducting junctions exhibit fascinating physical phenomena, making them promising building blocks for quantum computing. The competition between the two fundamental spin interactions—ferromagnetic exchange and spin-orbit interaction (SOI)—and superconductivity has already been demonstrated to substantially modify the spectroscopic and transport signatures of these junctions, and potentially results in topological superconductivity.

In this talk, we will focus on 2DEG-based S-N-S Josephson junctions that combine intrinsic SOI with proximity-induced superconductivity originating, e.g., from top Al islands. We will demonstrate that turning the nonsuperconducting (N) weak link additionally ferromagnetic—e.g., through a magnetic field—can imprint a strong direction dependence on the current-phase relation, which finally rises a substantial difference between positive and negative critical currents, and thereby a pronounced supercurrent diode effect. Motivated by pioneering experimental studies [1–3], we will elaborate on powerful theoretical approaches—such as numerical tight-binding simulations [2, 3] and analytical studies of the Andreev spectrum—to characterize and understand the features of this Josephson supercurrent diode effect.

[1] Phys. Rev. Lett. 126, 037001 (2021)
[2] Nat. Nanotechnol. 17, 39 (2022)
[3] J. Phys. Condens. Matter 34, 154005 (2022)

TT 27.7 Wed 12:00 HSZ 03

Plasmons and dynamical screening in layered superconducting heterostructures — •Yann in 't Veld[1], Mikhail Katsnelson[1], Andrew Millis[2,3], and Malte Rösner[1] — [1]Radboud University, Nijmegen, the Netherlands — [2]Flatiron Institute, New York, USA — [3]Columbia University, New York, USA

Layered metals host low-energetic plasmonic and phononic excitations, which both strongly couple to electrons. At the same time these excitations hybridize with each other, which can be tuned by the surrounding material, resulting in a complex interplay of different bosons. Here we investigate how this interplay affects superconductivity in layered materials and how it is affected by the substrate material. To this end we use a one-loop theory which consistently treats phonons, plasmons, their mutual interaction and environmental screening on the same footing. We find two regimes with large transition temperatures, controlled by the substrate screening. One is mediated by conventional phonon pairing, which shows a significantly reduced transition temperature due to consistent screening. The other regime is dominated by the unconventional electron-plasmon interaction, where we find strong effects of normal-state renormalization on the superconducting state. These results show how crucial a consistent treatment of all pairing and screening channels is for low-dimensional superconductivity.

TT 27.8 Wed 12:15 HSZ 03

Investigation of Nb gate-controlled superconducting nanoscale devices. — •Leon Ruf, Elke Scheer, and Angelo Di Bernardo — 78464 Konstanz, Konstanz Germany

The electrical conductance in nanoscale devices can be modulated by an applied electric field (EF). In semiconductors the charge density is low, and the EF can penetrate deeply. However, in superconductors the charge carrier density is high and the external EF decays exponentially over a short distance. In 2018, it was reported [1] that the superconducting state can be partially and fully suppressed in gated nano constrictions by a strong applied EF which they attribute to an EF induced perturbation of the superconducting state. Since then, the observations were controversially discussed attributing them to an EF effect [1], high-energy quasiparticle injection [2], low-energy-mediated phonon excitation [3] or hot-spot generation [4]. Here, we are studying Nb gated Dayem bridges. Our observations show reversible full suppression of the supercurrent for Nb devices made by lift off, not for geometrically comparable etched devices. We discuss our observations in the light of the suggested mechanisms [1-4].

[1] G. De Simoni *et al.*, Nat. Nanotechnol. 13, 802 (2018)
[2] L. D. Alegria *et al.*, Nat. Nanotechnol. 16, 404 (2021)
[3] M. F. Ritter *et al.*, Nat. Electron. 5, 71 (2022)
[4] J. Basset *et al.*, Phys. Rev. Res. 3, 043169 (2021)

TT 27.9 Wed 12:30 HSZ 03

Gate-controlled switching in non-centrosymmetric superconducting devices — •Jennifer Koch, Leon Ruf, Elke Scheer, and Angelo Di Bernardo — Universität Konstanz, Konstanz, Germany

Gate-controlled superconducting devices have become of great interest for the development of energy-efficient hybrid superconductor/semiconductor computing architectures. The idea behind this technology stems from the recent discovery that superconducting devices can be controlled electrically with the application of a gate voltage [1-3].

We investigate gate-controlled switching devices made of the non-centrosymmetric superconductor $Nb_{0.18}Re_{0.82}$ for different gate-to-wire distances. This material promises a low switching voltage due to its disordered structure and should therefore be more suitable for the realization of devices compatible with CMOS transistors.

[1] G. De Simoni et al., Nature Nanotech. 13, 802 (2018)
[2] F. Paolucci et al., Nano Lett. 18, 4195 (2018)
[3] F. Paolucci et al., Phys. Rev. Applied 11, 024061 (2019)

TT 27.10 Wed 12:45 HSZ 03

Microscopic theory of gate-voltage mediated surface pair breaking and its impact on a superconducting wire — •Subrata Chakraborty, Danilo Nikolic, and Wolfgang Belzig — Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany

Gate-induced supercurrent suppression in a superconducting nanobridge is a hot topic for research in present days. Recent experiments find supercurrent suppression in this nano-bridge for high gate electric fields [1-3]. The microscopic understanding of this effect is not clear till now. According to many experimental findings, there are three distinct tentative mechanisms, which could be responsible for this event, at high gate fields. In our work, we theoretically investigate the role of gate-mediated surface pair breaking on the supercurrent suppression. We show that in presence of a small concentration of magnetic impurities on the surface of the bridge, large gate-fields result in strong spin-flip scattering at the surface. Using microscopic modelling based on the quasiclassical Usadel equation we present the full phase diagram of the wire, that shows a supercurrent suppression very similar to some experiment. We speculate, that our generic theoretical predictions based on this microscopic effect can be tested experimentally by modifying the surface.

[1] G. De Simoni *et al.*, Nat. Nanotechnol.**13**, 802 (2018)
[2] I. Golokolenov *et al.*, Nat. Commun. **12**, 2747 (2021)
[3] L. D. Alegria *et al.*, Nat. Nanotechnol. **16**, 404 (2021)

TT 28: Unconventional Superconductors

Time: Wednesday 9:30–11:15 Location: HSZ 103

TT 28.1 Wed 9:30 HSZ 103

Fermi surface study of the putative spin-triplet superconductor UTe_2 — •Alexander Eaton[1], Theodore Weinberger[1], Zheyu Wu[1], Alexander Hickey[1], Nicholas Popiel[1], and Michal Valiska[2] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]MGML, Charles University, Prague

The unconventional superconductor UTe_2 exhibits numerous properties indicative of spin-triplet pairing, including an upper critical field far in excess of the Pauli paramagnetic limit, and re-entrant superconductivity at high magnetic fields > 40 T. However, a detailed understanding of the material's Fermi surface remains a key open question hampering efforts to attain a more detailed theoretical picture of the microscopic pairing mechanism(s) at play.

Here, we report a detailed de Haas-van Alphen study of the Fermi surface of UTe_2. We measured quantum oscillations in the magnetic torque and contactless resistivity of several high quality samples (RRR $\sim$ 900, Tc = 2.1 K) in a dilution refrigerator at temperatures down to 19 mK and magnetic fields up to 28 T, through two orthogonal rotation planes. Importantly, access to field strengths this high allowed us to measure directly along the [001] direction, which has previously been proposed to run parallel to the axis of cylindrical Fermi surface sections.

We present a summary of our angle- and temperature-dependent results performed to date, and compare to DFT and DMFT calculations that we find to capture the majority of the observed behaviour.

TT 28.2 Wed 9:45 HSZ 103

High pressure study of the unconventional superconductor $CeRh_2As_2$ — •Meike Pfeiffer[1], Konstantin Semeniuk[2], Seunghyun Khim[2], and Elena Hassinger[1] — [1]Technische Universität Dresden Institut für Festkörper- und Materialphysik, 01069 Dresden — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden

The heavy-fermion superconductor $CeRh_2As_2$ hosts two distinct superconducting states which are currently understood as even- and odd-parity states. The compound crystallizes in a layered lattice that is globally centrosymmetric but lacks local inversion symmetry at the Ce sites. This results in a strong spin-orbit coupling, believed to lead to a very high ratio of upper critical field (> 15 T) to critical temperature ($T_c = 0.26$ K). The normal state of the compound hosts an additional phase below 0.4 K, believed to be a quadrupole-density wave (QDW) order. We present a high-pressure electrical resistivity study of $CeRh_2As_2$ across different generations of samples. The QDW order is highly sensitive to lattice compression and gets fully suppressed at $P_c \approx 0.6$ GPa. The superconducting transition temperature T_c decreases at a significantly lower rate, and both superconducting phases persist well above 2 GPa. Thus, we confirm that the QDW is not responsible for the phase switching from even- to odd-parity state. At the same time, the in-plane magnetic field peaks at P_c, suggesting a different kind of interplay between the two orders.

TT 28.3 Wed 10:00 HSZ 103

Superconductivity versus quadrupole density wave in $CeRh_2As_2$ — •Konstantin Semeniuk[1], Daniel Hafner[1], Pavlo Khanenko[1], Javier Landaeta[1], Thomas Lühmann[1], Christoph Geibel[1], Seunghyun Khim[1], Elena Hassinger[2], and Manuel Brando[1] — [1]MPI-CPfS, Dresden, Germany — [2]TU Dresden, Dresden, Germany

A heavy-fermion superconductor $CeRh_2As_2$ ($T_c \approx 0.3\,$K) undergoes a phase transition at the temperature $T_0 \approx 0.5\,$K, proposed to be a quadrupole density wave (QDW) instability. The compound hosts two distinct superconducting (SC) phases, presumably of different parity. These are separated by a first order phase boundary at magnetic field $\mu_0 H^* = 4\,$T, applied along the c axis of the tetragonal lattice. Recent studies suggest that the QDW phase boundary could meet the $T_c(H)$ line at exactly at H^*. This would imply that the SC phase switching is driven by the field-induced suppression of the QDW order coexisting with the superconductivity. Inability to reliably track T_0 near 4 T has left the question standing.

We present a study of a new generation of $CeRh_2As_2$ crystals, showing sharper signatures of phase transitions. From our measurements of heat capacity and electrical resistivity in c-axis magnetic field, we produce a more detailed phase diagram which shows that the QDW and SC phase boundaries meet at 6 T. We conclude that the QDW state is not responsible for the SC phase switching at H^* and discuss the possible interplay between the two orders with reference to the Fermiology of $CeRh_2As_2$ as well as thermodynamic considerations.

TT 28.4 Wed 10:15 HSZ 103

Exploring the unconventional superconducting state in Ce_3PtIn_{11} — Jan Fikáček[1], Sarah R. Dunsiger[2], Sébastien Laughrea[3], Andrea D. Bianchi[3], Shinsaku Kambe[4], Hironori Sakai[4], Yo Tokunaga[4], Manuel Brando[5], and •Jeroen Custers[1] — [1]Charles University, Faculty of Mathematics and Physics, Department of Condensed Matter Physics, Ke Karlovu 5, 121 16 Prague 2, Czech Republic — [2]Centre for Molecular and Materials Science, TRIUMF, Vancouver, British Columbia, Canada V6T 2A3 — [3]Département de Physique, Université de Montréal, Montréal, Canada — [4]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai-mura, Ibaraki 319-1195, Japan — [5]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Strasse 40, D-01187, Dresden, Germany

The properties of the heavy fermion compound Ce_3PtIn_{11} are certainly enigmatic. At ambient pressure, the compound displays two consecutive magnetic transitions into antiferromagnetic (AFM) states at $T_{N1} = 2.2$K and $T_N = 2.0$K, respectively. Below $T_c = 0.32$K superconductivity (SC) is found. It has been speculated that AFM and SC coexist because the compound harbors two inequivalent Ce sites each having a specific environment favoring either a magnetic or superconducting state. We focus on the SC state and present specific heat, ^{115}In NQR and recent μSR experiments at ambient pressure and down to 20mK. The results sketch a picture of an unusual unconventional SC state.

TT 28.5 Wed 10:30 HSZ 103

Surface-acoustic-wave-induced unconventional superconducting pairing — •Viktoriia Kornich — Julius-Maximilians-Universität Würzburg

Exotic materials, topological states, and quantum collective phenomena are of high interest for fundamental science and technology, because they provide complex and stable performance even at a very small scale. The field of unconventional superconductivity investigates new features and phenomena occurring in superconducting materials and setups. However, the exact processes, which lead to unconventional superconducting states are usually not clear and subject to numerous hypotheses and attempts to experimentally verify them. Here, I will discuss how to use externally applied acoustic waves in order to induce unconventional superconducting pairing of different types in solid state matter, primarily in thin films and 2D materials. I will consider a simple setup consisting of a solid state material with conduction electrons and an applied surface acoustic wave, that breaks spatial translation symmetry. I will show that the symmetries of the possible surface-acoustic-wave-induced order parameters depend on the shape of the applied wave. As an example, I will show that even-frequency spin-triplet odd-parity order parameter can occur due to Rayleigh surface acoustic wave.

Invited Talk TT 28.6 Wed 10:45 HSZ 103

Studying the Fulde-Ferrell-Larkin-Ovchinnikov order parameter in quasi-2D organic superconductors — •Tommy Kotte[1], S. Molatta[1], D. Opherden[1], G. Koutroulakis[2], S. E. Brown[3], J. A. Schlueter[4,5], H. Kühne[1], G. Zwicknagl[6], and J. Wosnitza[1,7] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]UC Santa Barbara, USA — [3]UC Los Angeles, USA — [4]NSF, Alexandria, USA — [5]ANL, Argonne, USA — [6]IMP, TU Braunschweig — [7]IFMP, TU Dresden

The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state can emerge in superconductors for which the orbital critical field exceeds the Pauli limit. This unconventional superconducting state is characterized by a spatial modulation of the superconducting order parameter. Although evidence of the formation of an FFLO state has been found in various classes of materials, it is still theoretically debated and experimentally unexplored how the superconducting order parameter evolves within the FFLO phase. Here, we present two fundamental studies concerning this question in quasi-2D organic superconductors, which are well established to host an FFLO state: (i) By means of ^{13}C NMR spectroscopy on β"-$(ET)_2SF_5CH_2CF_2SO_3$, we were able to quantify the modulation amplitude of the spin polarization throughout the FFLO state. This quantity is related to the modulated superconducting gap, hence representing the order parameter. (ii) By means of angular-resolved specific-heat measurements on κ-$(ET)_2Cu(NCS)_2$, we furthermore show how the FFLO order parameter becomes unstable against orbital interactions, leading to a crossover from the FFLO into Abrikosov-like states of higher-order Landau levels.

TT 29: Frustrated Magnets: General

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

TT 29.1 Wed 9:30 HSZ 201

Possible stress-driven spiral-to-Néel transition in the triangular antiferromagnet $PdCrO_2$ — •Nina Stilkerich[1,2], Seunghyun Khim[2], Andrew Mackenzie[2,3], Jochen Geck[1], and Clifford Hicks[2,4] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany — [3]Scottish Universities Physics Alliance (SUPA), School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom — [4]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, United Kingdom

$PdCrO_2$ is a triangular antiferromagnet that undergoes a transition from a double-q to single-q magnetic structure under moderate uniaxial stress [1]. Due to a high sensitivity of the magnetic anisotropy to uniaxial stress, another transition from spiral order to a linear antiferromagnetic structure is predicted for higher stress of about 1 GPa [1]. We performed stress-strain measurements on $PdCrO_2$ and were able to identify the double- to single-q transition as a jump in strain. We report the discovery of an additional transition under higher stress, which might be the spin spiral to Néel transition suggested previously.

[1] D. Sun et al., New J. Phys. 23, 123050 (2021)

TT 29.2 Wed 9:45 HSZ 201

Thermodynamic study of the partially polarized state of the sawtooth chain atacamite, $Cu_2Cl(OH)_3$ — Leonie Heinze[1], Tommy Kotte[2], Albin de Muer[3], Sven Luther[2,4], Andrew Ammerlaan[5], Uli Zeitler[5], Anja U.B. Wolter[6], Bernd Büchner[6], Kirrily C. Rule[7], Hannes Kühne[2], and •Stefan Süllow[1] — [1]TU Braunschweig, Braunschweig, Germany — [2]HLD, HZ Dresden-Rossendorf, Germany — [3]LNCMI, CNRS, Grenoble, France — [4]TU Dresden, Dresden, Germany — [5]HFML, Radboud University, Nijmegen, The Netherlands — [6]ANSTO, Lucas Heights, Australia — [7]IFW Dresden, Dresden, Germany

Recently, the natural mineral atacamite, $Cu_2Cl(OH)_3$, has been established as a unique model compound of the $S = 1/2$ quantum sawtooth chain with a dominant magnetic exchange $J \sim 360$ K along the chain spine and $J' \sim 102$ K within the sawteeth [1]. Residual interchain couplings of a few Kelvin drive atacamite into an antiferromagnetic (AFM) ground state below $T_N = 8.4$ K. The AFM phase is suppressed in magnetic fields of ~ 30 T. Upon suppression of AFM order, the magnetization becomes plateau-like close to $M_{sat}/2$.

By now, we have been able to study the magnetic phase diagram up into the unusual partially polarized state by means of specific heat. Here, we present a corresponding study and present evidence for quantum critical behavior occuring upon suppression of AFM order.

[1] L. Heinze *et al.*, Phys. Rev. Lett. **126**, 207201 (2021).

TT 29.3 Wed 10:00 HSZ 201

Weakly coupled triangles forming a star lattice in an organic-inorganic copper sulfate — •Oleg Janson[1], Ulrich K. Rössler[1], and Hajime Ishikawa[2] — [1]Leibniz IFW Dresden, Germany — [2]ISSP, University of Tokyo, Japan

The recently synthesized organic-inorganic copper sulfate $[(CH_3)_2(NH_2)]_3[Cu_3(OH)(SO_4)_4]\cdot0.24H_2O$ has been proposed as a material realization of the $S = \frac{1}{2}$ star lattice model [1]. We report high-field magnetization measured on powder samples showing a broad plateau at $\frac{1}{3}$ of the saturation magnetization. Full saturation was reached at about 105 T in a destructive pulsed-field experiment. Low-field and low-temperature measurements on single crystals show no indications of magnetic ordering and reveal a sizable anisotropy of magnetization. Density-functional-theory (DFT) calculations indicate the relevance of two inequivalent exchanges J_T and J_D with $J_T \gg J_D$, placing this material in the limit of weakly coupled triangles. Anisotropic components of J_T were estimated by noncollinear DFT+U calculations. We demonstrate that a simple model of isolated triangles accounts for the thermodynamic behavior of this compound.

[1] M. Sorolla *et al.*, J. Am. Chem. Soc. **142**, 5013 (2020)

TT 29.4 Wed 10:15 HSZ 201

Temperature-dependent transitions of the rare-earth delafossite $NaGdS_2$ — •Justus Grumbach[1], Mathias Doerr[1], Ellen Haeussler[2], and Sergey Granovsky[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany

Rare-earth delafossites are materials containing ideal triangular magnetic planes, which are frustrated. Due to their properties, rare-earth delafossites are promising candidates for a QSL ground state. In recent years this state occured in some S=$\frac{1}{2}$-delafossites with transitions in the mK range.

Now a number of own new measurements were made on $NaGdS_2$ single crystals. This delafossite with magnetic Gd^{3+} ions, which has been extensively investigated for the first time, is of special interest due to the pure spin moment J=S=$\frac{7}{2}$. Measurements of several different thermodynamic and magnetic properties were performed on very small samples (size $\sim \mu$m) down to lowest temperatures (40 mK).

Essential physical data could be extracted, which show correspondingly a AFM-groundstate below ∼250 mK, which is kind of expected. An additionally investigated modification at 60 K, indicating an anisotropy in the system, is still under theoretical debate and will form a main part of the talk.

TT 29.5 Wed 10:30 HSZ 201

Study of $CoNb_2O_6$ magnetic properties from first principles — •Amanda Konieczna[1], Kira Riedl[1], Roser Valenti[1], and Radu Coldea[2] — [1]Goethe-Universität, Frankfurt am Main, Germany — [2]University of Oxford, Oxford, England

The quasi-one-dimensional ferromagnet $CoNb_2O_6$ offers an interesting playground to investigate the interplay of anisotropic magnetic interactions in real materials. A variety of magnetic models was proposed for this material, including longer-range Heisenberg exchange, dominant anisotropic Ising and bond-dependent Kitaev-type magnetic interactions.

In this talk, we discuss our theoretical approach to extract the magnetic exchange in $CoNb_2O_6$. We first obtain material-specific hoppings from ab-initio methods and proceed by moving from a description in terms of the Hubbard model to the Spin Hamiltonian using exact diagonalization and perturbation theory. Finally, we will discuss how our results fit into the picture of available results for this system, both on the theoretical and experimental side.

We gratefully acknowledge funding by the DFG (German Research Foundation): QUAST-FOR5249 - 449872909 (Project TP4).

TT 29.6 Wed 10:45 HSZ 201

Valence bond solid state in explicitly dimerized chain with magnetic frustration — •Jędrzej Wardyn[1], Satoshi Nishimoto[1,2], and Cliò Efthimia Agrapidis[3] — [1]IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Faculty of Physics, University of Warsaw, Pasteura 5, 02093 Warsaw, Poland;

We consider the spin-1/2 dimerized frustrated ferromagnetic (FM) $J_1-J_1'-J_2$ model, with $J_1, J_1' < 0$ FM first neighbours coupling and $J_2>0$ antiferromagnetic second neighbors coupling. This model serves as a minimal model for $LiCuSbO_4$ and $Rb_2Cu_2Mo_3O_{12}$. We introduce the frustration parameter $J_2/|J_1|=\alpha$ and the dimerization parameter $J_1'/J_1=\beta$. There are two special limits of dimerization: fully dimerized at β=0 and the undimerized J_1-J_2 model at β=1. Earlier studies have identified phases featured in the special limits as valence bond

solid with a finite spin gap for β=1 and a Haldane-like state for β=0. For our model, the spin gap and phase diagram was investigated in a 2017 study by Agrapidis *et al.* [1]. Thanks to new insight, we revisit these results with applying new boundary conditions, which allow us to correctly estimate the spin gap which was previously underestimated. We compute the spin gap, the string order parameter (SOP), and dimer-dimer correlations using the density matrix renormalization group method (DMRG). We prove that the model features a VBS state. Our results allow us to determine this state as $\mathcal{D}_3$-VBS state adiabatically connected to the Haldane-like state in the limit of β=0.
[1] C. E. Agrapidis *et al.*, Phys. Rev. B, 95, 220404 (2017).

TT 29.7 Wed 11:00 HSZ 201

The effect of nonlocal electronic correlations on different lattice geometries - A dynamical vertex approximation study — •Marvin Leusch[1], Andreas Hausoel[2], Alessandro Toschi[3], Giorgio Sangiovanni[4], and Georg Rohringer[1] — [1]Universität Hamburg, Hamburg, Germany — [2]IFW Dresden, Germany — [3]Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [4]TU Wien, Vienna, Austria

In the last decades, dynamical mean-field theory (DMFT) has become a standard tool for describing strongly correlated electron systems. It captures all purely local correlations effects and, hence, provides exact results in the limit of infinite coordination number and thus spacial dimensions. For finite dimensional systems, it neglects nonlocal correlation effects which are captured by diagrammatic extensions of DMFT such as the dynamical vertex approximation (DΓA). In our work, we analyze the three dimensional Hubbard model on various lattice types to investigate the effect of different coordination numbers on local and nonlocal correlations. In particular, we study the magnetic phase diagram of the Hubbard model on a simple cubic (sc), body-centered cubic (bcc) and face-centered cubic (fcc) lattice within DΓA and compare their transition temperatures to magnetically ordered states to corresponding DMFT results. Our numerical findings demonstrate, that the nonlocal correlations of DΓA generally reduce the size of the ordered region with respect to DMFT while the actual magnitude of this reduction depends on the specific lattice type and, in particular, on the coordination number.

15 min. break

TT 29.8 Wed 11:30 HSZ 201

Systematic analysis of diagonal ordering patterns in bosonic lattice models with algebraically decaying density-density interactions — •Jan Alexander Koziol[1], Antonia Duft[1], Giovanna Morigi[2], and Kai Phillip Schmidt[1] — [1]Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Theoretical Physics, Saarland University, Campus E2.6, D-66123 Saarbrücken, Germany

We propose a general approach to analyse diagonal ordering patterns in bosonic lattice models with algebraically decaying density-density interactions on arbitrary lattices. The key idea is a systematic search for the energetically best order on all unit cells of the lattice up to a given extent. Using resummed couplings we evaluate the energy of the ordering pattern in the thermodynamic limit using finite unit cells. We apply the proposed approach to the atomic limit of the extended Bose-Hubbard on a triangular lattice at fillings $f = 1/2$ and $f = 1$. We investigate the ground-state properties of the antiferromagnetic long-range Ising model on the triangular lattice and determine a six-fold degenerate plain-stripe phase to be the ground state for finite decay exponents. We also probe the classical limit of the Hamiltonian describing Rydberg atom arrangements on the sites and links of the Kagome lattice.

TT 29.9 Wed 11:45 HSZ 201

Phases of the spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice in a magnetic field — •Nils Caci[1], Katarína Karl'ová[2], Taras Verkholyak[3], Jozef Strečka[2], Stefan Wessel[1], and Andreas Honecker[4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia — [3]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, L'viv, Ukraine — [4]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France

The spin-1/2 Heisenberg antiferromagnet on the highly frustrated diamond-decorated square lattice is a spin system of orthogonal spin dimers that features various ground-state phases, consisting of extended monomer-dimer and dimer-tetramer ground states as well as a ferrimagnetic regime. By using a combination of density matrix renormalization group (DMRG), exact diagonalization, as well as unbiased sign-problem free quantum Monte Carlo (QMC) methods, we investigate this system in the presence of a finite magnetic field. We find at high magnetic fields the emergence of a spin-canted phase, with continuously rising magnetization, as well as the fully polarized paramagnetic phase. At intermediate field strength, we identify the presence of a first-order quantum phase transition line between a ferrimagnetic phase and the monomer-dimer regime, which extends to finite temperatures and terminates in a line of critical points belonging to the Ising universality class.

TT 29.10 Wed 12:00 HSZ 201

Ground-state degeneracy and magneto-thermodynamics of the spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice — •Andreas Honecker[1], Nils Caci[2], Taras Verkholyak[3], Katarína Karl'ová[4], Stefan Wessel[2], and Jozef Strečka[4] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [3]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, L'viv, Ukraine — [4]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia

The spin-1/2 Heisenberg antiferromagnet on the diamond-decorated square lattice exhibits a rich ground-state phase diagram in a magnetic field [1]. We investigate the thermodynamic properties of this model using a combination of analytical and numerical methods, including full diagonalization up to effectively $N = 30$ sites. We focus in particular on the vicinity of a "dimer-tetramer" phase at low magnetic fields that maps to a classical dimer model on the square lattice and retains a macroscopic ground-state ddegeneracy in a magnetic field. We discuss the consequences of this degeneracy for the thermodynamic and magnetocaloric properties of the system.
[1] N. Caci, K. Karlova, T. Verkholyak, J. Strečka, S. Wessel, A. Honecker, preprint arXiv:2210.15330

TT 29.11 Wed 12:15 HSZ 201

Thermodynamics of the frustrated Heisenberg model on the truncated hexagonal lattice — •Adrien Reingruber[1], Nils Caci[2], and Stefan Wessel[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen University, Aachen, Germany

The thermodynamical properties of the spin-1/2 Heisenberg antiferromagnet on the truncated hexagonal lattice are studied using trimer-based cluster quantum Monte Carlo simulations. The system consists of an arrangement of spin-trimers on a honeycomb lattice with dimer couplings interconnecting neighboring trimers. The physics of this frustrated quantum spin system is investigated for different spin-coupling strengths. The severeness of the quantum Monte Carlo sign problem with respect to the single-site, dimer and trimer basis is examined. In the parameter regime of weakly coupled trimers an effective spin-1/2 Hamiltonian can be derived to describe the low-temperature physics. This effective model yields antiferromagnetic effective spin-1/2 trimer-spin interactions with bond-dependent coupling strengths. Unbiased quantum Monte Carlo simulations confirm the validity of the effective model within the low-temperature regime.

TT 29.12 Wed 12:30 HSZ 201

Another exact ground state of a 2D quantum antiferromagnet — Pratyay Ghosh, •Tobias Müller, Jannis Seufert, and Ronny Thomale — Julius-Maximilians-Universität, Würzburg, Germany

We present the exact dimer ground state of a quantum antiferromagnet on the maple-leaf lattice. A coupling anisotropy for one of the three inequivalent nearest-neighbor bonds is sufficient to stabilize the dimer state. Together with the Shastry-Sutherland Hamiltonian, we show that this is the only other model with an exact dimer ground state for all two-dimensional lattices with uniform tilings. We futhermore discuss the stability of this ground state from the perspective of perturbation theory.

TT 29.13 Wed 12:45 HSZ 201

Bound states and plateaus: Magnetization behavior of the

maple leaf lattice — •Jannis Seufert, Pratyay Ghosh, Tobias Müller, and Ronny Thomale — Julius-Maximilians-Universität, Würzburg, Germany

Recently, the maple leaf lattice equipped with a Heisenberg-Hamiltonian was shown to exhibit an analytically exact antiferromagnetic dimer ground state analogous to the better known Shastry-Sutherland model. Anticipating that its even stronger frustration will lead to both familiar and exotic magnetic behavior, we present the calculation of magnetization plateaus in the maple leaf model with Ising- and Heisenberg-spins. For the latter, this is achieved within a perturbation theory of magnetic excitations incorporating triplet-triplet interactions and correlated hopping, which promotes the emergence of bound states.

TT 29.14 Wed 13:00 HSZ 201

Exact analytical solutions of a distorted spin-1/2 tetrahedron with ring exchange — Rolf Schumann[1] and •Stefan-Ludwig Drechsler[2] — [1]TU-Dresden, D-1169 Dresden, Germany — [2]IFW-Dresden, D-1169 Dresden, Germany

We present exact analytical solutions for the eigenvalues of a general spin-1/2 Hamiltonian with 6 bilinear (Heisenberg) J_i and 3 ring exchange K_i couplings. Focusing on the experimentally interesting orthorhombically, tetragonally, trigonally and non-distorted ideal tetrahedra (ITH) we consider their thermodynamic properties as the magnetization M, susceptibility, entropy, and specific heat at any temperature T and external magnetic field H and derive from the magnetization steps $M(H)$ at high-fields and low-T the saturation field H_s, the critical ferrimagnetic field H_{c1}, and the width of the corresponding plateau as a function of the cyclicity . As a result we find enhanced H_s and lowered H_{c1} values with increasing ring exchange $K > 0$ due to the reduced frustration. We present exact mapping equations to extract the relevant exchange integrals J_i and K_i from experimentally observed transition energies and provide an analytical mapping of the single-band Hubbard model on the ITH valid at any coupling strength U/t, where U is the onsite Coulomb repulsion and t the NN-hopping integral. The experimental situations with respect to the magnitude and sign of $\kappa = J/K$ for $Cu_2Te_2OBr_2$, Cu_2OSeO_3, and $Cu_4X_6L_4$ with X=Cl,Br and L being various ligands are briefly discussed.

TT 30: Complex Oxides

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

TT 30.1 Wed 9:30 HSZ 204

Planar superconducting resonators on $SrTiO_3$ and $KTaO_3$: GHz properties of quantum paraelectrics — Vincent T. Engl, Nikolaj G. Ebensperger, Lars Wendel, Marius Tochtermann, Ilenia Neureuther, Ishan Sarvaiya, Cenk Beydeda, and •Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

$SrTiO_3$ is a common substrate for perovskite thin films, and it hosts a superconducting interface when covered with $LaAlO_3$. Recently, similar superconducting interfaces based on $KTaO_3$ were realized. Any cryogenic electronics application using $SrTiO_3$ or $KTaO_3$ faces the quantum-paraelectric nature of both materials: upon cooling to temperatures of a few K, their very large real part ϵ_1 of the dielectric function complicates high-frequency device design, while the imaginary part ϵ_2 indicates rather high losses for $SrTiO_3$ at GHz frequencies.

Overcoming the challenges of the high ϵ_1, we present coplanar superconducting Nb microwave resonators on $SrTiO_3$ and $KTaO_3$ substrates, which we operate at temperatures down to 25 mK. For $SrTiO_3$ with $\epsilon_1 \approx 20000$ at low temperatures, we couple the coplanar resonator to a conventional 50 Ω feedline using a distant-flip-chip geometry.[1,2] With loaded quality factors exceeding 800 for $SrTiO_3$ and 8000 for $KTaO_3$ we advance the prospects of these quantum paraelectrics towards applications in oxide-based superconducting quantum circuitry.

[1] L. Wendel *et al.*, Rev. Sci. Instrum. **91**, 054702 (2020)
[2] V. T. Engl *et al.*, arXiv:1911.11456 [cond-mat.supr-con]

TT 30.2 Wed 9:45 HSZ 204

Revsisiting magnetic and orbital ordering in V_2O_3 — Louis-Victor Schäfer and •Maria Daghofer — Institut für funktionelle Materie und Quantentechnologien, Universität Stuttgart

We revisit the correlated bands of V2O3 using the variational cluster approximation. Starting from various sets of one-particle parameters discussed in the literature, double counting of correlations turns out to be relevant here, as also reported in the literature. Settling onto consistent parameters, we then find that a careful treatment of inter-layer dimers is crucial to reproduce the experimentally observed magnetic ordering. Additionally, bonds in the planes orthogonal to the dimers affects orbital densities. Antiferromagnetic ordering is the found to go in hand with orbital symmetry breaking within the e_g sector. We find any models that reproduce the measured a_{1g} orbital densities also leads to active orbital degrees of freedom above the Neel transition.

TT 30.3 Wed 10:00 HSZ 204

Direct imaging of valence orbitals using hard x-ray photoelectron spectroscopy — •Daisuke Takegami[1], Laurent Nicolaï[2], Yuki Utsumi[1], Anna Meléndez-Sans[1], Daria A. Balatsky[1], Cariad-A. Knight[1], Connor Dalton[1], Shao-Lun Huang[1], Chi-Sheng Chen[1], Li Zhao[1], Alexander C. Komarek[1], Yen-Fa Liao[3], Ku-Ding Tsuei[3], Ján Minár[2], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of West Bohemia, Pilsen, Czech Republic — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan

It was hypothesized already more than 40 years ago that photoelectron spectroscopy should in principle be able to image atomic orbitals. If this can be made to work for orbitals in crystalline solids, one would have literally a different view on the electronic structure of a wide range of quantum materials. Here, we demonstrate how hard x-ray photoelectron spectroscopy can make direct images of the orbitals making up the band structure of our model system, ReO3 [1]. The images are energy specific and enable us to unveil the role of each of those orbitals for the chemical bonding and the Fermi surface topology. The orbital image information is complementary to that from angle-resolved photoemission and thus completes the determination of the electronic structure of materials.

[1] D. Takegami *et al.*, Phys. Rev. Res. 4, 033108 (2022)

TT 30.4 Wed 10:15 HSZ 204

Orbital imaging of the spin state transition in $LaCoO_3$ — Brett Leedahl[1], Daisuke Takegami[1], Martin Sunderamnn[1,2], Hlynur Gretarsson[1,2], Alexander Komarek[1], Arata Tanaka[3], Maurits Haverkort[4], and •Liu Hao Tjeng[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Department of Quantum Matter, Hiroshima University, Japan — [4]Institute for Theoretical Physics, Heidelberg University, Germany

Here we have investigated the Co 3d orbital occupation in $LaCoO_3$ across the spin state transition using the recently developed x-ray-based orbital-imaging method. The images collected allow for a direct determination of the amount of the Co t_{2g} and e_g holes. We find that, at the lowest temperatures, the low-spin state with the nominally $t_{2g}^6 e_g^0$ electron configuration *does* have holes in the t_{2g} subshell which we attribute to the presence of spin-orbit interaction. The hole amount, however, sets limits to the minimum energy gap between the lattice-frozen low-spin and high-spin states. At high temperatures, we find that the high-spin state occupation is about $half$ (!) of the value reported in the most recent literature. Implications for the ab-initio modeling of the spin-state transition process are discussed.

TT 30.5 Wed 10:30 HSZ 204

Directional ballistics in ultra-pure delafossite metals — •Michal Moravec[1,2], Graham Baker[3], Maja D. Bachmann[1,2], Philippa H. McGuinness[1,2], Markus König[1], Seunghyun Khim[1], and Andrew P. Mackenzie[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom — [3]University of British Columbia, Vancouver, Canada

Studying electrical transport in extremely pure materials has led to the discovery of novel phenomena. The delafossite metals, with their two-dimensional electronic structure and mean free paths in excess of 20 μm, are a recent addition to the ultra-pure materials class. Here we study electrical transport in bars of varied width in delafossite metals

$PdCoO_2$ and $PtCoO_2$. The bar-like structures are sculpted in two crystal orientations using the focused ion beam and sequentially narrowed across the width corresponding to the mean free path. We observe a cross-over from Ohmic to ballistic transport and gradual increase in resistivity anisotropy between the two orientations, as the channel is narrowed. This anisotropy is not allowed by the symmetry of the bulk crystal lattice; it is an example of symmetry lowering due to the imposition of shapes of finite size and the Fermi surface anisotropy [1]. We also complement our measurements with numerical solutions to the Boltzmann equation including the ARPES Fermi surface parametrisation. We obtain a good qualitative agreement with resistivity the data.

[1] M.D. Bachmann et al. Nat. Phys. 18, 819 (2022)

TT 30.6 Wed 10:45 HSZ 204

Electronic structure of the Fe^{2+} compound $FeWO_4$: a combined experimental and theoretical X-ray photoelectron spectroscopy study — •Simone G. Altendorf[1], Daisuke Takegami[1], Anna Meléndez-Sans[1], Vanda M. Pereira[1], Chang-Yang Kuo[1,2,3], Chun-Fu Chang[1], Chien-Te Chen[2], Masato Yoshimura[2], Ku-Ding Tsuei[2], Antoine Maignan[4], Marcus Schmidt[1], Arata Tanaka[5], and Liu-Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan — [4]CRISMAT, Normandie Univ, ENSICAEN, UNICAEN, CNRS, Caen 14000, France — [5]Quantum Matter Program, Hiroshima University, Higashi-Hiroshima 739-8530, Japan

Iron tungstate ($FeWO_4$) is one of the rare oxide compounds with a nearly pure divalent iron valence state. We investigate the electronic structure of $FeWO_4$ experimentally by X-ray photoelectron spectroscopy. Using various photon energies, cross-section effects allow to identify the individual contributions of the Fe and W states to the valence band. A comparison with band structure and full atomic multiplet configuration interaction calculations yields important insights into the correlations in the material.

The research in Dresden is partially supported by the DFG through SFB 1143.

TT 30.7 Wed 11:00 HSZ 204

Imaging the orbital-switching in Ti_2O_3 across the metal-insulator transition — •Paulius Dolmantas[1], Chun-Fu Chang[1], Martin Sundermann[1,2], Brett Leedahl[1], Andrea Amorese[1], Hlynur Gretarsson[1,2], Alexander Komarek[1], Arata Tanaka[3], Maurits W. Haverkort[4], and Liu Hao Tjeng[1] — [1]MPI-CPfS, Dresden, Germany — [2]DESY/PETRA-III, Hamburg, Germany — [3]Department of Quantum Matter, Hiroshima University, Japan — [4]Institute for Theoretical Physics, Heidelberg University, Germany

Using the recently developed x-ray-based *orbital-imaging* method, we have been able to observe a switching of the Ti $3d$ orbital occupation across the metal-insulator transition in Ti_2O_3. We find that in the insulating state only the a_{1g} of the t_{2g} subshell is occupied, while in the metallic state also the e_g^π gets filled at the expense of the a_{1g}. The insulator-metal transition may then be viewed as a transition from a solid of isolated Ti-Ti c-axis singlet dimers into a solid of electronically partially broken dimers, where the Ti ions acquire additional hopping in the a-b plane via the e_g^π channel. These findings have implications for the ab-initio modeling of the metal-insulator transition.

15 min. break

TT 30.8 Wed 11:30 HSZ 204

Effect of cation dynamics on polar instabilities of perovskite derived structures — •Rinis Ferizaj[1], Florian Büscher[1], Peter Lemmens[1], Hiroshi Kageyama[2], and Tong Zhu[2] — [1]IPKM, TU Braunschweig — [2]Energy Chemistry, Univ. Kyoto, Japan

Perovskite derived structures have a huge variability in structural, electronic and magnetic properties. This makes them leading candidates for todays search for novel energy materials. Using Raman scattering we probe phonon dynamics in such material and focus to the cation dynamics to better understand transitions into different polar/nonpolar low temperature phases.

We acknowledge support by DFG GrK 1952/2, Metrology for Complex Nanosystems-NanoMet, and DFG EXC-2123 QuantumFrontiers - 390837967.

TT 30.9 Wed 11:45 HSZ 204

Anomalous magnetotransport in $SrIrO_3$ (111) films — •Ji Soo Lim[1], Merit Spring[1], Martin Kamp[1], Louis Veyrat[1,2], Axel Lubk[2], Bernd Büchner[2], Michael Sing[1], and Ralph Claessen[1] — [1]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Leibniz Institute for Solid State and Materials Research and Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany

Complex oxides provides an inexhaustible playground for the study of interactions between charge, spin, orbital, and lattice degrees of freedom. In particular, spin-orbit coupling can be of comparable magnitude to electron correlations in 5d iridates, leading to exotic quantum phases such as spin liquids and correlated topological semimetals [1]. Perovskite $SrIrO_3$ (SIO) films grown along the <111> direction exhibit a buckled honeycomb lattice, and are predicted to be topological crystalline insulators with a relatively large band gap [2].

Here we report on the epitaxial growth of ultrathin SIO films on $SrTiO_3$ (111) that display a twinned perovskite-like superlattice structure with a periodicity of 3 unit cells and the observation of unusual magnetotransport properties, namely the anomalous Hall effect. We observe a sign change of the magnetoresistance and hysteresis loops with increasing coercive fields below 10 K. By comparing with theoretical results, we discuss the origin of the unusual transport behavior.

[1] J. Chakhalian et al., APL Mater. 8, 050904 (2020)
[2] P. M. Gunnink et al., J. Phys.: Condens. Matter 33, 085601 (2021)

TT 30.10 Wed 12:00 HSZ 204

Magnetoelectric coupling of terbium orthotantalates — •Xiaotian Zhang[1], Nicola Kelly[2], Cheng Liu[1], Sian Dutton[1], and Siddharth Saxena[1] — [1]Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom — [2]Department of Chemistry, University of Oxford, Oxford, United Kingdom

Quantum multiferroic materials form a new and emerging area of physics where one expects to find emergence of novel quantum phases induced by subtle coupling between spin and charge degrees of freedom at low temperatures. Experimental study of such phenomena is limited by the lack of model materials where magnetism and dielectric properties can be tuned using magnetic fields at low temperatures.

In a recent breakthrough, we found that $TbTaO_4$ exhibits enhancement in dielectric response below 2 K on application of magnetic field, indicating magnetoelectric coupling. Previously, using susceptibility and heat capacity measurements we showed that $TbTaO_4$ orders at $T_N = 2.25$ K; powder neutron diffraction (PND) was used to solve the magnetic structure, which is A-type antiferromagnetic.

These rare-earth tantalates $LnTaO_4$ (Ln = Y, La-Lu) are of wide interest as a result of their luminescent, proton-conducting, oxide-ion-conducting and dielectric properties. In addition, in the monoclinic M polymorph of the tantalates with Ln = Nd-Er, the magnetic Ln^{3+} ions are arranged on an elongated diamond lattice. Materials with such a magnetic lattice have the potential for unusual magnetic behaviour owing to the interplay of the crystal electric field with the (possibly competing) J1 and J2 interactions.

TT 30.11 Wed 12:15 HSZ 204

$S = 1$ dimer system $K_2Ni(MoO_4)_2$: A candidate for magnon Bose-Einstein condensation — •Benjamin Lenz[1], Bommisetti Koteswararao[2], Silke Biermann[3,4,5], Panchanan Khuntia[6,7], Michael Baenitz[7], and Swarup K. Panda[8] — [1]IMPMC, Sorbonne Université, Paris, France — [2]IIT Tirupati, Tirupati, India — [3]CPHT, Ecole Polytechnique, Palaiseau, France — [4]Collège de France, Paris, France — [5]Lund University, Lund, Sweden — [6]IIT Madras, Chennai, India — [7]MPI for Chemical Physics of Solids, Dresden, Germany — [8]Bennett University, Greater Noida, India

Dimerized quantum magnets provide a unique possibility to investigate the Bose-Einstein condensation of magnetic excitations in crystalline systems at low temperature. Here, we model the low-temperature magnetic properties of the recently synthesized spin $S = 1$ dimer system $K_2Ni(MoO_4)_2$ and propose it as a candidate material for triplon and quintuplon condensation. Based on a first-principles analysis of its electronic structure, we derive an effective spin dimer model that we first solve within a mean-field approximation to refine its parameters in comparison to experiment. Finally, the model is solved by employing a numerically exact quantum Monte Carlo technique which leads to magnetic properties in good agreement with experimental magnetization and thermodynamic results. We discuss the emergent spin model of $K_2Ni(MoO_4)_2$ in view of the condensation of magnetic excitations in a broad parameter regime. Finally, we comment on a geometrical peculiarity of the proposed model and discuss how it could host a supersolid phase upon structural distortions.

TT 30.12 Wed 12:30 HSZ 204

The crucial influence of side groups on magnetic superexchange - a modification of the Goodenough-Kanamori-rules — Dijana Milosavljevic[1], Oleg Janson[2], Stefan-Ludwig Drechsler[2], and •Helge Rosner[3] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]IFW Dresden, 01069 Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

According to the famous Goodenough-Kanamori-Anderson rules, the key structural feature that determines the magnetic exchange coupling constant for superexchange in magnetic insulators is the magnetic ion-ligand-magnetic ion bond angle. Here, we demonstrate that this angle is not the only determining factor. An at least equally important influence on the exchange coupling has the presence of side groups attached to the ligands. Applying density functional calculations and subsequently derived realistic parameters for a multiband tight-binding model, we provide a quantitative analysis for the example case of edge-sharing Cu-O chains with bond angles near 90 degrees. We find that a single parameter, the difference in onsite-energies of the ligand orbitals parallel and perpendicular to the Cu-O chain, is at least as important as the bond angle for sign and size of the superexchange. This parameter strongly depends on the position of side groups outside the superexchange pathway. For a fixed bond angle, changes of a side group position, only, can cause changes in the superexchange of several hundred Kelvin and thus dramatic changes in the magnetic properties.

TT 30.13 Wed 12:45 HSZ 204

A consistent microscopic magnetic model of the edge-sharing chain cuprate $CuSiO_3$ — •Dijana Milosavljevic[1,2], Andrei Gippius[3], Oleg Janson[4], Michael Baenitz[1], Yurii Prots[1], Johannes Richter[5], and Helge Rosner[1] — [1]MPI for Chemical Physics of Solids, Dresden — [2]MPI of Microstructure Physics, Halle — [3]Moskow, Russia — [4]IFW, Dresden — [5]MPI Physics of Complex Systems, Dresden

A unique place in the family of low-dimensional magnets occupies the Cu^{2+} compounds featuring a series of square-planar CuO_4 plaquettes connected via their edges, forming in this way a chain. The edge-shared plaquettes in Li_2CuO_2 show ferromagnetic ordering [1], whereas similar chains with increased Cu-O-Cu bond angle bridging neighboring Cu atoms in $CuGeO_3$, undergo a spin-Peierls transition [2]. A compound with a Cu-O-Cu angle essentially identical to the one in Li_2CuO_2 and isostructural to the famous Spin-Peierls system $CuGeO_3$ is spin-1/2 cuprate $CuSiO_3$ [3]. In a combined experimental-theoretical approach, we derive a new magnetic model of $CuSiO_3$, consistent with all reported experimental results.

[1] E.L.M Chung et al., Phys. Rev. B **68**, 144410 (2003)
[2] M. Hase et al., Phys. Rev. Lett. **70**, 3651 (1993)
[3] H. H. Otto et al., Z. Kristallogr. **214**, 558 (1999)

TT 31: Topology: Majorana Physics

Time: Wednesday 9:30–12:45 Location: HSZ 304

TT 31.1 Wed 9:30 HSZ 304

Photonic noise as a probe of Majorana bound states — •Lena Bittermann[1], Fernando Dominguez[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

We propose a route to detect Majorana bound states (MBSs) by coupling a topological superconductor to a quantum dot (QD) in a pn-junction. Here, two MBSs are coherently coupled to electrons on the QD, which recombine with holes in situ to photons. Importantly, the polarization of the emitted photons provides direct information on the spin structure [1,2] and nonlocality [2,3] of the MBSs. Here, we focus on the shot noise of the emitted photons which allows to clearly distinguish the cases of well separated MBSs at zero energy from overlapping MBSs. In addition, we show that quasiparticle poisoning changes the shot noise from super-Poissonian to sub-Poissonian [4]. Furthermore, this setup can be extended by coupling a second QD close to the second MBS which gives rise to nonlocal shot noise correlations leading to additional signatures of MBSs.

[1] D. Sticlet, C. Bena, and P. Simon, PRL 108, 096802 (2012)
[2] E. Prada, R. Aguado, and P. San-Jose, PRB 96, 085418 (2017)
[3] A. Schuray, L. Weithofer, and P. Recher, PRB 96, 085417 (2017)
[4] L. Bittermann, C. De Beule, D. Frombach, and P. Recher, PRB 106, 075305 (2022)

TT 31.2 Wed 9:45 HSZ 304

Statistical Majorana bound state spectroscopy — •Alexander Ziesen[1], Alexander Altland[2], Reinhold Egger[3], and Fabian Hassler[1] — [1]JARA Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Köln, Germany — [3]Institut für Theoretische Physik, Heinrich-Heine-Universität, Düsseldorf, Germany

Tunnel spectroscopy data for the detection of Majorana bound states (MBS) is often criticized for its proneness to misinterpretation of genuine MBS with low-lying Andreev bound states. Here, we suggest a protocol removing this ambiguity by extending single shot measurements to sequences performed at varying system parameters. We demonstrate how such sampling, which we argue requires only moderate effort for current experimental platforms, resolves the statistics of Andreev side lobes, thus providing compelling evidence for the presence or absence of a Majorana center peak.

TT 31.3 Wed 10:00 HSZ 304

Disentanglement, disorder lines, and Majorana edge states in a solvable quantum chain — Gennady Y. Chitov[1], •Karun Gadge[2,3], and Pavel N. Timonin[4] — [1]Département de Physique, Institut Quantique, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1, Canada — [2]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany — [3]School of Basic Sciences, Indian Institute of Technology Mandi, Mandi 175005, India — [4]Rostov-on-Don, Russia

We study the exactly solvable one-dimensional model: the dimerized XY chain with uniform and staggered transverse fields, equivalent upon fermionization to the noninteracting dimerized Kitaev-Majorana chain with modulation. The criticality is controlled by the properties of zeros of model's partition function, analytically continued onto the complex wave numbers. In the ground state they become complex zeros of the spectrum of the Hamiltonian. The analysis of those roots yields the phase diagram which contains continuous quantum phase transitions and weaker singularities known as disorder lines (DLs) or modulation transitions. The salient property of zeros of the spectrum is that the ground state is shown to be separable (factorized), and the model is disentangled on a subset of the DLs. From analysis of those zeros we also find the Majorana edge states and their wave functions. Reference: PRB 106, 125146 (2022)

TT 31.4 Wed 10:15 HSZ 304

Unifying the theoretical description of Andreev, Majorana, quasi-Majorana bound states — •Pasquale Marra[1,2] and Angela Nigro[3] — [1]Graduate School of Mathematical Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8914, Japan — [2]Department of Physics, and Research and Education Center for Natural Sciences, Keio University, 4-1-1 Hiyoshi, Yokohama, Kanagawa 223-8521, Japan — [3]Dipartimento di Fisica 'E. R. Caianiello', Università degli Studi di Salerno, 84084 Fisciano (Salerno), Italy

In one-dimensional topological superconductors systems, zero-energy Majorana edge modes localize at the domain walls between topologically distinct phases, similar to the case of Jackiw-Rebbi solitons, which are solutions of the Majorana-Dirac equation on an inhomogeneous background. On the other hand, topologically trivial Andreev states below the particle-hole gap can originate from disorder or spatial inhomogeneities. Distinguishing between Majorana and Andreev states is an ongoing challenge that generated intense debate in the scientific community. Indeed, there is a continuous crossover between topologically nontrivial Majorana and trivial Andreev states induced by smooth inhomogeneities, which can occur without closing the bulk gap. Here, we describe nontrivial Majorana and Andreev bound states induced by spatial inhomogeneities and disorder, Shockley states, and Jackiw-Rebbi solitons in a unifying framework, introducing a characteristic length scale that can unambiguously distinguish between different regimes.

TT 31.5 Wed 10:30 HSZ 304

Majorana zero modes in fermionic wires coupled by Aharonov-Bohm cages — •Niklas Tausendpfund[1,2], Sebastian Diehl[2], and Matteo Rizzi[1,2] — [1]Peter Grünberg Institut 8, Forschungszentrum Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, Germany

We devise a number-conserving scheme for the realization of Majorana Zero Modes in an interacting fermionic ladder coupled by Aharonov-Bohm cages. The latter provide an efficient mechanism to cancel single-particle hopping by destructive interference. The crucial parity symmetry in each wire is thus encoded in the geometry of the setup, in particular, its translation invariance. A generic nearest-neighbor interaction generates the desired correlated hopping of pairs. We exhibit the presence of an extended topological region in parameter space, first in a simplified effective model via bosonization techniques, and subsequently in a larger parameter regime with matrix-product-states numerical simulations. We demonstrate the adiabatic connection to previous models, including exactly-solvable ones, and we briefly comment on possible experimental realizations in synthetic quantum platforms, like cold atomic samples.

TT 31.6 Wed 10:45 HSZ 304

Tunable coupling of quantum dots via Andreev bound states - towards a Kitaev chain — Chun-Xiao Liu, Guanzhong Wang, Tom Dvir, and •Michael Wimmer — Qutech and Kavli Institute for nanophysics, TU Delft, Niederlande

We show that the coupling between two quantum dots can be effectively mediated via Andreev bound states in a central superconducting segment. This gives rise to an effective superconducting and normal coupling between quantum dot states. Both coupling strengths can be independently controlled by changing the properties of the Andreev bound states, e.g. by a gate voltage. This allows to implement a Kitaev chain that can easily be tuned to a topological phase [1]. We will also discuss first experimental results implementing a two-site Kitaev chain [2, 3].

[1] arXiv:2203.00107
[2] arXiv:2205.03458
[3] arXiv:2206.08045

TT 31.7 Wed 11:00 HSZ 304

Odd-frequency pairing in Floquet topological superconductors — •Eslam S. Ahmed, Shun Tamura, and Yukio Tanaka — Department of Applied Physics, Nagoya University, Japan

Time-periodic (Floquet) Hamiltonians offer a unique and tunable way to engineer topological systems with intriguing edge modes. In particular, Floquet superconductors can possess multi-Majorana edge modes at energies $E = 0$ and $E = \pi$.

It is well-established that there is a direct relationship between odd-frequency Cooper pairing amplitudes and the topological invariants in the static superconductors. In our study, we discuss this relationship in the time-periodic regime.

We consider a Kitaev chain alternating in time between two different values for chemical potential. By tuning the time-periodicity of the alternating chemical potential, we show that the chain admits multiple zero and π energy Majorana modes at the edge of the chain. Furthermore, We show that odd-frequency Cooper pairing amplitude at the edge of the chain is correlated to the presence of Zero and π Majorana modes.

15 min. break

TT 31.8 Wed 11:30 HSZ 304

Phase diagram of an extended parafermion chain — Jurriaan Wouters[1], Fabian Hassler[2], Hosho Katsura[3], and •Dirk Schuricht[1] — [1]Institute for Theoretical Physics, Center for Extreme Matter and Emergent Phenomena, Utrecht University — [2]JARA-Institute for Quantum Information, RWTH Aachen University — [3]Department of Physics, Graduate School of Science, The University of Tokyo

We study the phase diagram of an extended parafermion chain, which, in addition to terms coupling parafermions on neighbouring sites, also possesses terms involving four sites. Via a Fradkin–Kadanoff transformation the parafermion chain is shown to be equivalent to the non-chiral $\mathbb{Z}_3$ axial next-nearest neighbour Potts model. We discuss a possible experimental realisation using hetero-nanostructures. The phase diagram contains several gapped phases, including a topological phase where the system possesses three (nearly) degenerate ground states, and a gapless Luttinger-liquid phase.

TT 31.9 Wed 11:45 HSZ 304

Interacting Majorana fermions — •Lukas Janssen[1] and Urban F. P. Seifert[2] — [1]Technische Universität Dresden, Dresden, Germany — [2]University of California, Santa Barbara, USA

I will present our study of models of interacting Majorana fermions with global SO(N) symmetry. The models can be understood as real counterparts of the SU(N) Hubbard-Heisenberg models and may be realized in Abrikosov vortex phases of topological superconductors, or in fractionalized phases of strongly frustrated spin-orbital magnets. I will describe the zero-temperature phase diagrams and discuss the natures of the occurring quantum phase transitions, with the help of mean-field, renormalization group, and quantum Monte Carlo approaches.

[1] L. Janssen and U. F. P. Seifert, Phys. Rev. B 105, 045120 (2022)

TT 31.10 Wed 12:00 HSZ 304

Multiplicative Majorana zero modes — •Adipta Pal — Max Plank Institute for the Physics of Complex Systems, Dresden, Germany

Topological qubits composed of unpaired Majorana zero-modes are under intense experimental and theoretical scrutiny in efforts to realize practical quantum computation schemes. In this work, we show the minimum four 'unpaired' Majorana zero-modes required for a topological qubit according to braiding schemes and control of entanglement for gate operations are inherent to multiplicative topological phases, which realize symmetry-protected tensor products—and maximally-entangled Bell states—of unpaired Majorana zero-modes known as multiplicative Majorana zero-modes. We introduce multiplicative Majorana zero-modes as topologically-protected boundary states of both one and two-dimensional multiplicative topological phases, using methods reliant on multiplicative topology to construct relevant Hamiltonians from the Kitaev chain model. We furthermore characterize topology in the bulk and on the boundary with established methods while also introducing techniques to overcome challenges in characterizing multiplicative topology. In the process, we explore the potential of these multiplicative topological phases for an alternative to braiding-based topological quantum computation schemes, in which gate operations are performed through topological phase transitions.

TT 31.11 Wed 12:15 HSZ 304

Controlling Majorana modes via Fulde-Ferrell-Larkin-Ovchinnikov phases in topological superconductors and superfluids — •Pasquale Marra[1,2], Daisuke Inotani[2], Takeshi Mizushima[3], and Muneto Nitta[2] — [1]Graduate School of Mathematical Sciences, The University of Tokyo, 3-8-1 Komaba, Meguro, Tokyo 153-8914, Japan — [2]Department of Physics, and Research and Education Center for Natural Sciences, Keio University, 4-1-1 Hiyoshi, Yokohama, Kanagawa 223-8521, Japan — [3]Department of Materials Engineering Science, Osaka University, Toyonaka, Osaka 560-8531, Japan

The next milestones in the route to topological quantum computation with Majorana modes are demonstrating their nonabelian braiding statistics and realizing Majorana-based topological qubits. To achieve this, most proposals require the manipulation of electric gates or magnetic fields in networks of proximitized semiconducting nanowires. Here, we focus on an alternative platform to obtain Majorana modes by employing inhomogeneous Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) phases in topological superconductors and superfluids. The FFLO state spontaneously breaks translational symmetry, inducing a periodic and spatial modulation of the superconducting pairing. We explore the interplay between FFLO order, nontrivial topology, and emergent quantum-mechanical supersymmetry and consider possible routes to realize nonabelian braiding in these platforms.

TT 31.12 Wed 12:30 HSZ 304

Time-reversal invariant topological superconductor in the Coulomb blockade regime — •Steffen Bollmann[1], Elio König[1], and Jukka Väyrynen[2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Purdue University, West Lafayette, In-

diana USA

Floating topological superconductors coupled to conduction electrons can realize unconventional O(N), Sp(2N), or multi-channel Kondo effects. Here, we introduce a new topological superconducting mesoscopic device, a time-reversal invariant version of the Majorana Cooper pair box in the Coulomb blockade regime. In this setup of Cartan-Altland-Zirnbauer class DIII, spinful Majorana zero modes appear at the edges of a topological triplet superconductor with fluctuating Cooper pair spin and charge. We study the Kondo effect in the limit of dominating charging energy and in the limit of both small and large spin fluctuations. Beyond its value in the context of exotic mesoscopic Kondo effects, our study sheds light on the intricate interplay of band topology and strong quantum fluctuations of non-Abelian order parameter fields.

TT 32: Molecular Electronics and Excited State Properties (joint session CPP/TT)

Time: Wednesday 9:30–12:30 Location: GÖR 226

TT 32.1 Wed 9:30 GÖR 226

Strong Solvatochromism in a Two Metal Center Photocatalyst Molecule — •Miftahussurur Hamidi Putra[1] and Axel Gross[1,2] — [1]Universität Ulm Institut für Theoretische Chemie Mez-Starck-Haus Oberberghof 7 89081 Ulm Deutschland — [2]Helmholtz Institute Ulm (HIU) Electrochemical Energy Storage, 89069 Ulm, Deutschland

In the theoretical study presented here, we show that the electronic and optical properties of a molecular photocatalyst can strongly depend on the solvent it is dissolved in [1]. Ground-state density functional theory and linear response time dependent density functional theory calculations are applied in order to investigate the influence of implicit solvents on the structural, electronic and optical properties of a two metal center molecular photocatalyst $[(tbbpy)_2Ru(tpphz)PtI_2]^{2+}$ ($RuPtI_2$) [2]. These calculations predict a significant dependence of the HOMO-LUMO gap of the photocatalyst on the dielectric constant of the solvent. We elucidate the electronic origins of this strong solvatochromic effect and sketch the consequences of these insights for the use of photocatalysts in different environments.

[1] M. K. Nazeeruddin, S. M. Zakeeruddin, R. Humphry-Baker, M. Jirousek, P. Liska, N. Vlachopoulos, V. Shklover, C.-H. Fischer, M. Grätzel, Inorg. Chem. **38**, 6298-6305 (1999).
[2] M. G. Pfeffer, T. Kowacs, M. Wächtler, J. Guthmuller, B. Dietzek, J. G. Vos, S. Rau, Angew. Chem. **54**, 6627-6631 (2015).

TT 32.2 Wed 9:45 GÖR 226

Dynamic Charge-Transport and Charge-Transfer Regimes for Electron-Phonon-Coupled Molecular Systems — •Michel Panhans, Sebastian Hutsch, and Frank Ortmann — Department of Chemistry, TU München

Different approaches for charge transport in organic solids exist but they differ significantly in the described physics of the electron-phonon coupling. In our recent work, we investigate the charge-transfer dynamics, the fading of transient localization (TL) and the formation of polarons for a large range of vibration frequencies and temperatures in the phase space of the two-site Holstein model. The combined numerical and analytical method is based on the time-domain Kubo formula of electrical conductivity to describe the highly correlated electron-phonon dynamics from femtoseconds to very large time scales, reaching nanoseconds. We identify three charge-transport regimes, which are TL, soft gating, and polaron transport. Of particular interest is the built up of correlations between the electronic motion and the nuclei manifesting in the crossover between TL and polaron transport. We find, that the transition between these two limiting cases is seamless at all temperatures and all adiabatic ratios even for the low-frequency vibrational modes that were often considered to be frozen.

TT 32.3 Wed 10:00 GÖR 226

Multichromophore Macrocycles of Perylene Bisimide Dyes as Fluorescent OLED Emitters — •Björn Ewald[1], Ulrich Müller[1], Peter Spenst[2], Philipp Kagerer[1], Theodor Kaiser[1], Matthias Stolte[2], Frank Würthner[2], and Jens Pflaum[1] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institut für Organische Chemie and Center for Nanosystems Chemistry, University of Würzburg, 97074 Würzburg

Highly efficient electroluminescence from Organic Light Emitting Diodes (OLEDs) is limited by the non-radiative character of triplet states for conventional fluorophores. While fluorescent emitters benefit from high radiative recombination rates on the order of 10^9 s^{-1}, they lack from dark triplet states with lifetimes up to several μs or ms. Here we elucidate the potential of perylene bisimide macrocycles as a novel class of fluorescent OLED emitters by applying photon-correlation studies. The correlation experiments unfold additional excitonic relaxation pathways shortening the dark state lifetime for the covalently linked perylene bisimide chromophores. A trimeric chemical design leads to efficient single-photon emission from optically excited thin film samples and even under electrical operation in OLEDs. To the best of our knowledge this is the first indication of electrically-driven single-photon emission from a fluorescent molecule [1]. Therefor we consider our work to constitute an important step towards the design of state-of-the art fluorescent OLED emitters that might also feature a high potential for application in non-calssical single-photon sources.

[1] Ulrich Müller et al., Adv. Optical Mater. 2022, 10, 2200234.

TT 32.4 Wed 10:15 GÖR 226

A Tool Kit for Analyzing Emission Spectra of Multi-Molecular States — •Sebastian Hammer[1,4], Theresa Linderl[2], Kristofer Tvingstedt[1], Wolfgang Bruetting[2], and Jens Pflaum[1,3] — [1]Experimental Physics VI, University of Würzburg, 97074 Würzburg — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg — [4]Departments for Physics and Chemistry, McGill University, Montreal, Canada

The performance of opto-electronic devices is often crucially impacted by multi-molecular excited states such as charge-transfer (CT) states or excimers. Hence, the spectroscopic analysis of these states is a common tool in the characterization of such systems. Due to the many parameters at play full quantum mechanical interpretations are tedious and therefore the analysis is often performed on a phenomenological level only. Here we present a tool kit to analyze temperature dependent emission spectra using a Franck-Condon based approach with a single effective inter-molecular vibrational mode and discuss the implications of considering different potentials for the ground and excited state harmonic oscillators [1]. Finally, we show that fundamental parameters of the potential energy landscape can be extracted from temperature dependent steady state emission spectra using the example of a tetraphenyldibenzoperiflanthene:C_{60} CT hetero-structure [2]. Funding from the DFG (Project 490894053) is greatfully acknowledged.

[1] Hammer et al., *Mater. Horiz.*. (2022). doi: 10.1039/D2MH00829G
[2] Linderl et al., *Phys. Rev. Appl.*. **13** 024061 (2020)

TT 32.5 Wed 10:30 GÖR 226

Singlet Fission search in polyacene molecules in gas-phase and on rare-gas clusters using ab initio methods — •Selmane Ferchane and Michael Walter — Institute of Physics, University of Freiburg, Germany

Singlet fission (SF), is a spontaneous photo-excited splitting phenomenon. Where an organic chromophore dimer, converts its singlet exciton into a pair of triplet excitons. A great promise for future photon-to-current conversion of solar energy using organic materials with high efficiency. To get more insight into these processes of SF, we employed different ab initio theories and approaches in our investigation, namely, density functional theory (DFT), TD-DFT, MCTDH, and CASPT2/CASSCF. Since the spatial orientation is crucial to whether the molecule will go SF and the rate of it due to the orbital coupling of both molecules, based on recent studies. We calculate the most favorable orientation of the chromophores with the binding energies in the gas phase and adsorbed on Argon and Neon surfaces. Then we calculate the lowest-lying excited states that contribute to the singlet and triple transition plus the search for the possible conical intersection that crosses the surface potential energies.

TT 32.6 Wed 10:45 GÖR 226

Template-Designed Organic Electronics — •Klaus Meerholz

— Chemistry Department, University of Cologne, Greinstr. 4-6, 50939 Cologne, Germany

Worldwide, organic electronic devices such as OLEDs and solar cells have revolutionized the field of electronics; however, technological progress has been largely made by empirical research and development, while fundamental knowledge is often still incomplete.

This presentation will report results from the DFG-funded Research Training Group Template-Designed Organic Electronics addressing the question, how structural order influences the optoelectronic properties of pi-conjugated materials, and how these properties can be improved via the use of templates for the optimization of devices. Our approach spans all the way from the design of appropriate pi-conjugated molecular building blocks and surface-active templates, investigation of surfaces and interfaces by different spectroscopies, fabrication of optoelectronic devices, and finally theoretically modelling.

TT 32.7 Wed 11:00 GÖR 226

Optically detected magnetic resonance of TADF OLED emitters — •Pascal Schady, Mona Löther, Fabian Binder, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

Thermally activated delayed fluorescence (TADF) is an efficient triplet harvesting mechanism for organic light-emitting diodes (OLED). Molecular TADF Donor-Acceptor type emitters are limited by low reverse intersystem crossing (rISC) rates and broad spectra, making them less suitable for potential OLED devices. In contrast, so-called multiple resonance (MR) effect emitters, are very promising as they show narrowband emission, even for deep blue wavelengths. MR-TADF emitters consist mostly of planar and rigidly bound benzyl groups with boron and nitrogen substituents for HOMO and LUMO pinning. As a result, the exchange integral is small, therefore the energy gap between singlet and triplet states is low enough to efficiently populate emissive singlet states by up-converting long-lived triplet states via thermal excitation, even at room temperature. However, many MR-TADF materials, like the DABNA-series behave differently in solution or as a solid. We therefore are investigating the spin system of those emitters by optically detected magnetic resonance (ODMR) in order to shed light on spin-dependent efficiency limiting pathways and how to address them to improve future OLED devices.

15 min. break

TT 32.8 Wed 11:30 GÖR 226

Influence of Fluorination on the Temperature Dependent Optical Transition in β- Phase ZnPc Single Crystals — •Lisa Schraut-May[1], Kilian Strauss[1], Sebastian Hammer[2], Kilian Frank[3], Bert Nickel[3], and Jens Pflaum[1] — [1]Experimental Physics VI, University of Würzburg — [2]Departments of Physics and Chemistry, McGill University, Montreal, Canada — [3]Department of Physics, LMU Munich

The possibility of fluorination renders zinc phthalocyanine (ZnPc) an excellent model system to study the interplay between molecular packing and opto-electronic properties [1]. Here, we conduct temperature as well as polarisation dependent photoluminescence (PL) studies on β-phase ZnPc single crystals with different degrees of fluorination to modify the microscopic packing and, thus, the interaction between the molecules. For plain ZnPc an exceptionally sharp PL peak can be observed at temperatures below 100 K, which can be attributed to a superradiant enhancement [2]. Since this coherent coupling between several molecules strongly depends on the intermolecular spacing, we show, that this phenomenon can be steered by the fluorination of the molecules involved. We interpret the resulting PL signal and its temperature dependence in combination with X-ray studies by a model based on coupled excitons whose coupling is affected by the spatial anisotropy of the thermal contraction of the crystal lattice.

We thank the Bavarian research network SolTech for financial support. [1] Rödel et al., J. Phys. Chem. C (2022) [2] Hestand et al., Chem. Rev. (2018)

TT 32.9 Wed 11:45 GÖR 226

Charge Delocalization and Vibronic Couplings in Quadrupolar Squaraine Dyes — Daniel Timmer[1], Fulu Zheng[2], Moritz Gittinger[1], Thomas Quenzel[1], •Daniel C. Lünemann[1], Katrin Winte[1], Yu Zhang[3], Mohamed E. Madjet[2], Jennifer Zablocki[4], Arne Lützen[4], Jin-Hui Zhong[1], Antonietta De Sio[1], Thomas Frauenheim[2], Sergei Tretiak[3], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]University of Bremen, Germany — [3]Los Alamos National Laboratory, USA — [4]University of Bonn, Germany

Squaraines are prototypical quadrupolar charge-transfer chromophores. Their optical properties are often rationalized using an essential state model, predicting that optical transitions to the lowest excited state (S1) are one-photon allowed and to the next higher state (S2) are only two-photon-allowed and that vibronic coupling to high-frequency modes is greatly reduced. Here, we combine time-resolved spectroscopy techniques and quantum-chemical simulations to test and rationalize these predictions. We find the one-photon-allowed S1 and two-photon-allowed S2 states to be energetically well-separated. Also, we find small Huang-Rhys factors, especially for the high-frequency modes. The resulting concentration of the oscillator strength in a narrow spectral region around the S1 transition makes squaraines almost perfect optical two-level. Thus, these molecules and their aggregates are exceptionally interesting for e.g. strong coupling applications. [1]: Timmer, Daniel, et al., J. Am. Chem. Soc., 144, 41, 19150-19162 (2022)

TT 32.10 Wed 12:00 GÖR 226

In-operando observation of polaron formation in SAMFETs using NEXAFS spectroscopy — Manuel Johnson, •Andreas Späth, Baolin Zhao, Marcus Halik, and Rainer H. Fink — FAU Erlangen-Nürnberg, Erlangen, Germany

We present an in-operando near-edge x-ray absorption fine structure (NEXAFS) study on p-type BTBT-based self-assembled monolayer (BTBT-SAM) films. As a 2D-model system, the BTBT-SAM offers direct electron spectroscopic insight into the active organic semiconductor layer without interfering bulk contributions. This optimized geometry allows for the first time the observation of polaronic states caused by charged species at the dielectric/organic interface using a core-level spectroscopic tool. Linear NEXAFS dichroism is employed to derive the molecular orientation of the BTBT subunit. In addition to the conventional C K-edge NEXAFS resonances, we observe modifications in the density of unoccupied states. The spectral changes are affected by the strength and polarity of the applied gate voltage. Furthermore, the related energies match the energy levels of polaronic states. Thus, we have clear indications to interprete the data in the context of polaron formation due to charge accumulation induced by the applied electric field in our ultrathin device.[1] The study has been funded by the DFG within GRK 1896 and the SolTECH initiative. [1] M. Johnson et al., Appl. Phys. Lett.121 (2022) 183503.

TT 32.11 Wed 12:15 GÖR 226

Machine learning for molecular design of organic molecules and reaction optimization — •Julia Westermayr[1], Reinhard J. Maurer[2], and Detlev Belder[3] — [1]Artificial Intelligence in Theoretical Chemistry Group, Leipzig University, Germany — [2]Computational Surface Chemistry Group, University of Warwick, UK — [3]Analytical Chemistry, Leipzig University, Germany

High-throughput screening of reaction conditions and electronic properties of molecules plays a crucial role in chemical industry and can be facilitated by automated workflows and machine learning. However, the high combinatorial complexity of the various parameters affecting molecular properties leaves unguided searches in chemical space highly inefficient and the optimization of reactions to synthesize these molecules often fails as theoretical protocols are usually decoupled from experiments. In this talk, we will show how predictive and generative deep learning models can be combined to theoretically design new molecules with potential relevance to organic electronics [1]. Further, we will present how these tools can be coupled with experiments to enable automated micro-laboratories [2] for targeted chemical synthesis. [1] JW et al. Nat. Comp. Sci, in press (2023). [2] R. J. Beulig et al., Lab Chip 17, 1996 (2017).

TT 33: Many-Body Quantum Dynamics (joint session DY/TT)

Time: Wednesday 9:30–13:00 Location: MOL 213

Invited Talk TT 33.1 Wed 9:30 MOL 213

Many-body localization from Hilbert- and real-space points of view — •Ivan Khaymovich[1], Giuseppe De Tomasi[2], Frank Pollmann[3], and Simone Warzel[3] — [1]Nordic Institute for Theoretical Physics, Stockholm, Sweden — [2]University of Illinois Urbana-Champaign, USA — [3]Technical University Munich, Germany

Many-body localization (MBL), known as a generic mechanism to break quantum ergodicity, has been recently shown to be not the Hilbert-space Anderson localization. Instead, the MBL eigenstate occupies a fractal support [1-2], with extensive number of configurations. On the other hand, the well-established and accepted by the community picture of an emergent set of local integrals of motion [3] provides the structure of the MBL in the real space.

In this talk, I will provide the observable (later measured in the experiment [4]) which combines the fractality in the Hilbert space with the presence of local integrals of motion [2]. This observable, being the radial profile of the eigenstate over the Hamming distance, keeps the information about both the Hilbert-space fractal dimensions and the real-space localization lengths and uncovers the structure of these measures across the MBL transition. Phenomenological picture behind this behavior is consistent with the Kosterlitz-Thouless scenario of the MBL transition, suggested in the literature.

Literature: [1] N. Macé et al., PRL 123, 180601 (2019). [2] G. De Tomasi, I. M. Khaymovich et al. PRB 104, 024202 (2021). [3] Abanin et al., RMP 91, 021001 (2019). [4] Y. Yao et al arXiv:2211.05803.

TT 33.2 Wed 10:00 MOL 213

Bridging classical and quantum many-body information dynamics — •Andrea Pizzi[1,2], Daniel Malz[3,4], Andreas Nunnenkamp[5], and Johannes Knolle[6,4,7] — [1]Department of Physics, Harvard University, Cambridge 02138, Massachusetts, USA — [2]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [3]Max-Planck-Institute of Quantum Optics, Hans-Kopfermann-Str. 1, 85748 Garching, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [5]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1190 Vienna, Austria — [6]Department of Physics, Technische Universität München, James-Franck-Stra. 1, 85748 Garching, Germany — [7]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The fundamental question of how information spreads in closed quantum many-body systems is often addressed through the lens of the bipartite entanglement entropy. Among its most striking features are unbounded linear growth in the thermodynamic limit, asymptotic extensivity in finite-size systems, and measurement-induced phase transitions. Here, we show that these key qualitative features emerge naturally also for the classical bipartite mutual information, the natural classical analogue of the quantum entanglement entropy. Key for this observation is treating the classical many-body problem on par with the quantum one, that is, explicitly accounting for the exponentially large probability distribution. Our analysis is supported by extensive numerics on prototypical cellular automata and Hamiltonian systems.

TT 33.3 Wed 10:15 MOL 213

Performance boost of a collective qutrit refrigerator — •Dmytro Kolisnyk[1] and Gernot Schaller[2] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

A single qutrit with transitions selectively driven by weakly-coupled reservoirs can implement one of the world's smallest refrigerators. We analyze the performance of N such fridges that are collectively coupled to the reservoirs. We observe a quantum boost, manifest in a quadratic scaling of the steady-state cooling current with N. As N grows further, the scaling reduces to linear, since the transitions responsible for the quantum boost become energetically unfavorable. Fine-tuned inter-qutrit interactions may be used to maintain the quantum boost for all N and also for not-perfectly collective scenarios.

[1] D. Kolisnyk and G. Schaller, Performance boost of a collective qutrit refrigerator, arXiv:2210.07844.

[2] M. Kloc, K. Meier, K. Hadjikyriakos, and G. Schaller, Superradiant Many-Qubit Absorption Refrigerator, Phys. Rev. Applied 16, 044061 (2021).

[3] N. Linden, S. Popescu, and P. Skrzypczyk. How small can thermal machines be? The smallest possible refrigerator. Phys. Rev. Lett. 105:130401, 2010.

TT 33.4 Wed 10:30 MOL 213

Hidden Phase of the Spin-Boson Model — •Florian Otterpohl[1,2], Peter Nalbach[3], and Michael Thorwart[2,4] — [1]Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA — [2]I. Institut für Theoretische Physik, Universität Hamburg, Notkestraße 9, 22607 Hamburg, Germany — [3]Fachbereich Wirtschaft und Informationstechnik, Westfälische Hochschule, Münsterstraße 265 46397 Bocholt, Germany — [4]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

A quantum two-level system immersed in a sub-Ohmic bath experiences enhanced low-frequency quantum statistical fluctuations which render the nonequilibrium quantum dynamics highly non-Markovian. Upon using the numerically exact time-evolving matrix product operator approach, we investigate the phase diagram of the polarization dynamics. In addition to the known phases of damped coherent oscillatory dynamics and overdamped decay, we identify a new third region in the phase diagram for strong coupling showing an aperiodic behavior. We determine the corresponding phase boundaries. The dynamics of the quantum two-state system herein is not coherent by itself but slaved to the oscillatory bath dynamics.

TT 33.5 Wed 10:45 MOL 213

Exploring anomalies by many-body correlations — •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 quantum anomaly can be written alternatively into a form violating conservation laws or as non-gauge invariant currents seen explicitly on the example of chiral anomaly. By reinterpreting the many-body averaging, the connection to Pauli-Villars regularization is established which gives the anomalous term a new interpretation as arising from quantum fluctuations by many-body correlations at short distances. This is exemplified by using an effective many-body quantum potential which realizes quantum Slater sums by classical calculations. It is shown that these quantum potentials avoid the quantum anomaly but approaches the same anomalous result by many-body correlations. A measure for the quality of quantum potentials is suggested to describe these quantum fluctuations in the mean energy. Consequently quantum anomalies might be a short-cut way of single-particle field theory to account for many-body effects. This conjecture is also supported since the chiral anomaly can be derived by a completely conserving quantum kinetic theory. [Eur. Phys. J. B 92 (2019) 176, Phys. Lett. A 383 (2019) 1362, Phys. Status Solidi B (2021) 2100316]

TT 33.6 Wed 11:00 MOL 213

Non-Markovian Stochastic Schrödinger Equation: Matrix Product State Approach to the Hierarchy of Pure States — Xing Gao[1], Jiajun Ren[2], Zhigang Shuai[2], and •Alexander Eisfeld[3] — [1]Sun Yat-sen University, Shenzhen, Guangdong, China — [2]Tsinghua University, Beijing, China — [3]MPI-PKS, Dresden

We derive a stochastic hierarchy of matrix product states (HOMPS) for non-Markovian dynamics in open quantum system at finite temperature, which is numerically exact and efficient. HOMPS is obtained from the stochastic hierarchy of pure states (HOPS) by expressing HOPS in terms of formal creation and annihilation operators. The resulting stochastic first order differential equation is then formulated in terms of matrix product states and matrix product operators. In this way the exponential complexity of HOPS can be reduced to scale polynomial with the number of particles. The validity and efficiency of HOMPS is demonstrated for the spin-boson model and long chains where each site is coupled to a structured, strongly non-Markovian environment.

[1] X. Gao, J. Ren, A. Eisfeld, Z. Shuai, *Phys. Rev. A* 105, L030202 (2022)

TT 33.7 Wed 11:15 MOL 213

ultrafast gap dynamics near the zone boundary in a cuprate superconductor — •qinda guo, maciej dendzik, magnus berntsen, cong li, wanyu chen, yang wang, dibya phuyal, and oscar tjernberg — Department of Applied Physics, KTH Royal Institute of Technology, Hannes Alfvéns väg 12, 114 19 Stockholm, Sweden

The time- and angle- resolved photoemission spectroscopy (tr-ARPES) is a powerful technique to directly probe the ultrafast electron dynamics in the momentum space. Our recently developed narrow-bandwidth tr-ARPES setup enabled us to access the ultrafast dynamics of the quasiparticle population as well as the superconducting gap, in the whole surface Brillouin zone of the photoexcited cuprate superconductor (Bi2212). The results show non-trivial dynamics at the d-wave antinode and provide new insights into the enigma of the Cooper-pair formation process and condensation that takes place in the high-temperature cuprate superconductor.

15 min. break

TT 33.8 Wed 11:45 MOL 213

Controlling Many-Body Quantum Chaos — •Lukas Beringer[1], Steven Tomsovic[1,2], Juan Diego Urbina[1], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany — [2]Department of Physics and Astronomy, Washington State University, Pullman, WA USA

Targeting in classical chaos control problems makes optimal use of the system's exponential instabilities to direct a given initial state to a predetermined final target state. A generalization to chaotic quantum systems in the semiclassical regime is possible [1], but also requires controlling an initially localized evolving quantum state's spreading. A coherent procedure of this kind enables directing highly excited, far-out-of-equilibrium states from an initial to some final target quantum state. Such methods have been successfully developed and applied to initially minimum uncertainty wave packets in a quantum kicked rotor system. The aim of our work is to extend those procedures to bosonic many-body systems. More specifically, we demonstrate how to make a localized quantum initial state follow special chaotic mean-field solutions of a Bose-Hubbard system toward an arbitrary localized target final state.

[1] S. Tomsovic, J. D. Urbina, and Klaus Richter, Controlling Quantum Chaos: Optimal Coherent Targeting, arXiv:2211.07408

TT 33.9 Wed 12:00 MOL 213

Environment-induced decay dynamics of antiferromagnetic order in Mott-Hubbard systems — •Gernot Schaller[1], Friedemann Queisser[1,2], Nikodem Szpak[3], Jürgen König[3], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

We study the dissipative Fermi-Hubbard model in the limit of weak tunneling and strong repulsive interactions, where each lattice site is tunnel-coupled to a Markovian fermionic bath. For cold baths at intermediate chemical potentials, the Mott insulator property remains stable and we find a fast relaxation of the particle number towards half filling. On longer time scales, we find that the antiferromagnetic order of the Mott-Néel ground state on bipartite lattices decays, even at zero temperature. For zero and nonzero temperatures, we quantify the different relaxation time scales by means of waiting time distributions, which can be derived from an effective (non-Hermitian) Hamiltonian and obtain fully analytic expressions for the Fermi-Hubbard model on a tetramer ring.

[1] G. Schaller *et al.*, Phys. Rev. B **105**, 115139 (2022).

TT 33.10 Wed 12:15 MOL 213

Arrow of time concept based on properties of Lanczos coefficients — •Christian Bartsch, Mats H. Lamann, Robin Heveling, Lars Knipschild, Jiaozi Wang, Robin Steinigeweg, and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, DE-49076 Osnabrück

We introduce an arrow of time concept based on a specifically defined class of arrow of time functions (ATF) consisting of a limited number of Krylov space generating observables. These ATF'S are found to be essentially monotonously decaying in time which is measured by some quantifying parameter. The ATF's are constructed to be upper bounds for pertinent autocorrelation functions. Employing certain features of the Lanczos coefficients and the wave package-like excitation moving on the Krylov chain, we find reasonable agreement with corresponding numerics.

TT 33.11 Wed 12:30 MOL 213

Fast Time-Evolution of Matrix-Product States using the QR decomposition — •Jakob Unfried[1,2], Johannes Hauschild[1], and Frank Pollmann[1,2] — [1]Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MC-QST), Schellingstr. 4, 80799 München, Germany

Numerical simulations of quantum many-body dynamics in and out of equilibrium is essential for the understanding of a wide range of physical phenomena. Efficient matrix product state simulation techniques, such as time evolution block decimation (TEBD), are widely successful in extracting experimentally relevant signatures, such as dynamical correlation functions. We propose and benchmark a modified TEBD algorithm that uses a truncation scheme based on the QR decomposition instead of the singular value decomposition (SVD). The modification reduces the scaling with the dimension of the physical Hilbert space d from d^3 down to d^2. Unlike the SVD, the QR decomposition allows for highly efficient implementations on GPU hardware. In a benchmark simulation of a global quench in a quantum clock model, we observe a speedup of orders of magnitude comparing the QR based scheme on a GPU to the SVD based TEBD on CPU.

TT 33.12 Wed 12:45 MOL 213

Simulating infinite temperature spin dynamics by a dynamic mean-field theory — •Timo Gräßer[1], Kristine Rezai[2], Alexander O. Sushkov[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Boston University, Boston, MA 02215, USA

We develop a dynamic mean-field theory for spin systems at infinite temperature (spinDMFT) [1]. The idea is to replace the large environment of a spin by a dynamic mean-field which displays a random Gaussian temporal evolution. Its autocorrelations are self-consistently linked to the quantum mechanic expectation values of spin-spin correlations. This approach becomes exact in the limit of large lattice coordination numbers. We improve the approach by considering spin clusters quantum-mechanically (cluster spinDMFT). The extended model is able to describe dynamic spin correlations measured in recent experiments [2] where an inhomogeneous spin-$\frac{1}{2}$ ensemble on a diamond surface is probed using nitrogen-vacancy centers as sensors.

[1] T. Gräßer et al., Phys. Rev. Research **3**, 043168 (2021).

[2] K. Rezai et al., arXiv:2207.10688 (2022).

TT 34: Fe-based Superconductors

Time: Wednesday 11:30–13:00 Location: HSZ 103

TT 34.1 Wed 11:30 HSZ 103

Efficient tuning of the superconductor $BaNi_2As_2$ by Calcium substitution - Single crystal Growth and Characterization — •Fabian Henssler, Kristin Willa, Mehdi Frachet, Tom Lacmann, Christoph Meingast, Michael Merz, Amir-Abbas Haghighirad, and Matthieu Le Tacon — Institut für Quantenmaterialien und Technologien, KIT Karlsruhe, Deutschland

$BaNi_2As_2$ is a highly tunable superconductor, which is non-magnetic and isostructural to the Fe-based parent compound $BaFe_2As_2$. Beyond superconductivity, recent publications reinforce the strong interplay between nematicity, charge density waves (CDW), and structural distortions [1,2,3]. At about 145 K, an incommensurate CDW forms, which coincides with a small lattice distortion ($\delta \sim 10^{-4}$) [4]. At slightly lower temperatures (T_S), the system undergoes a first-order transition, which can be suppressed e.g. by P- or Sr-substitution. Thereby, the superconducting transition temperature T_c can be enhanced by a factor of six [5]. In the case of Sr substitutions, however, a concentration as large as $x_{Sr} \sim 0.7$ is required. As an alternative, we report on the growth of Ca-substituted single crystals with Ca content up to $x_{Ca} \sim 0.1$. Specific heat and electrical transport measurements indicate that Ca is about eight times more efficient than Sr to suppress T_S.

[1] M. Frachet et al., arXiv:2207.02462 (2022)
[2] C. Meingast et al., Phys. Rev. B 106, 144507 (2022)
[3] S. M. Souliou et al., arXiv:2207.07191 (2022)
[4] M. Merz et al., Phys. Rev. B 104, 184509 (2021)
[5] C. Eckberg et al., Nat. Phys. 16, 346-350 (2020)

TT 34.2 Wed 11:45 HSZ 103

Electronic theory for FFLO state in KFe_2As_2 superconductor — •Luka Jibuti and Ilya Eremin — Ruhr Universität Bochum, Bochum, Germany

Following the experimental observation of the Frude-Ferrel-Larnik-Ovchinnikov (FFLO) state in heavily hole-doped KFe_2As_2, we develop a microscopic theory of multi-orbital FFLO phase in this system, based on the microscopic low-energy model consisting of two Γ-centered hole pockets created by xz and yz orbitals and the sizeable spin-orbit coupling between them. We use the leading angular harmonics approximation (LAHA) to write down the general form of the interaction, that involves both s-wave and d-wave channels. By decomposing the interaction into s- and d-wave channels, employing the mean-field approximation and solving the self-consistent equations for the order parameters, we analyse the creation of the FFLO phase, with the appearance of the non-zero, symmetry preserving q vector for the nodal d-wave state and s-wave with accidental nodes. We also discuss the role of spin-orbit coupling and possible orbital FFLO state, discussed recently in the context of Ising superconductors.

TT 34.3 Wed 12:00 HSZ 103

Superconductivity of $CaKFe_4As_4$ under anisotropic strains — B. Zúñiga Céspedes[1], A. Valadkhani[2], S. Mandloi[1], M. Xu[3,4], J. Schmidt[3,4], S. L. Bud'ko[3,4], P. C. Canfield[3,4], A. P. Mackenzie[1,5], R. Valentí[2], and •E. Gati[1] — [1]MPI CPfS, 01187 Dresden, DE — [2]Inst. for Theor. Physics, Goethe University, 60438 FFM, DE — [3]Ames Lab, US DOE, Ames, IA 50011, USA — [4]Dept. of Physics and Astronomy, Iowa State Uni, Ames, IA 50011, USA — [5]Scottish Universities Physics Alliance, School of Physics and Astronomy, Uni of St Andrews, UK

$CaKFe_4As_4$ is an exceptional member of the family of Fe-based superconductors. First, it is a stochiometric superconductor at ambient pressure with high critical temperature $T_c \sim 35$ K. Second, this superconducting phase can be found in close proximity to a so-called hedgehog vortex magnetic order (SVC), which does preserve tetragonal symmetry. This is in contrast to the ubiquitous stripe-type magnetic order (SSDW) in the Fe-based superconductors that is accompanied by a vestigial nematic phase. Thus, $CaKFe_4As_4$ is an important testbed to investigate the interplay of superconductivity with different magnetic orders and nematicity. Here, we will discuss the impact of anisotropic strains, which couple directly to the nematic order parameter, on superconductivity. To this end, we present measurements of T_c as well as results of DFT calculations of the stability of SVC vs. SSDW order under large strains. Our results support the notion that nematic fluctuations contribute to superconducting pairing in this high-T_c superconductor.*Funded through the SFB/TRR288 (Elasto-Q-mat).*

TT 34.4 Wed 12:15 HSZ 103

The resistive anisotropy of FeSe in the nematic state — •Clifford Hicks[1,2], Jack Bartlett[2], Alexander Steppke[2], Suguru Hosoi[3], Takasada Shibauchi[4], and Andrew Mackenzie[2] — [1]University of Birmingham, U.K. — [2]Max Planck Institute for Chemical Physics of Solids, Dresden — [3]Osaka University, Japan — [4]University of Tokyo, Japan

We employed strain tuning to adjust the degree of twinning of samples of FeSe. By doing so, we were able to measure the resistive anisotropy in the nematic state. The resistive anisotropy of the nematic state, along with the dependence of the resistivity and the superconducting critical temperature on biaxial strain suggest a strong role for the yz orbital in electronic scattering in FeSe.

TT 34.5 Wed 12:30 HSZ 103

The low-temperature specific heat and thermal expansion of YFe_2Ge_2 — •Pavlo Khanenko[1,2], Jiasheng Chen[2], Jacintha Banda[1], Thomas Luehmann[1], F. Malte Grosche[2], and Manuel Brando[1] — [1]Max Planck Institute for Chemical Physics of Solids, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge, UK

We present specific heat and thermal expansion coefficient measurements of the layered iron-based superconductor YFe_2Ge_2 down to 40 mK and in magnetic field. A new generation of crystals [1] with residual resistivity ratios larger than 500 and $T_c = 1.2$ K have been investigated. These crystals display a sharp superconducting anomaly in both specific heat and thermal expansion. From the jump magnitudes and using the Ehrenfest relation we derive a small positive pressure dependence of T_c, $dT_c/dp = 24.4$ mK/GPa. Despite the high purity of the crystals, the residual Sommerfeld coefficient is relatively large $\gamma_0 \approx 40\,\mathrm{mJ/K^2mol}$, i.e., less than about half of the value in the normal state ($100\,\mathrm{mJ/K^2mol}$). The field dependences of $\gamma_0(B)$ and its respective coefficient in thermal expansion $\alpha_0(B)$ are analyzed within the frame of two gap scenario.

[1] J. Chen *et al.*, Phys. Rev. Lett. 125, 237002 (2020)

TT 34.6 Wed 12:45 HSZ 103

Spin-density-wave order and evidence for superconductivity in single-crystal $LuFe_2Ge_2$ — •Jiasheng Chen and F. Malte Grosche — Cavendish Laboratory, Cambridge, UK

The discovery of unconventional superconductivity in YFe_2Ge_2 [1, 2] has encouraged the search for more iron-based superconductors in the germanide family. The isostructural and isoelectronic compound, $LuFe_2Ge_2$, exhibits physical properties that closely resemble those of YFe_2Ge_2. Despite the additional spin-density-wave order observed below 9 K in $LuFe_2Ge_2$, the overall shape and magnitude of the resistivity and susceptibility above 10 K, and the similarly enhanced Sommerfeld coefficient $C/T > 70\,\mathrm{mJ/molK^2}$ suggest a similar underlying physics in the two systems [3]. Using the liquid transport flux growth method [2], we investigated the effect of changing growth conditions on the crystal quality and on the spin-density-wave order in $LuFe_2Ge_2$. In the best samples with RRR reaching 170, we observe evidence of superconductivity, making it the second iron-germanide superconductor discovered to date.

[1] J. Chen et al., PRL 116, 127001 (2016)
[2] J. Chen *et al.*, PRL 125, 237002 (2020)
[3] M. Avila *et al.*, J. Magn. Magn. Mater. 270 , 51 (2004)

TT 35: Focus Session: Correlations in Moiré Quantum Matter I

Topological quantum phenomena and breakthroughs in time-resolved spectroscopy pose new challenges for many-body theory: Spatio-temporal electronic correlations often strongly impact topological and dynamical material properties but at the same time hinder an unambiguous interpretation of experiments, let alone a reliable quantitative prediction of material properties. Moiré quantum matter, i.e. systems where fundamental electronic properties and correlation phenomena emerge beyond the atomic scale exemplify these challenges. This Focus Session brings together the most recent developments in the field.

Organizers: Roser Valentí (Goethe-Universität Frankfurt) and Tim Wehling (Universität Hamburg)

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

Invited Talk TT 35.1 Wed 15:00 HSZ 03
Strongly correlated excitons in atomic double layers — •Phuong Nguyen[1], Liguo Ma[1], Raghav Chaturvedi[1], Kenji Watanabe[2], Takashi Taniguchi[2], Kin Fai Mak[1,3,4], and Jie Shan[1,3,4] — [1]School of Applied and Engineering Physics, Cornell University, Ithaca, NY, USA — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY, USA — [4]Kavli Institute at Cornell for Nanoscale Science, Ithaca, NY, USA

Excitons (bound electron-hole pairs) in solids have been proposed as a platform to achieve high temperature Bose-Einstein condensation. The small exciton binding energy in conventional semiconductors has limited the condensation temperature to about 1 K. In the past several years, a new class of two-dimensional semiconductors with much larger exciton binding energy has emerged. In this talk, we discuss the development of transition metal dichacogenide double layer structures and electrical injection of interlayer excitons up to 10^{12} cm^{-2}. We establish electrical control of the chemical potential of interlayer excitons and probe their thermodynamic properties by capacitance measurements. We present experimental evidence for an excitonic insulating state and discuss the possibility of probing exciton superfluidity in the atomic double layer system.

Invited Talk TT 35.2 Wed 15:30 HSZ 03
The Quantum Twisting Microscope — •Shahal Ilani — Weizmann Institute

In this talk I will present a fundamentally new type of scanning probe microscope, the Quantum Twisting Microscope (QTM), capable of performing local quantum interference measurements at a twistable interface between two quantum materials. Its working principle is based on a unique tip, made of an atomically-thin two-dimensional material. This tip allows electrons to coherently tunnel into a sample at many locations at once, with quantum interference between these tunneling events, making it a scanning electronic interferometer. With an extra twist degree of freedom, our microscope becomes a momentum-resolving local probe, providing powerful new ways to study the energy dispersions of interacting electrons. I will present various experiments performed with this microscope, demonstrating quantum interference at room temperature, probing the conductance of in-situ twisting interfaces, and imaging local energy dispersions in a variety of quantum materials.

Invited Talk TT 35.3 Wed 16:00 HSZ 03
Light-driven phenomena in two-dimensional and correlated quantum materials — •Angel Rubio — Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — Center for Computational Quantum Physics Flatiron Institute, Simons Foundation, 10010 NY, USA

We will introduce our newly developed quantum electrodynamics density-functional formalism (QEDFT) as a first principles framework to predict, characterize and control the appearance of ordered phases of strongly interacting light-matter hybrid. We will pursue whether it is possible to create these new states of materials as ground-states of the system. To this end we will show how the emerging (vacuum) dressed states resembles Floquet states in driven systems. Strong light*matter coupling in cavities provides a pathway to break fundamental materials symmetries, like time-reversal symmetry in chiral cavities. We will discuss how to realize non-equilibrium states of matter that have so far been only accessible in ultrafast and ultrastrong laser-driven materials. We illustrate the realization of those ideas in molecules and 2D materials and show that the combination of cavity-QED and 2D twisted vdW heterostructures provides a novel and unique platform for the seamless realization of a plethora of interacting quantum phenomena, including exotic and elusive correlated and topological phases of matter.

15 min. break

Invited Talk TT 35.4 Wed 16:45 HSZ 03
Cascade of transitions in twisted and non-twisted graphene layers within the van Hove scenario — •Laura Classen[1], Dmitry Chichinadze[2], Yuxuan Wang[3], and Andrey Chubukov[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Minnesota, Minneapolis, USA — [3]University of Florida, Gainesville, USA

Fermions in layered graphene structures are described by both spin and valley degrees of freedom. Due to weak coupling between valleys, this can lead to an approximate SU(4) symmetry made from combined spin and valley transformations, which plays out differently depending on filling and interactions. Motivated by measurements of compressibility and STM spectra in twisted bilayer graphene, we analyze the pattern of symmetry breaking for itinerant fermions near a van Hove singularity. Making use of the approximate SU(4) symmetry of the Landau functional, we show that the structure of the order parameter changes with increasing filling via a cascade of transitions. We compute the feedback from different spin/valley orders on fermions and argue that each order splits the initially 4-fold degenerate van Hove peak in a particular fashion, consistent with the STM data and compressibility measurements, providing a unified interpretation of the cascade of transitions in twisted bilayer graphene. Our results follow from a generic analysis of an SU(4)-symmetric Landau functional and are valid beyond a specific underlying fermionic model. We argue that an analogous van Hove scenario explains the cascade of phase transitions in non-twisted Bernal bilayer and rhombohedral trilayer graphene.

Invited Talk TT 35.5 Wed 17:15 HSZ 03
Topology and strong correlation: From twisted bilayer graphene to the boundary zeros of Mott insulators — •Giorgio Sangiovanni[1], Niklas Wagner[1], Gautam Rai[2], Lorenzo Crippa[1], Tim Wehling[2], and Roser Valentí[3] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]I. Institut für Theoretische Physik, Universität Hamburg — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main

Strong electronic correlations drive materials towards atomic-like Mott phases. How to topologically classify these many-body insulators is an open and highly debated question. In this talk I am going to start from twisted bilayer graphene, an example of the interplay between low-energy protection of single-particle eigenvalues and non-perturbative effects of electron-electron interactions. From this, I plan to move to a broader concept which has been spelled out in rather different ways in the recent literature: topological Mott insulators. Most of the proposed realizations rely either on Hartree-Fock approximations or on appropriately defined auxiliary degrees of freedom. I am going to present a novel, remarkably simple way of describing a topological Mott insulator without long-range order, based on the topological properties of their Green's function zeros in momentum space. After discussing the fate of the bulk-boundary correspondence in these systems, I will show how the zeros can be seen as a form of "topological antimatter" with distinctive features associated to the annihilation with conventional topologically protected edge modes.

TT 35.6 Wed 17:45 HSZ 03

Transport and electron correlations in magic-angle twisted bilayer graphene: A dynamical mean field theory study — •Gautam Rai[1], Lorenzo Crippa[2], Giorgio Sangiovanni[2], Roser Valenti[3], and Tim Wehling[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany — [2]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [3]Institut für Theoretische Physik, Goethe-Universität Frankfurt am Main, Frankfurt am Main, Germany

Fully characterising the low-temperature phase diagram of magic-angle twisted bilayer graphene (MATBG) has proven to be one of the most compelling challenges in recent condensed matter physics. Correlation effects dominate due to the flatness of the low-energy bands. By varying doping and temperature, one can tune between superconductor, correlated-insulator, and strange metal phases. It has been difficult to apply standard strong-correlation computational techniques because of a topological obstruction, which precludes the existence of exponentially localized, symmetry-preserving Wannier functions for the flat bands. Recently, a heavy Fermion model has been proposed that successfully treats the hybrid localised-delocalised nature of MATBG [1]. We apply dynamical mean field theory (DMFT) to the heavy Fermion model to describe electron correlation effects in MATBG. In particular, we demonstrate how filling commensurability affects transport at low temperatures.

[1] Z. D. Song and B. A. Bernevig, PRL 129, 047601 (2022)

TT 35.7 Wed 18:00 HSZ 03

Moiré minibands of twisted MoS_2 heterostructures — •Chithra H. Sharma[1,2], Marta Prada[1], Jan-Hendrick Schmidt[1], Lars Tiemann[1], Tobias Stauber[3], Takashi Taniguchi[4], Kenji Watanabe[4], Robert Zierold[1], Kai Rossnagel[2], and Robert H. Blick[1,5] — [1]Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg — [2]CAU Kiel, Leibnitzstrasse 19, 24118 Kiel — [3]ICMM-CSIC, Sor Juana Inés de la Cruz 3, Madrid 28049 Spain — [4]Research Center for Functional Materials, National Institute for Materials Science, Namiki 1-1, Tsukuba, 305-0044, Ibaraki, Japan — [5]Material Science and Engineering, University of Wisconsin-Madison, University Ave. 1550, Madison, 53706, Wisconsin, USA

In the last decade, the evolution of van der Waals material systems has provided a multitude of options to manipulate, control, and engineer materials properties to various needs by combination, proximity, and twisting. Moiré superlattices formed as a result of lattice mismatch or twist angle modify the electronic structure to create flat bands and host exotic correlated electron phases. Here we observe the existence of low-dispersing mini-bands near the conduction band edge of MoS_2 twisted devices. We employ transport measurements and resolve discrete states within the band gap at low temperatures, in agreement with first-principles density functional theory calculations. We could also infer that the mini-bands correspond to iso-spin flavors as a result of interaction in the system coherent with our temperature dependence.

TT 36: Topological Insulators

Time: Wednesday 15:00–17:45 Location: HSZ 103

TT 36.1 Wed 15:00 HSZ 103

In-plane magnetic field induced asymmetric magnetoconductance in topological insulator kinks — •Gerrit Behner[1,2], Abdur Rehman Jalil[1,2], Kristof Moors[1,2], Erik Zimmermann[1,2], Peter Schüffelgen[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

The study of the transport properties of quasi one-dimensional topological insulator (TI) nanostructures under the application of an in-plane magnetic field is crucial for the later realization of topological quantum computation building blocks. We present low temperature measurements of selectively grown TI-kinks under the application of an in-plane magnetic field. A dependence of the TI-kink resistance on the the in-plane magnetic field angle is visible in the magnetotransport data resulting in a π-periodic change of the conductance. This phenomenon originates from an orbital effect, leading to a periodic alignment of the phase-coherent states on the bottom and top surface of the topological insulator. Respectively, once the states are aligned an increased conductance in the device is observed. The measurement results are supported theoretically by an analysis of a surface Rashba-Dirac model and tight-binding calculations of an effective three-dimensional model.

TT 36.2 Wed 15:15 HSZ 103

Topological quantum chemistry with a twist — •Axel Fünfhaus, Marius Möller, and Roser Valentí — Goethe Uni Frankfurt, Frankfurt am Main, Germany

It is well known that many topological phases can be indicated by the symmetry behavior of their band structure at high symmetry points, which culminated in the development of topological quantum chemistry. This approach becomes problematic once interactions are added, as this does not permit conserved particle occupation numbers in reciprocal space. We face this challenge by generalizing the Brillouin zone for translation invariant many-body wave functions via a torus of twisted boundary conditions. This allows for a symmetry analysis of the ground state wave function in twisted boundary space. We apply this ansatz to detect topological phases in interacting Chern insulators and fractional Chern insulators as well as Mott insulating systems that cannot adiabatically be connected to atomic limits.

TT 36.3 Wed 15:30 HSZ 103

Phonon-induced breakdown of Thouless pumping in the Rice-Mele-Holstein model — •Suman Mondal, Eric Bertok, and Fabian Heidrich-Meisner — Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

Adiabatic and periodic variations of the lattice parameters can make it possible to transport charge through a system even without net external electric or magnetic fields, known as Thouless charge pumping. The amount of charge pumped in a cycle is quantized and entirely determined by the system's topology, which is robust against perturbations such as disorder and interactions. However, coupling to the environment may play a vital role in topological transport in many-body systems. In this talk, we will discuss the topological Thouless pumping, where the charge carriers interact with local optical phonons. The semi-classical multi-trajectory Ehrenfest method is employed to treat the phonon trajectories classically and charge carriers quantum mechanically. We find a breakdown of the quantized charge transport in the presence of phonons. It happens for any finite electron-phonon coupling strength at the resonance condition when the pumping frequency matches the phonon frequency, and it takes finite phonon coupling strength away from the resonance. Moreover, there exist parameter regimes with non-quantized negative and positive charge transport. The modified effective pumping path due to electron-phonon coupling accurately explains the underlying physics.

textitSupported by DFG (Deutsche Forschungsgemeinschaft) via FOR 2414.

TT 36.4 Wed 15:45 HSZ 103

Large thermal Hall effect in a disordered topological insulator — •Rohit Sharma, Mahasweta Bagchi, Oliver Breunig, Yoichi Ando, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln, Germany

Topological insulators mother compounds (Bi_2Se_3,Bi_2Te_3) are notorious for their high thermoelectric figure of merit and to quantify that, they have been under scrutiny in the past for their longitudinal thermal transport. Surprisingly no attention has been paid on the transverse part of heat transport. Motivated by the recent findings of thermal Hall effect in some oxide and magnetic insulators[1], we have experimentally observed a large thermal Hall effect in disordered topological insulator $TlBi_{0.15}Sb_{0.85}Te_2$[2]. By comparing thermal conductivity κ_{xx} and thermal Hall effect κ_{xy} data with the electrical counterparts (σ_{xx} & σ_{xy}), we study a possible influence of phonon drag on thermal transport. Electrical hall conductivity (σ_{xy}) shows multi-band behaviour in the whole temperature range (4-300K). Electronic contribution to thermal transport κ_e was calculated by using Wiedemann-Franz law and then compared with the measured thermal transport

data, where it was found that both κ_{xx} and κ_{xy} shows phonon dominated behaviour. When compared κ_{xy} and κ_e, former shows an order of magnitude higher signal then the latter one.Possible reasons for large thermal Hall effect in $TlBi_{0.15}Sb_{0.85}Te_2$ will be discussed.
Funded by the DFG via CRC 1238 Projects A04 and B01
[1] M. Boulanger et al., Nat. Commun. 11, 5325 (2020)
[2] O. Breuning et al., Nat. Commun. 8, 15545 (2017)

TT 36.5 Wed 16:00 HSZ 103

Mixed higher-order topology: boundary non-Hermitian skin effect induced by a Floquet bulk — •Hui Liu and Ion Cosma Fulga — Leibniz Institute for Solid State and Materials Research, Dresden

We show that anomalous Floquet topological insulators generate intrinsic, non-Hermitian topology on their boundary. As a consequence, removing a boundary hopping from the time-evolution operator stops the propagation of chiral edge modes, leading to a non-Hermitian skin effect. This does not occur in Floquet Chern insulators, however, in which boundary modes continue propagating. By evaluating the local density of states, we found that the resulting non-Hermitian skin effect is critical, i.e. scale-invariant, due to the nonzero coupling between the bulk and the edge. Further, it is a consequence of the nontrivial topology of the bulk Floquet operator, which we show by designing a real-space topological invariant. Our work introduces a form of 'mixed' higher-order topology, where a bulk system characterized by Floquet topology produces a boundary system characterized by non-Hermitian topology, without the need for any added perturbations. This opens an alternate direction in the study of topological classifications, and provides a route towards generating non-Hermitian skin effects by means of periodic driving.

15 min. break

TT 36.6 Wed 16:30 HSZ 103

PT-symmetric photonic topological insulator — •Alexander Fritzsche[1,2], Tobias Biesenthal[2], Lukas Maczewsky[2], Karolin Becker[2], Max Erhardt[2], Matthias Heinrich[2], Ronny Thomale[1], Yogesh Joglekar[3], and Alexander Szameit[2] — [1]Fakultät für Physik und Astronomie, Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [2]Institut für Physik, University of Rostock, Rostock, Germany — [3]Department of Physics, Indiana University-Purdue University Indianapolis (IUPUI), Indianapolis, Indiana, USA

Gain and loss are characteristic features of open or non-Hermitian systems and lead, in general, to instable, exponentially increasing and decreasing states. However, these instabilities can be avoided when parity-time (PT) symmetry is added to such arrangements. Because of its unique properties it has been tried to combine PT symmetry with the unrivalled robustness of transport in topological insulators. In this work we propose and experimentally realize a periodically driven topological insulator with two counterpropagating boundary states where gain and loss are distributed not only spatially but also temporally using photonic waveguides as the experimental platform. Here, the periodic driving allows us to circumvent the problems that have so far hindered the combination of PT symmetry and topological insulators thereby providing the missing link between these two realms.

TT 36.7 Wed 16:45 HSZ 103

Time-reversal invariant finite-size topology — •Rafael Alvaro Flores Calderon, Roderich Moessner, and Ashley Cook — Max Planck Institut for the Physics of Complex Systems, Dresden,Germany

We report finite-size topology in the quintessential time-reversal (TR) invariant systems, the quantum spin Hall insulator (QSHI) and the three-dimensional, strong topological insulator (STI): previously-identified helical or Dirac cone boundary states of these phases hybridize in wire or slab geometries with one open boundary condition for finite system size, and additional, topologically-protected, lower-dimensional boundary modes appear for open boundary conditions in two or more directions. For the quasi-one-dimensional (q(2-1)D) QSHI, we find topologically-protected, quasi-zero-dimensional (q(2-2)D) boundary states within the hybridization gap of the helical edge states, determined from q(2-1)D bulk topology characterized by topologically non-trivial Wilson loop spectra. We show this finite-size topology furthermore occurs in 1T'-WTe2 in ribbon geometries with sawtooth edges, based on analysis of a tight-binding model derived from density-functional theory calculations, motivating experimental investigation of our results. In addition, we find quasi-two-dimensional (q(3-1)D) finite-size topological phases occur for the STI, yielding helical boundary modes distinguished from those of the QSHI by a non-trivial magneto-electric polarizability linked to the original 3D bulk STI.

TT 36.8 Wed 17:00 HSZ 103

Spectral functions of a topological Fermi-Hubbard model in one dimension — •David Mikhail and Stephan Rachel — School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

We study the effects of electron-electron interactions on the charge excitation spectrum of the spinful Su-Schrieffer-Heeger model, a prototype of a one-dimensional bulk obstructed topological insulator. In light of recent progress in the fabrication of dopant-based quantum simulators we focus on experimentally detectable signatures of interacting topology in finite lattices. Importantly, these semiconductor platforms allow for local high-precision measurements using scanning tunnelling spectroscopy (STS). To this end we use Lanczos-based exact diagonalization to calculate the single-particle spectral function in real space which generalizes the local density of states to interacting systems. Its spatial and spectral resolution allows for the direct investigation and identification of edge states. While the non-trivial topology is manifested in zero-energy spin-like edge excitations for any finite interaction strength, our analysis of the spectral function shows that the single-particle charge excitations are gapped out on the boundary. Despite the loss of topological protection, we find that these edge excitations are quasiparticle-like as long as they remain within the bulk gap and as such serve as an indicating signature of the correlated topological phase measurable in single-particle measurement techniques such as STS. Our results are available at Phys. Rev. B 106, 195408 (2022).

TT 36.9 Wed 17:15 HSZ 103

Topological phases of one and two Su-Schrieffer-Heeger wires on a semiconducting substrate — •Keshab Sony[1], Anas Abdelwahab[2], and Eric Jeckelmann[3] — [1]Leibniz universität, Hannover, Germany — [2]Leibniz universität, Hannover, Germany — [3]Leibniz universität, Hannover, Germany

Atomic wires deposited on semiconducting substrates attracted lots of attention in the last two decades as a platform of quasi one-dimension (1D) properties. The Su-Schrieffer-Heeger (SSH) model is one of the simplest models that manifests the typical features of topological phases in quasi 1D characterized by topological invariant (winding number) and corresponding number of zero edge states. In this study, we consider models of one and two SSH wires coupled to semiconducting three-dimensional (3D) substrates and investigate the topological phases of these models with respect to the model parameters, eg. dimerization, wire-wire coupling, wire-substrate hybridization. The phase diagram of single wire coupled to the substrate shows stability of the existing phases without substrate but with changing effectively the wire parameters. We also address the issue of how the presence of the substrate change or preserve the phase diagrams of the two-leg ladders without substrate. We discuss the local density of states for different cases we consider.

TT 36.10 Wed 17:30 HSZ 103

Thermal diode effect in Dirac hybrid junctions — •Phillip Mercebach and Pablo Burset — Autonomous University of Madrid, Madrid, Spain

Thermo-electric devices are utilized for nano-scale refrigeration or to harness waste heat to produce electric power in electronic circuits. These devices usually require semiconductor materials or complex geometries to induce thermo-electric effects which may suffer from a narrow range of operation or poor efficiency. To counteract these shortcomings, we propose a simple device consisting of a ferromagnet (F) in proximity to a Dirac semi-metal (N) creating a ballistic NFN junction with a large operating window. We theoretically study the heat and electric currents through the junction and show strong Seebeck and Peltier effects arising from the Dirac physics and Klein tunneling in the ballistic junction. We use the device's high tunability to create a thermal diode allowing for refrigeration of a hot reservoir or for power production induced by a temperature gradient. Finally, we discuss refrigeration efficiency and the effective electron cooling temperature taking into account the phonon contribution in quasi-two-dimensional materials, like graphene or topological insulators.

TT 37: Ruthenates

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

TT 37.1 Wed 15:00 HSZ 201

Elastocaloric determination of the phase diagram of Sr_2RuO_4 — •You-Sheng Li[1], Markus Garst[2,3], Jörg Schmalian[3,4], Sayak Ghosh[5], Naoki Kikugawa[6], Dmitry Sokolov[1], Clifford Hicks[1,7], Fabian Jerzembeck[1], Matthias Ikeda[8], Zhenhai Hu[1], Brad Ramshaw[5], Andreas Rost[9], Michael Nicklas[1], and Andrew Mackenzie[1,9] — [1]Max Planck Institute for Chemical Physics of Solids — [2]Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie — [3]Institut für Quantenmaterialien und -technologien, Karlsruher Institut für Technologie — [4]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie — [5]Laboratory of Atomic and Solid State Physics, Cornell University — [6]National Institute for Materials Science — [7]School of Physics and Astronomy, University of Birmingham — [8]Department of Applied Physics, Stanford University — [9]School of Physics and Astronomy, University of St Andrews

Uniaxial pressure has shown the capabilities of tuning the electronic structures of Sr_2RuO_4 across a Van Hove singularity (VHS). By performing high precision ac-elastocaloric effect (ECE) measurements under uniaxial strain along <100> direction, we mapped out the phase diagram of Sr_2RuO_4 in detail. Similar to many unconventional superconductors, Sr_2RuO_4 has a SC dome in proximity to a magnetic phase. Besides, we observe a strong reversal of the ECE around the VHS upon entering the SC state. Together with a model calculation, these results strongly suggest a node-less gap opening at the VHS and, thus, put a strong constraint on possible SC order parameters.

TT 37.2 Wed 15:15 HSZ 201

High-resolution elastocaloric effect measurement of 110-Sr_2RuO_4 — •Zhenhai Hu[1,2], You-Sheng Li[1], Fabian Jerzembeck[1], Michael Nicklas[1], Andrew P. Mackenzie[1,2], and Clifford W. Hicks[1,3] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Scottish Universities Physics Alliance, School of Physics and Astronomy, University of St Andrews, St Andrews, UK — [3]School of Physics and Astronomy, University of Birmingham, Birmingham, UK

The symmetry of the order parameter of superconducting Sr_2RuO_4 remains an undetermined question. Whether the order parameter has more than one component is still under debate. If the superconducting order parameter is degenerate and protected by lattice symmetry, the degeneracy will be lifted when the lattice symmetry is broken. Uniaxial pressure, which can continuously break the lattice symmetry, is thus a powerful tool to distinguish whether there is a degeneracy. However, the second transition was not observed in the previous heat capacity and elastocaloric effect measurements with strain applied along <100>. Although stringent constraints on the nature of superconducting states at zero strain were placed by the absence of the second transition with <100> strain, there remains a possibility that a second transition exists under <110> strain. Here we report the latest progress on elastocaloric measurement of Sr_2RuO_4 crystal with strain applied along <110>. Within our experimental precision, no signal indicating a second phase transition below T_c is observed.

TT 37.3 Wed 15:30 HSZ 201

Strain dependence of the superconducting state of Sr_2RuO_4 under <110> uniaxial pressure: No evidence for multi-component order parameter — •Fabian Jerzembeck[1], You-Sheng Li[1], Zhenhai Hu[1], Naoki Kikugawa[2], Dmitry Sokolov[1], Yoshiteru Maeno[3], Michael Niklas[1], Andrew Mackenzie[1], and Clifford Hicks[4] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]National Institute for Materials Science, Tsukuba 305-0003, Japan — [3]Department of Physics, Kyoto University, Kyoto 606-8502, Japan — [4]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, United Kingdom

After more than 25 years of intense research, the order parameter of the unconventional superconductor Sr_2RuO_4 is still unknown. Recent experiments suggest that the order parameter is even-parity and multi-component [1,2], which would result in distinct features in the strain dependence of the superconducting state, such as a kink in the strain dependence of T_c around zero strain [3]. Here, we present uniaxial pressure results along the crystallographic <110>-axis and find no evidence for a discontinuity in T_c, predicted for a multi-component order parameter. However, we can place tight constraints on the thermodynamics of several discussed two-component order parameters.

[1] Pustogow et al., Nature 574, 72 (2019)
[2] Ghosh et al., Nat. Phys. 17, 199 (2021)
[3] Kivelson et al., npj Quantum Materials 5, 43 (2020)

TT 37.4 Wed 15:45 HSZ 201

Giant lattice softening at a Lifshitz transition in the normal state of Sr_2RuO_4 — •Hilary M. L. Noad[1], Kousuke Ishida[1], You-Sheng Li[1], Veronika Stangier[2], Naoki Kikugawa[3], Dmitry A. Sokolov[1], Bongjae Kim[4], Igor I. Mazin[5], Markus Garst[2], Jörg Schmalian[2], Andrew P. Mackenzie[1,6], and Clifford W. Hicks[1,7] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]National Institute for Materials Science, Tsukuba, Japan — [4]Kunsan National University, Gunsan, Korea — [5]George Mason University, Fairfax, USA — [6]University of St Andrews, St Andrews, UK — [7]University of Birmingham, Birmingham, UK

The interplay between lattice and electronic degrees of freedom is a central theme in condensed matter physics. In Sr_2RuO_4, the quasi-two-dimensional Fermi surface can be tuned through a Lifshitz transition—a change in its topology—with uniaxial pressure along the ⟨100⟩ direction. We investigated the influence of this electronic transition on the lattice by using a piezo-based uniaxial pressure cell to measure the stress-strain relation of Sr_2RuO_4 across the Lifshitz transition. We find a large and strongly temperature-dependent softening of the [100] Young's modulus at the Lifshitz transition. From thermodynamic arguments and comparison to a tight-binding model, we establish that the softening is indeed driven by conduction electrons.

TT 37.5 Wed 16:00 HSZ 201

Effect of superconductivity on the stress-strain relationships of Sr_2RuO_4 — •Kousuke Ishida[1], Hilary Noad[1], You-sheng Li[1], Veronika Stangier[2], Naoki Kikugawa[3], Dmitry Sokolov[1], Michael Nicklas[1], Markus Garst[2], Jörg Schmalian[2], Andrew Mackenzie[1,4], and Clifford Hicks[1,5] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]National Institute for Materials Science, Tsukuba, Japan — [4]University of St. Andrews, St. Andrews, United Kingdom — [5]University of Birmingham, Birmingham, United Kingdom

In the unconventional superconductor Sr_2RuO_4, applying uniaxial stress along a ⟨100⟩ crystalline direction induces a Lifshitz transition. Here we report on measurement of the stress-strain relationships across this transition down to temperatures below the superconducting transition. In the normal state, the Young's modulus softens by ≈ 10 % in the vicinity of the Lifshitz transition, indicating that this is a local maximum in the electronic free energy. We find that the onset of superconductivity causes a slight hardening of the lattice, though the electronic free energy remains a local maximum at the Lifshitz transition.

TT 37.6 Wed 16:15 HSZ 201

Effect of strain and momentum dependent spin-orbit coupling on the superconducting phase of Sr_2RuO_4 — •Jonas Hauck[1,2], Sophie Beck[1], Dante Kennes[2,3], Antoine Georges[1,4,5,6], and Olivier Gingras[1] — [1]Center for Computational Quantum Physics, Flatiron Institute, NY 10010, USA — [2]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52056 Aachen, Germany and JARA - Fundamentals of Future Information Technology — [3]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [4]Collège de France, 75005 Paris, France — [5]CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France — [6]DQMP, Université de Genève, CH-1211 Genève, Switzerland

The nature of Sr_2RuO_4's superconducting order parameter is a long-standing puzzle. First proposed to be a triplet superconductor, the current preferred picture is that of a degenerate singlet order parameter. The main driving force behind this development is the unification of experimental measurements and theoretical predictions. In this talk, we will employ a functional renormalization group approach to first-principles derived tight binding models to study the behavior of the leading order parameter under strain. Additionally, we examine the influence of momentum dependent spin-orbit coupling. Our results suggest the possible pairing candidates should be restricted to combinations of a d-wave pseudospin singlet with another order parameter whose critical temperature is not influenced by strain.

15 min. break

TT 37.7 Wed 16:45 HSZ 201

Gate-controlled superconductivity in Sr_2RuO_4 — •Priyana Puliyappara Babu[1], Roman Hartmann[1], Rosalba Fittipaldi[2], Antonio Vecchione[2], Elke Scheer[1], and Angelo Di Bernardo[1] — [1]University of Konstanz, 78457 Konstanz, Germany — [2]University of Salerno, I-84084 Fisciano, Italy

The electrical field effect was believed to be inapplicable for superconductors until 2018 when it was found that the supercurrent I_c in nanowires can be controlled by the application of strong enough voltages to gate electrodes, which has been interpreted as field effect. This discovery has great potential in the future to build hybrid superconductor/semiconductor architectures which might serve reducing the increasing energy demands of modern supercomputers. The majority of observations of such gate effects have been made for BCS superconductors like Ti, Va, Nb, Al etc. Here we report gate control of I_c in transistors made of Sr_2RuO_4 flakes. Sr_2RuO_4 is an unconventional superconductor found in 1994 which has been intensively studied to understand the nature of its superconducting order parameter. Single crystals of Sr_2RuO_4 were mechanically exfoliated to produce flakes which were then patterned into gated nanodevices using a gallium focused ion beam. Total suppression of I_c was observed for gate voltages V_G above 8.3 V. The V_G dependence of I_c at different temperatures and different fields were also investigated. We will also discuss the role of leakage currents between wire and gate and possibilities to further minimize them.

TT 37.8 Wed 17:00 HSZ 201

Non-local electrodynamics and field angle dependence of the superfluid density in Sr_2RuO_2 — •Javier Landaeta[1], Konstantin Semeniuk[1], Joost Aretz[1], Ismardo Bonalde[2], and Elena Hassinger[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Centro de Física, Instituto Venezolano de Investigaciones Científicas, Caracas 1020-A, Venezuela

Although being extensively studied for more than 25 years, the nature of the superconducting order parameter (SOP) of the weak type II superconductor Sr_2RuO_4 is still strongly debated. To get insight into the nodal structure of the SOP, we carried out a comprehensive study of the temperature dependence of the superfluid density n_s at various field orientations. By measuring the superconducting lower critical field $H_{c1}(T)$ in a spherical sample with ac-susceptibility, we obtained the temperature dependence of $n_s = H_{c1}(T)/H_{c1}(0)$ down to $0.03\,T_c$. Our results show that follows a low-temperature power law of T^2 up to $0.7T_c$ irrespective of the field angle. The observed behavior is in excellent agreement with what is expected of a type II superconductor with vertical nodes, with a strong influence of non-local electrodynamics. The discussed mechanisms are highly relevant for all weak type II superconductors.

TT 37.9 Wed 17:15 HSZ 201

Propagating charge carrier plasmon in Sr_2RuO_4 — Martin Knupfer[1], Fabian Jerzembeck[2], Naoki Kikugawa[3], Friedrich Roth[4], and •Jörg Fink[1] — [1]Leibniz Institute of Solid State an Materials Research, Dresden — [2]MPI for Chemical Physics of Solids, Dresden — [3]National Institute for Material Science, Tsukuba, Japan — [4]Institute of Exp. Physics, TU Bergakademie Freiberg

We report on studies of charge carrier plasmon excitations in Sr_2RuO_4 by transmission Electron Energy-Loss Spectroscopy. In particular, we present results on the plasmon dispersion and its width as a function of momentum transfer. The dispersion can be qualitatively explained in the framework of RPA calculations, using an unrenormalized tight-binding band structure. The constant long-wavelength width of the plasmon indicates, that it is caused by a decay into inter-band transition and not by quantum critical fluctuations. The results from these studies on a prototypical highly correlated metal system show that the long-wavelength plasmon excitations near 1 eV are caused by resilient quasiparticles and are not influenced by correlation effects.

TT 37.10 Wed 17:30 HSZ 201

Transport and structural characterisation of the metal to insulator transition in Ca_2RuO_4 nanoflakes — •Roman Hartmann[1], Anita Guarino[2], Rosalba Fittipaldi[2], Mario Cuoco[2], Elke Scheer[1], Antonio Vecchione[2], Gerardina Carbone[3], and Angelo di Bernardo[1] — [1]Department of Physics, Universität Konstanz, Konstanz, Germany — [2]CNR-Spin, Salerno, Italy — [3]Max IV Laboratory, Lund, Sweden

The Mott-insulator Ca_2RuO_4 (CRO) has attracted considerable attention due to its insulator to metal transition (IMT) with a transition temperature of 357 K (insulating below, metallic above) and the ability to trigger the IMT using pressure, current or an electric field of just 40 V/cm [1,2]. Unfortunately, stress from a structural transition (orthorombic to tetragonal) during the IMT with an increase in unit cell volume [1] generally breaks bulk crystals. To overcome this limitation we have developed a method to fabricate CRO nanoflakes (despite it not being a layered material) that we can contact using standard lithographic methods. In these nanoflakes we can reversibly trigger the IMT thousands of times by passing current without breaking the sample. The robustness of the devices also enabled us to perform spatially resolved nano-diffraction measurements showing the current-dependent local formation of the metallic phase, confirming the reversibility and giving first insights in the timescale of the IMT.

[1] F. Nakamura et al. Sci. Rep. 3, 2536 (2013)
[2] R. Okazaki et al., JPSJ 82, 103702 (2013)

TT 37.11 Wed 17:45 HSZ 201

Tuning van Hove singularities in strontium ruthenate with isovalent Barium doping — •Caitlin I O'Neil[1,2], Maximillian T Pelly[1,2], Ben Gade[1], Alexandra S Gibbs[1,3,4], and Andreas W Rost[1,2] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, UK — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]MPI for Solid State Research, Stuttgart, Germany — [4]ISIS Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, OX11 0QX, UK

Controlling a van Hove singularity (VHS) close the Fermi energy (E_F) of a compound allows control of the low temperature phases as shown for example in recent experiments in single layer ruthenates [1,2]. This study pursues a new direction of structural doping of $Sr_3Ru_2O_7$ by the substitution of barium onto the strontium site. Powder samples of $(Sr_{1-x}Ba_x)_3Ru_2O_7$ were synthesised from x=0.0 - 0.12. The samples were analysed with X-ray and neutron diffraction, magnetic susceptibility and heat capacity measurements. The unit cell volume changes linearly with doping with the primary structural change being an adjustment of the RuO_6 octahedral rotation mode magnitude. Using heat capacity we map the evolution of the VHS towards the E_F, crossing it at x=0.08. Intriguingly, heat capacity shows that the strength of the singularity is decreased, contrary to standard scenarios. In combination with DFT calculations we trace this back to the primary role of the rotation mode in controlling the VHS in ruthenates.

[1] Y.-S. Lie *et al.*, Nature **607**, 276 (2022)
[2] C. A. Marques *et al.*, Adv. Mater. **33**, e21005

TT 37.12 Wed 18:00 HSZ 201

Imaging of compass-like control of the electronic structure in $Sr_3Ru_2O_7$ — Masahiro Naritsuka[1], Izidor Benedičič[1], Luke Rhodes[1], Carolina Marques[1], Christopher Trainer[1], Zhiwei Li[2], Alexander Komarek[2], 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]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straβe 40, 01178 Dresden, Germany

Electronic nematicity results in a surprisingly strong symmetry-breaking reconstruction of electronic states without a significant lattice distortion. An enigmatic example of a nematic state is found in $Sr_3Ru_2O_7$, where a large resistivity anisotropy is stabilized by external magnetic field. The direction of the anisotropy can be controlled by the in-plane component of the magnetic field. Recently, STM measurements have revealed symmetry breaking of the electronic structure at the surface of $Sr_3Ru_2O_7$ even in zero magnetic field. Here, we use low-temperature scanning tunnelling microscopy to study the electronic structure in $Sr_3Ru_2O_7$ in vector magnetic fields. We find that the electronic structure is strongly affected even by relatively small external field when applied in the crystallographic a-b-plane, and is evolving continuously as a function of in-plane field direction. Our result establishes compass-like control over the electronic structure in the surface layer of $Sr_3Ru_2O_7$. We can rationalise the continuous evolution of the electronic structure with field direction through the interplay of magnetism and spin-orbit coupling.

TT 37.13 Wed 18:15 HSZ 201

Optical study of domains and domain walls in $Ca_3Ru_2O_7$ as a function of temperature and uniaxial pressure tuning — •Simli Mishra[1], Fei Sun[1], Elena Gati[1], Hilary Noad[1], Andrew P Mackenzie[1,2], and Veronika Sunko[1,3] — [1]Max Planck Institute, Chemical Physics of Solids, 01187, Dresden, Germany — [2]School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY16 9SS, UK — [3]Department of Physics, University of California, Berkeley, California, 94720, USA

Using optical methods to investigate a material is a powerful non-contact method to explore fundamental physics. In our experiment, we use optics as a versatile microscope to investigate birefringence as well as thermal transport with micron-scale spatial resolution. It can be combined with an in-situ controllable uniaxial pressure device, which has recently been shown to be a powerful tuning parameter to control lattice symmetries in quantum materials. In this contribution, we present the birefringence of an anisotropic material, $Ca_3Ru_2O_7$, which has structural domains at room temperature and can be tuned through a structural phase transition by lowering the temperature at ambient pressure. We will discuss the spatial evolution of its domains as a function of temperature and uniaxial pressure.

TT 38: Nonequilibrium Quantum Many-Body Systems II (joint session TT/DY)

Time: Wednesday 15:00–18:30 Location: HSZ 204

TT 38.1 Wed 15:00 HSZ 204

Hilbert space fragmentation in open quantum systems — •Yahui Li, Pablo Sala, and Frank Pollmann — Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Several mechanisms have been identified that can lead to a breakdown of thermalization in closed quantum systems-including integrability and many-body localization. Recently, a novel mechanism for ergodicity breaking has been discovered in systems with certain dynamical constraints, where the Hilbert space fragments into exponentially many disconnected subspaces. An open question is how such systems evolve when they are coupled to a dissipative bath.

We find that the Hilbert space fragmentation can be utilized to preserve coherence in the presence of dissipation. We study a quantum fragmented model, which fragments in an entangled basis due to unconventional non-Abelian symmetries. We investigate the Lindblad dynamics under two different couplings, which either preserves or destroys the quantum fragmentation structure. At sufficiently large couplings, the operator space entanglement is suppressed, which allows for an efficient numerical simulation using tensor networks. Surprisingly, under the structure-preserving noise, we observe finite Renyi negativity, indicating non-vanishing quantum correlations. Using an analytic approach, we derive the stationary states under both couplings, which explains the long-time behaviors observed in numerical simulations.

TT 38.2 Wed 15:15 HSZ 204

Hilbert space fragmentation and interaction-induced localization in the extended Fermi-Hubbard model — •Philipp Frey, Lucas Hackl, and Stephan Rachel — University of Melbourne

We study Hilbert space fragmentation in the extended Fermi-Hubbard model with nearest and next-nearest neighbor interactions. Using a generalized spin/mover picture and saddle point methods, we derive lower bounds for the scaling of the number of frozen states and for the size of the largest block preserved under the dynamics. We find fragmentation for strong nearest and next-nearest neighbor repulsions as well as for the combined case. Our results suggest that the involvement of next-nearest neighbor repulsions leads to an increased tendency for localization. We then model the dynamics for larger systems using Markov simulations to test these findings and unveil in which interaction regimes the dynamics becomes spatially localized. In particular, we show that for strong nearest and next-nearest neighbor interactions random initial states will localize provided that the density of initial movers is sufficiently low.

[1] arXiv:2209.11777 (accepted for publication in PRB Letter)

TT 38.3 Wed 15:30 HSZ 204

Rate functions and the approach to adiabaticity in quantum many body systems — •Vibhu Mishra, Salvatore Manmana, and Stefan Kehrein — Institute for Theoretical Physics, Georg-August-Universität Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen

The quantum adiabatic theorem is a fundamental result in quantum mechanics with applications ranging from quantum adiabatic computation to topological systems, while also serving as a theoretical foundation to many body perturbation theory via the Gell-Mann Low theorem.

We establish an inherent competition between ramp times T for an adiabatic process vs the system size N, in the behavior of relevant many body overlaps. We study this interplay between T and N by analyzing the properties of rate functions which are defined to be intensive quantities that give us a quantitative measure of the deviation from adiabaticity in the thermodynamic limit.

We analyze the Transverse Field Ising Model and the XXZ chain in $1D$ using exact diagonalization. We find that the rate functions show algebraic decay with increasing ramp time T. The decay exponent of the rate function for ramps within the gapped phase is 2, for ramps across Ising critical point it is 0.5 and within the Luttinger Liquid phase it is 1. The immediate implication is that the many body adiabatic time scales grow unavoidably with system size, namely as the $\sqrt{N}$ for ramps within the gapped phase, and with N within the Luttinger Liquid phase.

TT 38.4 Wed 15:45 HSZ 204

Classical route to ergodicity and scarring phenomena in a two-component Bose-Josephson junction — Debabrata Mondal[1], Sudip Sinha[1], •Sayak Ray[2], Johann Kroha[2], and Subhasis Sinha[1] — [1]Indian Institute of Science Education and Research Kolkata, Mohanpur, Nadia 741246, India — [2]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115 Bonn, Germany

We consider a Bose-Josephson junction (BJJ) formed by the binary mixture of ultracold atoms to investigate the manifestation of coherent collective dynamics on ergodicity and quantum scars, unfolding the connection between them. By tuning the inter and intra-species interaction, we demonstrate a rich variety of Josephson dynamics and transitions between them, which plays a crucial role in controlling the overall ergodic behaviour. The signature of underlying classicality is revealed from the entanglement spectrum, which also elucidates the formation of quantum scars of unstable steady states and of periodic orbits leading to athermal behaviour in a reduced Hilbert space. We show how the degree of ergodicity across the energy band and the scarring phenomena can be probed from the auto-correlation function as well from the phase fluctuation of the condensates, which has relevance in cold atom experiments. The model can also be realized in spin systems with application to information processing and lattice-gauge simulation.

[1] D. Mondal, S. Sinha, S. Ray, J. Kroha, and S. Sinha, Phys. Rev. A **106**, 043321 (2022)

TT 38.5 Wed 16:00 HSZ 204

Ultrafast dynamics of cold Fermi gas after a local quench — Nikolay Gnezdilov[1], •Andrei Pavlov[2,3], Vladimir Ohanesjan[4], Yevheniia Cheipesh[4], and Koenraad Schalm[4] — [1]Department of Physics, University of Florida, Gainesville, USA — [2]The Abdus Salam International Centre for Theoretical Physics (ICTP) Strada Costiera 11, Trieste, Italy — [3]Institut für QuantenMaterialien und Technologien, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, Eggenstein-Leopoldshafen, Germany — [4]Instituut-Lorentz, Universiteit Leiden, Leiden, The Netherlands

We consider energy dynamics of two initially independent reservoirs A and B filled with a cold Fermi gas coupled and decoupled by two quantum quenches following one another. The energy change in the system adds up the heat transferred between A and B and the work done by the quench to uncouple the reservoirs. In case when A and B interact for a short time, we find an energy increase in both reservoirs upon decoupling. This energy gain results from the quenches' work and does not depend on the initial temperature imbalance between the reservoirs. We relate the quenches' work to the mutual correlations of A and B expressed through their von Neumann entropies. Utilizing this relation, we show that once A and B become coupled, their von Neumann entropies grow (on a timescale of the Fermi time) faster than thermal transport within the system. For a metallic setup, this implies the characteristic timescale of correlations' growth to be in the femtosecond range, while for the ultracold atoms, we expect it to be in the millisecond range.

TT 38.6 Wed 16:15 HSZ 204

A conjecture regarding the overlap of different ground states within the same phase — •Sarah Damerow and Stefan Kehrein — Georg-August Universität Göttingen

An extension of the adiabatic theorem to quantum quenches, i.e. non-adiabatic changes, is presented. Using exact diagonalisation, we numerically study the Transverse Field Ising Model (TFIM) and the Axial Next Nearest Neighbour Ising Model (ANNNI). We numerically test the following conjecture: Within the same phase, the overlap between the initial ground state and the ground state of the quenched Hamiltonian is the largest possible eigenstate overlap. In the TFIM, this conjecture is confirmed for both the paramagnetic (PM) and the ferromagnetic (FM) phases. In the ANNNI model results are ambiguous in some phases, due to both numerical errors and finite size effects.

15 min. break

TT 38.7 Wed 16:45 HSZ 204

Charge, spin, and heat shot noises in the absence of average currents — •Ludovico Tesser, Matteo Acciai, Christian Spånslätt, Juliette Monsel, and Janine Splettstoesser — Chalmers University of Technology, Gothenburg, Sweden

Shot noise in electronic conductors occurs when the system is brought out of equilibrium, e.g., by a stationary bias. However, nonequilibrium does not imply that an average current flows. Indeed, the situation where selected currents are suppressed is of interest in fields like thermoelectrics and spintronics, raising the question of how the related noises behave.

I will present results on zero-current charge, spin, and heat noises in two-terminal mesoscopic conductors induced by voltage, spin and temperature biases. The nonequilibrium shot noises can be arbitrarily large, even if the respective average currents vanish. However, as soon as a temperature bias is present, additional equilibrium (thermal-like) noise necessarily occurs. This equilibrium noise sets an upper bound on the zero-current nonequilibrium charge and spin shot noise [1,2]. We have shown that the bound on the charge noise for strictly two-terminal conductors even extends into the finite-frequency regime. By contrast, these bounds can be overcome for heat transport by breaking the spin and electron-hole symmetries, respectively.

[1] J. Eriksson, M. Acciai, L. Tesser, J. Splettstoesser, Phys. Rev. Lett. 127, 136801 (2021)
[2] L. Tesser, M. Acciai, C. Spånslätt, J. Monsel, J. Splettstoesser, arXiv:2210.06051 [cond-mat.mes-hall] (2022)

TT 38.8 Wed 17:00 HSZ 204

Maximally chaotic to Fermi liquid crossover in a generalized SYK model — •Nick von Selzam and Stefan Kehrein — Institute for Theoretical Physics, University of Göttingen, Germany

We consider a generalized Sachdev-Ye-Kitaev (SYK) model: Majorana fermions on $\mathcal{N}$ sites with random $\frac{q}{2}$-body all to all interactions plus a kinetic energy term.

The SYK model can be seen as a toy model for quantum chaos and does not allow for a quasiparticle description. We discuss the continuous crossover between the Fermi liquid regime, dominated by the kinetic term, and the maximally chaotic regime, dominated by the SYK interaction, by studying the quantum Lyapunov exponents.

For fixed interaction strength there exists a crossover temperature for which the Lyapunov exponent becomes maximal. For lower temperatures the Lyapunov exponent is exponentially small. For larger temperatures the behaviour is close to indistinguishable from the pure SYK term.

TT 38.9 Wed 17:15 HSZ 204

Vibrationally-coupled electron transport in a quantum shuttle: A study using the hierarchical equations of motion approach — •Salvatore Gatto, Christoph Kaspar, and Michael Thoss — Institute of Physics, Albert-Ludwigs-Universität Freiburg

A quantum shuttle is an archetypical nanoelectromechanical device, in which the coupling of electronic and mechanical degrees of freedom is crucial [1]. In this contribution, we investigate transport properties of quantum shuttles, with a particular focus to the so-called shuttling regime, in which the transport of electrons is synchronized with the mechanical motion. The transport characteristics are strongly influenced by the interplay of electronic and vibrational degrees of freedom, which manifests itself in step structures of the current-voltage characteristics. An effective molecule-lead coupling results in an increase of the current with respect to the tunneling regime. The study uses the hierarchical equations of motion approach, which allows a numerically exact simulation of nonequilibrium transport in general open quantum systems involving multiple bosonic and fermionic environments [2].

[1] Novotný et al., Phys. Rev. Lett. 92, 248302 (2004)
[2] J. Bätge, Y. Ke, C. Kaspar, and M. Thoss, Phys. Rev. B 103, 235413 (2021)

TT 38.10 Wed 17:30 HSZ 204

Effective form factors for finite temperature correlation functions — •Oleksandr Gamayun — University of Warsaw, ul. Pasteura 5, 02-093 Warsaw, Poland

The behavior of dynamical correlation functions in one-dimensional quantum systems at zero temperature is now very well understood in terms of linear and non-linear Luttinger models. The "microscopic" justification of these models consists in exactly accounting for the soft-mode excitations around the vacuum state and at most few high-energy excitations. At finite temperature, or more generically for finite entropy states, this direct approach is not strictly applicable due to the different structure of soft excitations. To address these issues we study the asymptotic behavior of correlation functions in one-dimensional free fermion models. On the one hand, we obtain exact answers in terms of Fredholm determinants. On the other hand, based on "microscopic" resummations, we develop a phenomenological approach that introduces the effective form factors and reduces the problem to the zero temperature case. The information about the initial state is transferred into the scattering phase of the effective fermions. I will demonstrate how this works for correlation functions in the XY model, mobile impurity, and the sine-kernel Fredholm determinants.

TT 38.11 Wed 17:45 HSZ 204

Transfer-matrix summation of path integrals for transport through nanostructures — Simon Mundinar, •Alexander Hahn, Jürgen König, and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

On the basis of the method of iterative summation of path integrals (ISPI), we develop a numerically exact transfer-matrix method to describe the nonequilibrium properties of interacting quantum-dot systems. For this, we map the ISPI scheme to a transfer-matrix approach [1], which is more accessible to physical interpretation, allows for a more transparent formulation of the theory, and substantially improves the efficiency. In particular, the stationary limit is directly implemented, without the need of extrapolation. The resulting new method, referred to as "Transfer-matrix Summation of Path Integrals" (TraSPI), is then applied to resonant electronic transport through a single-level quantum dot [2].

[1] S. Mundinar, P. Stegmann, J. König, and S. Weiss, Phys. Rev. B **99**, 195457 (2019)
[2] S. Mundinar, A. Hahn, J. König, and A. Hucht, Phys. Rev. B **106**, 165427 (2022)

TT 38.12 Wed 18:00 HSZ 204

Quasi-particle excitations at Mott-metal interfaces — •Jan Verlage[1], Friedemann Queisser[2,3], Peter Kratzer[1], and Ralf Schützhold[2,3] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Institut für Theoretische Physik, Helmholtz-Zentrum Dresden-Rossendorf — [3]Institut für Theoretische Physik, Technische Universität Dresden

We investigate excitations at the interface between a metallic bulk and a strongly correlated Mott insulator. Employing a hierarchy of correlations we identify effective quasi-particle and hole excitations in the heterostructure. To leading order in the hierarchy, the modes satisfy an effective two-component evolution equation. This allows the investigation of evanescent modes at the interface and tunneling through a Mott insulating layer.

The project is funded by the DFG, grant # 278162697 (CRC 1242).

TT 38.13 Wed 18:15 HSZ 204

Configuration interaction based nonequilibrium steady state impurity solver — •Daniel Werner, Jan Lotze, and Enrico Arrigoni — ITPCP, Graz, Austria

We present a solver for correlated impurity problems out of equilibrium based on a combination of the so-called auxiliary master equation approach (AMEA) and the configuration interaction (CI) expansion. Within AMEA one maps the original impurity model onto an auxiliary open quantum system with a restricted number of bath sites which can be addressed by numerical many-body approaches such as ED or MPS. While the mapping becomes exponentially more accurate with increasing number of bath sites, ED implementations are severely limited due to the fast increase of the Hilbert space dimension for open systems, and the MPS solver typically requires rather long runtimes. Here, we propose to adopt a CI approach to solve numerically the correlated auxiliary open quantum system. This allows access to a larger number of bath sites at lower computational costs than for ED. We benchmark the approach with NRG results in equilibrium and with MPS out of equilibrium. We evaluate the current, the conductance as well as the Kondo peak and its splitting. We obtain a rather accurate scaling of the conductance as a function of the bias voltage and temperature rescaled by TK for moderate to strong interactions in a wide range of parameters. The approach combines the fast runtime of ED with an accuracy close to the one achieved by MPS making it an attractive solver for nonequilibrium DMFT. (arXiv: 2210.09623)

TT 39: Superconducting Electronics

Time: Wednesday 15:00–18:15 Location: HSZ 304

Invited Talk TT 39.1 Wed 15:00 HSZ 304

Sensing and control of MHz photons with microwave photon-pressure — Ines C. Rodrigues[1,2], Gary A. Steele[1], and •Daniel Bothner[1,3] — [1]Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands — [2]Department of Physics, ETH Zürich, Switzerland — [3]Physikalisches Institut, Center for Quantum Science (CQ) and LISA+, Universität Tübingen, Germany

Superconducting microwave circuits have emerged as one of the leading platforms for quantum information science and quantum sensing in the recent decade. In 2018, a new type of interaction between a superconducting microwave circuit and a low frequency (LF) circuit has been realized, so called photon-pressure coupling, which is the all-circuit analogue of the radiation-pressure interaction between a mechanical oscillator and an optical cavity in optomechanics. Since 2020, several milestone experiments with photon-pressure circuits have been reported, such as the interferometric thermometry of an LF circuit, the observation of parametric strong-coupling or sideband-cooling of an LF mode into its quantum groundstate. Quite recently, we have realized a series of experiments in these circuits, for which we add a strong parametric drive to the Kerr-nonlinear high-frequency mode. This approach allows for parametrically enhanced interaction strengths, for the observation of nonreciprocal heat flow and for the implementation of photon-pressure with a "negative mass" microwave mode that inverts dynamical backaction and sideband-cooling effects. In our presentation, we will give an overview of photon-pressure circuits, discuss the most recent developments and possible future directions.

TT 39.2 Wed 15:30 HSZ 304

Waveguide quantum electrodynamics in high impedance networks — •Miriam Resch[1], Ciprian Padurariu[1], Björn Kubala[1,2], Frank Grossmann[3], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, Dresden, Germany

The emerging field of high impedance quantum circuits aims to exploit the extraordinary properties of high kinetic inductance materials, such as granular superconductors. The low propagation speed of electromagnetic excitations in such devices enables to strongly couple various types of qubits or resonators and waveguides. Theoretical description of such strongly coupled systems is challenging as the localized modes of the sub-unit couple to many waveguide modes simultaneously so that many common approximation schemes break down. Furthermore for a more realistic description of the system, Kerr nonlinearities are included in the model of the granular superconductor. To tackle this challenging regime in a numerically efficient way, we use the multi Davydov-Ansatz [1], where the wave function of the full system is described by a superposition of coherent states. As a first step we investigate how Kerr nonlinearities modify properties of qubit decay or readout, with the ultimate goal of identifying strong-coupling signatures in those observables, which are accessible to our experimental collaborators.

[1] M. Werther and F. Großmann, Phys. Rev. B **101**, 174315 (2020).

TT 39.3 Wed 15:45 HSZ 304

High-impedance resonators based on granular aluminum — •Mahya Khorramshahi, Martin Spiecker, Patrick Paluch, Nicolas Zapata, Ritika Dhundhwal, Ioan M. Pop, and Thomas Reisinger — Karlsruhe Institute of Technology, Germany

Superconductors with characteristic impedance larger than the resistance quantum are a valuable resource in superconducting circuits. They enable the design of protected qubits such as Fluxoniums or 0-pi qubits and can improve the coupling to small-dipole-moment objects, which may be useful for interfacing to spin-qubits, donor spins, etc. Here we present compact resonators in the lower GHz regime with a high characteristic impedance given by a high-kinetic-inductance material, namely granular aluminum, with spurious modes above 10GHz. We fabricated the resonators with an electron-beam lithography lift-off process, and we coupled them using a 50 Ohm coplanar waveguide architecture. Measurements performed in a dilution cryostat reveal that the resonators maintain high-quality factors in the single photon regime, a valuable resource for future quantum hardware implementations.

TT 39.4 Wed 16:00 HSZ 304

Surface acoustic wave resonators on thin film piezoelectric substrates for quantum acoustics — •Thomas Luschmann[1,2,3], Alexander Jung[1,2], Stephan Geprägs[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Technische Universität München, TUM School of Natural Sciences, Physics Department, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Lithium Niobate (LNO) is a well established material for Surface Acoustic Wave (SAW) devices including resonators, delay lines and filters. Recently, multi-layer substrates based on LNO thin films have become commercially available. Here, we present a systematic study of the performance of SAW devices fabricated on LNO-on-Insulator (LNOI) and LNO-on-Silicon substrates and compare them to bulk LNO devices. Our study aims at applications of these substrates for quantum acoustics, i.e. the integration with superconducting circuits operating in the quantum regime. To this end, we design SAW resonators with a target frequency of 5 GHz and perform our experiments at millikelvin temperatures and microwave power levels corresponding to single photons or phonons. We investigate the device quality factors as a function of the excitation power and temperature and model the observed losses by the coupling of the resonator to a bath of two-level-systems (TLS). Our results suggest that SAW devices on thin film LNO on Silicon have sufficient performance to be used in future SAW based quantum acoustic devices.

TT 39.5 Wed 16:15 HSZ 304

Towards hybrid quantum systems coupling superconducting qubits to cold atoms — •Benedikt Wilde, Nicolas Albenge, Manuel Kaiser, Conny Glaser, Malte Reinschmidt, Andreas Günther, József Fortágh, Dieter Koelle, Reinhold Kleiner, and Daniel Bothner — Physikalisches Institut, Center for Quantum Science (CQ) and LISA+, Universität Tübingen

Coupling superconducting quantum circuits to ultracold atom clouds promises the possibility of exploiting the advantages of both systems, enabling new advances in both fundamental research and potential technological applications. One can realize such a hybrid quantum system by using a superconducting microwave resonator that is simultaneously coupled to both sub-systems. While coupling superconducting resonators to superconducting qubits is state-of-the-art, several challenges arise when trying to couple cold atoms to the integrated circuit. These challenges include achieving the required microwave field homogeneity, engineering a sufficiently large interaction strength and keeping a high resonator quality factor despite environmental factors suitable to deteriorate the performance of superconducting circtuits, such as laser beams or magnetic atom traps. We present our recent developments and advances, discussing design considerations, simulations and intermediate results.

15 min. break

TT 39.6 Wed 16:45 HSZ 304

Parameter spread in Josephson traveling-wave parametric amplifiers: Vulnerabilities and tolerances — •Christoph Kissling, Victor Gaydamachenko, Fabian Kaap, Marat Khabipov, Ralf Dolata, Alexander B. Zorin, and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Josephson traveling-wave parametric amplifiers (JTWPAs) hold great promise for wideband amplification of few-photon-level signals at microwave frequencies. These devices typically consist of thousands of nominally identical circuit elements, which are subject to fabrication variations. We analyse the effect of circuit parameter variation on the performance of a JTWPA using transient circuit simulations. Using this tool, we analyze two dispersion engineering concepts, resonant phase matching and periodic capacitance modulation, and compare their parameter spread tolerances. We identify circuit elements, which are critical concerning parameter spread, and explore ways to mitigate the impact of spread. Furthermore, we present the status of our practical implementation of rf-SQUID based JTWPAs and show experimental results.

TT 39.7 Wed 17:00 HSZ 304

Fabrication of low-loss Josephson parametric circuits — •Kedar E. Honasoge[1,2], Yuki Nojiri[1,2], Daniil E. Bazulin[1,2], Leon Koch[1,2], Thomas Luschmann[1,2], Niklas Bruckmoser[1,2], Maria-Teresa Handschuh[1], Florian Fesquet[1,2], Michael Renger[1,2], Fabian Kronowetter[1,2,4], Achim Marx[1], Rudolf Gross[1,2,3], and Kirill G. Fedorov[1,2] — [1]Walther-Meißner-Institut, 85748 Garching, Germany — [2]Physik- Department, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 München, Germany — [4]Rohde & Schwarz GmbH, 81671 München, Germany

The emergence of quantum information processing with superconducting circuits has stimulated the development of various interest in Josephson parametric devices. The latter offer a wide range of applications ranging from quantum-limited amplification to the generation of entangled squeezed states of light. We fabricate low-loss devices by employing careful cleaning steps during the fabrication of the superconducting circuits. Upon optimization, we fabricate Josephson parametric devices with internal quality factors in excess of 10^5. We characterize bandwidth, gain, noise, dynamic range, and other properties of the realized devices. Based on these investigations, we derive useful criteria for the development of more intricate devices incorporating Josephson parametric circuits.

TT 39.8 Wed 17:15 HSZ 304

Nb SQUIDs patterned by He and Ne focused ion beams — •Simon Koch[1], Timur Griener[1], Simon Pfander[1], Julian Linek[1], Thomas Weimann[2], Reinhold Kleiner[1], Oliver Kieler[2], and Dieter Koelle[1] — [1]Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany — [2]Department Quantum Electronics, Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

Nanopatterning of superconducting thin film structures with focused He or Ne ion beams (He/Ne-FIB) offers a flexible tool for creating constriction-type Josephson junctions (cJJs) which can be integrated into strongly miniaturized superconducting quantum interference devices (nanoSQUIDs) for magnetic sensing on the nanoscale. We present our attempts to use He/Ne-FIB for fabricating Nb cJJs and nanoSQUIDs which shall provide ultra-low noise and high spatial resolution for their application in scanning SQUID microscopy (SSM). Moreover, we address the possibility to implement multiterminal, multi-JJ SQUIDs that provide flexibility in SQUID readout. The nanoSQUIDs are designed as sensors for magnetic flux and dissipation. They shall be integrated on custom-made Si cantilevers, which will provide the possibility of simultaneous conventional topographic imaging by atomic force microscopy (AFM). We will discuss the status of this project and challenges that have to be met on the way to combine SSM and AFM on the nanoscale.

We acknowledge the European Commission under H2020 FET Open grant FIBsuperProbes (number 892427).

TT 39.9 Wed 17:30 HSZ 304

Synchronization in Josephson photonics devices in the presence of shot noise — Florian Höhe[1], Ciprian Padurariu[1], Brecht Donvil[1], Lukas Danner[1,2], Joachim Ankerhold[1], and •Björn Kubala[1,2] — [1]ICQ and IQST, Ulm University, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany

For many quantum sources the exploitation and characterization of their quantum properties, such as entanglement and squeezing, is hampered by phase instability. Josephson photonics devices, where microwave radiation is created by inelastic Cooper pair tunneling across a *dc-biased* Josephson junction in-series with a microwave resonator are particularly vulnerable lacking the reference phase provided by an ac-drive. To counter this issue, sophisticated measurement schemes have been used in [1] to prove entanglement, while in [2] a weak ac-signal was put in to lock phase and frequency of the emission. Intrinsic shot noise of the Josephson-photonics device inevitably diffuses the oscillators phase and requires an extension of classical synchronization theories to the quantum regime.

Performing multi-time scale perturbation theory we derive an effective Fokker-Plank equation for the phase to analyze quantum locking and synchronization in an Adler-type equation. Injection locking and synchronization lead to a narrowing of the photon emission statistics, while the shot noise induces phase slips.

[1] A. Peugeot et al., Phys. Rev. X 11, 031008 (2021).
[2] M. C. Cassidy et al., Science 355, 939 (2017).

TT 39.10 Wed 17:45 HSZ 304

Mitigating losses in NbTiN superconducting circuits under magnetic fields. — •Arne Bahr, Matteo Boselli, Benjamin Huard, and Audrey Bienfait — Laboratoire de Physique - École normale supérieure de Lyon, France

Quantum superconducting circuits enable quantum information processing as well as quantum sensing at microwave frequencies. One predominant factor limiting their performance is the presence of impurities creating microwave losses, triggering intense research effort for their identification and mitigation[1]. Here we probe these impurities in the context of using superconducting circuits under magnetic fields, which has application for coupling to other spin systems[2] and also detecting electron spin resonance (ESR) at the few spin levels[3].

We report continuous wave ESR measurements on spin impurities in resonators fabricated in NbTiN on a sapphire substrate. A simple etch through a resist layer process results in the presence of many spin impurities, preventing any ESR measurement near the spin 1/2 line. Following the characterization and identification of these spin signals, we improve our fabrication process to remove these spurious spin signals so that the resonators exhibit internal quality factors above $5 \cdot 10^5$ that remain constant up to 350 mT.

[1] N. P. de Leon et al., Science (2021)
[2] A. J. Landig et al., Nat. Com. (2019)
[3]V. Ranjan et al., Appl. Phys. Lett. (2020)

TT 39.11 Wed 18:00 HSZ 304

Pressure drop measurements and flow simulations of different regenerator fillings in a single stage GM-type pulse tube cryocooler — •Bernd Schmidt[1,2], Elias Eisenschmidt[1,3], Jack-André Schmidt[1,2], Jens Falter[1], Hardy Weisweiler[3], and André Schirmeisen[1,2] — [1]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [2]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany — [3]Technische Hochschule Mittelhessen, Friedberg, Germany

Although pulse tube cryocoolers (PTCs) reaching liquid Helium temperature were already presented in the 1990s[1], they are still subject to vivid development in many directions. Much of this development is done with the help of simulations and empirical values. A crucial part of a PTC is the regenerator, which is usually filled with multiple layers of porous materials with high heat capacity. These porous materials come in different shapes, mainly packed spheres and wire meshes.

In this talk we present measurements and simulations of pressure drop and gas flow through different regenerator fillings. We show the differences between the different kinds of fillings from the fluid mechanics point of view.

[1] C. Wang et al., Cryogenics, 37, 159 (1997)

TT 40: Focus Session: Wissenschaftskommunikation / Outreach (joint session HL/O/TT)

Im wissenschaftlichen Umfeld wird Maßnahmen der Öffentlichkeitsarbeit eine zunehmend größere Bedeutung zugemessen, - aus der Gesellschaft heraus und auch durch die großen Fördereinrichtungen und die DPG. Dabei geht es nicht nur um die Ergebnisse der Forschung, sondern auch darum, Prozesse und Methoden von wissenschaftlicher Arbeit transparent abzubilden – eine Aufgabe, die prinzipiell alle Forschenden übernehmen können. In diesem Symposium sollen erfolgreiche Projekte der Wissenschaftskommunikation, insbesondere aus dem Bereich der Festkörperphysik, vorgestellt werden. In ihrer Gesamtheit sollen sie das Spektrum der Wissenschaftskommunikation hinsichtlich des finanziellen und zeitlichen Aufwands aufzeigen und Methoden für unterschiedliche Zielgruppen vorstellen.

So dient diese Session sowohl als Ideengeber und Inspiration als auch als eine Art Netzwerk-Treffen zum Austausch über die Wissenschaftskommunikation in unterschiedlichen Kontexten.

Time: Wednesday 15:00–18:30 Location: POT 81

Invited Talk TT 40.1 Wed 15:00 POT 81

experimentamus! Forschendes Lernen von Physik und Chemie in der Grundschule — •Sebastian Schlücker — Universität Duisburg-Essen, Campus Essen

Der Sachunterricht in der Primarstufe ist ein Konglomerat aus allen Natur- und Gesellschaftswissenschaften, erst in der Sekundarstufe findet eine Aufspaltung in die einzelnen Fächer statt. Zudem unterrichten viele Grundschul-Lehrkräfte fachfremd. Auch der Zeitaufwand für die Vorbereitung von Experimenten ist nicht unerheblich. Wie also kann man trotz dieser Hürden kindgerechte physikalische und chemische Experimente bereits in der Grundschule einführen?

Ich berichte aus 10 Jahren Erfahrung mit dem Projekt experimentamus!. Dabei handelt es sich um einen Kanon aus ca. 40 Experimenten für die Klassen 2 bis 4, welcher die Themen Licht, Wärme, Magnetismus, Wasser, Luft, Feuer und Elektrizität mit einem kindgerechten Alltagsbezug abdeckt. Anstelle des darlegenden Lernens wird auf das Forschende Lernen gesetzt: Frage - Hypothese - Experiment - Beobachtung - Erklärung; diese fünf Stationen des wissenschaftlichen Erkenntnisprozesses werden immer wieder durchlaufen. Ganz im Sinne Martin Wagenscheins wird dabei nach der exemplarischen und sokratischen Methode vorgegangen. Die praktische Implementierung umfasst 1. Materialkisten für alle Themen, 2. kompakte und leicht verständliche Informationshefter für die Lehrkräfte, sowie 3. Lernheftchen für alle SuS. Am Ende möchte ich über Erfahrungen und Herausforderungen im Rahmen dieses Projektes berichten und Ideen für eine mögliche weitere Verbreitung vorstellen.

TT 40.2 Wed 15:30 POT 81

Internal interfaces - goals and realisation of a scientific image film — •Ulrich Höfer[1,2] and Michael Dürr[2,3] — [1]Fachbereich Physik, Philipps-Universität Marburg — [2]SFB 1083, www.internal-interfaces.de — [3]Institut für Angewandte Physik, Justus-Liebig-Universität Giessen, Germany

Funded by the German Science Foundation (DFG), a professional film maker has produced an image film about the research conducted in the Collaborative Research Center SFB 1083 "Structure and Dynamics of Internal Interfaces". The six-minute video clip takes the non-specialist on a journey down to atomic scale to show the progress at the forefront of research at solid/solid interfaces. It is not a demanding educational film. Rather, it is a visually stunning piece that looks like science fiction taken straight out of a movie, with tracking shots that take the viewer down to the nanometer scale, with flights through luminous molecules, exotic excitons, and space-filling laser labs. The film also has a very impressive soundtrack. Gustav Holst's (1874-1934) composition "The Planets" was re-orchestrated especially for this film. It is available on the youtube channel of the DFG (https://www.youtube.com/watch?v=_-mDt0NzHrc). Visitors of Chemikum Marburg can watch the German version on a 4K OLED screen, a device actually based on microscopic processes at interfaces investigated by SFB 1083.

The idea behind the creation of a professional film, its conceptional design and the necessary steps towards its realization will be outlined.

TT 40.3 Wed 15:45 POT 81

Outreach activities of SFB 1083 @ Chemikum Marburg — •Christof Wegscheid-Gerlach, Luise Cleres, Ina Budde, Karl-Heinz Muth, and Marion Enssle — Chemikum Marburg / SFB1083

The diffusion of concepts, methods, and visions of the SFB 1083 on Structure and Dynamics of Internal Interfaces into the general public is our general goal. To this end project Ö makes use of the institution Chemikum Marburg e.V., whose basic idea is to fascinate the public excited about natural sciences. The experiments offered here, stand for chemical, biological, pharmaceutical, and physical subjects related with daily phenomena or beyond. We will give an overview about the introduction of basic ideas and methods of SFB 1083 to the public as well as the institution Chemikum Marburg. The contents of the individual offers, such as experiments within the regular workspace, the workshops for the Girls' Day and the compilation of special workshops that are offered to give high-school students an understanding of the research content of the SFB 1083 are presented. An additional topic is the linking of basic research to applications for regenerative energy resources. Hydrogen fuel cells are well-known to the general public and rely on functional internal interfaces. An additional workshop which was prepared in cooperation with the district Marburg-Biedenkopf gives an overview about production, storage, and application of hydrogen as a new energy resource. We will also share various occasions at Chemikum Marburg where further outreach activities represent SFB 1083.

Invited Talk TT 40.4 Wed 16:00 POT 81

Under the Microscope – spotlighting materials and nano science — •Svenja Lohmann and Pranoti Kshirsagar — The Science Talk, Germany

Real Scientists Nano is a science communication project dedicated to materials and nano science. Despite the widespread relevance of materials science to everyday life, we feel that dedicated science communication in this area is much rarer than in other fields. Our aim is to provide a platform for active materials and nano scientists to directly communicate their science and life as a scientist to the public. The use of social media thereby provides a very low threshold to science communication as basically the only requirement is to have an account. We have the goal to showcase the scientific community in all its diversity, and so far (12/2022) had guest scientists from more than 30 countries of origin as well as various fields and career stages. The two main pillars of the Real Scientists Nano project are the @RealSci_Nano Twitter account and the Under the Microscope podcast. Our guest scientists are interviewed for one podcast episode, and subsequently get to tweet from the account for one week following the rotation curation concept. We let curating scientist decide for themselves what they would like to tweet about. The form and content therefore vary greatly. Many of our scientists report from their everyday life, and are for example livetweeting from a conference, uploading videos or photos from the lab or sending the occasional "stuck in meetings, will return later" tweet. Science communication on social media thus gives the opportunity to open a direct and real-time window into the scientist's life.

30 min. break

Invited Talk TT 40.5 Wed 17:00 POT 81

Phyphox – A pocketful of physics — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Most smartphones are used to make phone calls, to write short messages, surf the Internet or check e-mails. However, they can do much more: With the help of the integrated sensors and the free app "phyphox" (abbreviation for Physical Phone Experiments), pupils, students, and teachers and interested others can independently perform and develop physics experiments. For example, the app can use the accelerometer to record pendulum movements and determine the rotational acceleration in a salad spinner, or the air pressure sensor to determine time-resolved differences in altitude and thus the speed of an elevator. The didactic potential of the app is great, as the students are picked up on ground that is very familiar and attractive to them (smartphones) and are introduced to experimental natural sciences in a playful way and with an extremely low barrier (zero cost, i.e. only one click away). The app helps to get students excited about scientific and technical questions and contexts at an early age. The app is available free of charge for Android and iOS (more information can be found at www.phyphox.org). In my presentation, I will go into the concept of phyphox, introduce the range of functions and show a number of application examples.

TT 40.6 Wed 17:30 POT 81

Chair PR representative as a doctoral student's secondary task: A field report — •Paula M. Weber, Felix Friedrich, and Manuel Seitz — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Especially in recent years, it has become more important to communicate one's scientific work and methods to the public in order to show that in the scientific world, knowledge can only be created through research and the scientific process. Yet, extra time besides research is often limited and it is thus difficult to get into science communication. In this talk, I would like to present how PhD students can use their interest in science communication to benefit their own research group as a part-time PR representative.

In the first part of my talk, I will report on our efforts to attract new bachelor and master students. This advertising is focused on an audience with a scientific background, such that lab tours and advertising posters may contain scientific language and references. The second part is about communication with the general public, who usually know physics from their school days. Here, I will report on how we presented our research activities at the Night of Science in Physics and at the "Highlights der Physik" in Würzburg.

Working part-time as a PR representative could encourage doctoral students to try their hand at science communication and develop the associated communication skills.

TT 40.7 Wed 17:45 POT 81

Real or Fake - A format in science communication that encurages critical thinking — •Tobias Löffler — Institut für Angewandte Physik Düsseldorf

The outreach format "Real or Fake" aims to train the audience in an critical approach to credible-sounding facts.

It is aimed at the general public and specifically at young people. At the same time, it offers an easy introduction for scientists to audience-oriented communication of science on stage. The format can be performed in front of a live audience or as an interactive online event. It has been proven to work as implemented into science festivals, nights of sciences, as a public individual event and also as part of events with constrained settings - such as outreach events at schools or as part of conferences.

"Real or Fake" was developed in 2017 by scientists around the Berlin March for Science who later founded Besserwissen e.V. with the goal to promote the format and support new organisers. I do cooprate with them since 2019 and have organized more than ten "Real or Fake" events since then.

In my talk, I will present the concept and its origins, give an overview of successful events and show what to do and what support one can get, if one wants to organize a "Real or Fake" event.

Invited Talk TT 40.8 Wed 18:00 POT 81

Physics for school and the public at the LMU — •Dr. Cecilia Scorza-Lesch — Fakultät für Physik der LMU, München

Germany lives from research and technology. Physics, as the basis of all empirical sciences and technologies, has a very special, fundamental role to play. The Faculty of Physics at LMU, the largest in Germany, comprises nine research areas, three centres and two excellence clusters. In this talk we will present the approach we use to successfully communicate our various topics of modern research, the role of physics in our daily lives and in the fight against global warming to the schools and the public in a participatory way.

TT 41: Quantum Transport and Quantum Hall Effects II (joint session HL/TT)

Time: Wednesday 15:00–17:00 Location: POT 251

TT 41.1 Wed 15:00 POT 251

Aharonov-Bohm-type oscillations in phase-pure core/shell GaAs/InAs nanowires — •Farah Basaric[1,2], Anton Faustmann[1,2], Erik Zimmermann[1,2], Gerrit Behner[1,2], Alexander Pawlis[1,2], Christoph Krause[1,2], Hans Lüth[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

Epitaxially grown phase-pure GaAs/InAs core/shell nanowires offer uniformity in their electrical, mechanical and optical properties due to the absence of a crystallographic disorder. Magnetotransport measurements were carried out at variable temperatures and for different gate voltages, under an applied in-plane magnetic field. Pronounced Aharonov-Bohm-type oscillations in the conductance are observed for this nanowire type. In measurements at different gate voltages, significantly higher oscillation amplitudes are observed in comparison to the corresponding measurements on polymorphic core/shell nanowires. Furthermore, measurements at different temperatures show robustness of these oscillations against high temperatures as a result of reduced disorder. Finally, strong indications of a quasi-ballistic transport regime could be recognized for the phase-pure nanowire type. Obtained results indicate a strong effect of disorder reduction in GaAs/InAs nanowire transport properties, manifested in superior transport properties.

TT 41.2 Wed 15:15 POT 251

Spin valves based on bilayer graphene quantum point contacts — •Eike Icking[1,2], Christian Volk[1,2], Christopher Schattauer[3], Luca Banszerus[1,2], Kenji Watanabe[4], Takashi Taniguchi[5], Florian Libisch[3], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]RWTH Aachen University, Germany — [2]Forschungszentrum Jülich, Germany — [3]TU Vienna, Austria — [4]Research Center for Functional Material, Japan — [5]International Center for Materials Nanoarchitectonics, Japan

Bernal bilayer graphene (BLG) is a unique material as it allows opening and electrostatically tuning a sizeable band gap by applying a perpendicular electric field. Recently, charge carriers have been confined successfully in one dimension to form quantum point contacts (QPC) based on split gates separated by a channel of a few hundred nanometers. Moreover, spin-polarized quantum transport through such structures has been demonstrated up to 6 e^2/h using a high in-plane magnetic field. The threshold magnetic field at which the lowest modes become spin-polarized depends on the subband spacing and thus on the width of the split gate channel. In this work, we combine two QPCs of different geometric widths, resulting in different threshold magnetic fields, to spin-polarize the first QPC and use it as a filter for the second QPC. In particular, we report on a spin-valve achieving spin-polarized channels with a total conductance of up to 10 e^2/h.

TT 41.3 Wed 15:30 POT 251

Optical and electrical tuning between the normal insulating and topological insulating phase of InAs/GaSb bilayer quantum wells — •Manuel Meyer[1], Tobias Fähndrich[1], Sebastian Schmid[1], Sebastian Gebert[1], Gerald Bastard[1,2], Fabian Hartmann[1], and Sven Höfling[1] — [1]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, D-97074 Würzburg, Germany — [2]Physics Department, École Normale Supérieure, PSL 24 rue Lhomond, 75005 Paris, France

Topological insulators (TI) based on InAs/GaSb bilayer quantum wells (BQW) are appealing due to their rich phase diagram with a TI and normal insulating (NI) phase[1]. The switching between both phases can be achieved by external electric fields using a top and back gate (TG and BG)[2]. However, especially a fully functional BG is difficult to realize in antimonides due to leakage issues. To overcome this bottleneck we present another tuning knob using optical excitation to switch from the NI to the TI phase over the TI gap[3]. By monitoring the charge carrier densities we can identify the hybridized band structure and in-plane magnetic field measurements evidence the TI gap. Furthermore, a top-gated sample is investigated. Without a back gate we find properties from both phases for magnetransport measurements which points to a mixing of NI and TI states. This is further indicated by the resistance peak evolutions with temperature for both samples.

[1] C. Liu et al., PRL 100, 236601 (2008)
[2] F. Qu et al., PRL 115, 036803 (2015)
[3] G. Knebl et al., PRB 98, 041301(R) (2018)

30 min. break

TT 41.4 Wed 16:15 POT 251

Transport in high mobility HgTe heterostructures — •Michael Kick, Lena Fürsst, Johannes Kleinlein, Saquib Shamim, Hartmut Buhmann, and Laurens W. Molenkamp — Experimentelle Physik III, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The Fractional Quantum Hall Effect (FQHE) has not yet been observed in the material system of HgTe. Due to recent progress in MBE growth, routinely charge carrier mobilities of HgTe heterostructures of over $\mu > 1 \cdot 10^6$ cm^2/Vs are obtained which is in the same order of magnitude as in the first reported experimental observation of the FQHE in GaAs/GaAlAs heterostructures. This opens up new prospects for transport investigations into the long time still open question of fractional states in this material system.

In 2-dimensional HgTe quantum wells, transport measurements show well pronounced quantum Hall plateaus for all filling factors, but no indication of any fractional state. High magnetic field measurements show a prolonged $\nu = 1$ plateau and a transition to an insulating state. Intriguingly, the $\nu = 1$ plateau exhibits a transition to an insulating state for filling factor $\nu = 1/2$.

Another possibility to observe the FQHE in HgTe is provided by the 2D surface states of a 3D topological insulator. High mobility layers, $\mu > 1 \cdot 10^6$ cm^2/Vs, of tensil strained HgTe are subject of extensive magneto-transport investigations. First results reveal a good and detailed correspondence to recent k.p band structure calculations for non-interacting electron systems.

TT 41.5 Wed 16:30 POT 251

Electron Density Depended Giant Negative Magnetoresistance — •Lina Bockhorn and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Ultra-high mobility two-dimensional electron gases not only show an increasing number of new fractional filling factors, but also an astonishing robust negative magnetoresistance at zero magnetic field [1 -5]. The theoretical description of this negative magnetoresistance is still an open issue due to its complex dependencies on several parameters.

The behavior of the giant negative magnetoresistance is affected by different scattering events, e. g. interface roughness, oval defects, background impurities and remote ionized impurities, which leads to a strong dependence on different parameters. Here, we take a closer look on the temperature dependence of the giant negative magnetoresistance for different electron densities. At low temperatures we observe the predicted temperature dependence of $T^{1/2}$ [6].

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] A. T. Hatke et al., Phys. Rev. B 85, 081304 (2012).
[3] R. G. Mani et al., Scientific Reports 3, 2747 (2013).
[4] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[5] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[6] I. V. Gornyi et al., Phys. Rev. B. 69, 045313 (2004).

TT 41.6 Wed 16:45 POT 251

Massless Dirac fermions on a space-time lattice with a topologically protected Dirac cone — •Michal Pacholski[1], Alvaro Donís Vela[3], Gal Lemut[3], Jakub Tworzydlo[2], and Carlo Beenakker[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Warsaw University, Warsaw, Poland — [3]Lorentz Institute, Leiden, The Netherlands

The symmetries that protect massless Dirac fermions from a gap opening may become ineffective if the Dirac equation is discretized in space and time, either because of scattering between multiple Dirac cones in the Brillouin zone (fermion doubling) or because of singularities at zone boundaries. Here we introduce an implementation of Dirac fermions on a space-time lattice that removes both obstructions. The quasienergy band structure has a tangent dispersion with a single Dirac cone that cannot be gapped without breaking both time-reversal and chiral symmetries. We show that this topological protection is absent in the familiar single-cone discretization with a linear sawtooth dispersion, as a consequence of the fact that there the time-evolution operator is discontinuous at Brillouin zone boundaries.

TT 42: Poster: Correlated Electrons I

Time: Wednesday 15:00–18:00 Location: P2/OG2

TT 42.1 Wed 15:00 P2/OG2

Single crystal growth and characterization of $CeCoIn_5$ and Ce_2IrIn_8 — •Anja Philipp, Kristin Kliemt, and Cornelius Krellner — Max-von-Laue-Straße 1

The heavy-fermion series $Ce_nT_mIn_{3n+2}$ (n=1,2; T = Co, Rh, Ir) with the unique tetragonal crystal structure, leading to a quasi-two dimensional Fermi surface, received growing attention over the past decades [1],[2],[3]. In these compounds, there are strong electronic interactions between conduction electrons and localized 4f-electrons of the Ce ions, which lead to a variety of interesting phenomena like spin and valence fluctuations, Kondo effect, magnetic order, non Fermi-liquid behaviour and unconventional superconductivity [3].

In this contribution, the results of the self-flux growth of $CeCoIn_5$ and Ce_2InIr_8 single crystals are shown. The crystallographic orientation of the single crystals was determined using microscopy and Laue X-ray diffraction. The physical properties like resistivity, heat capacitiy and magnetic susceptibility down to 2K were measured for both compounds and were analyzed in this work.

[1] R.T. Maculso et al., Chem Mater. 15, 1394 (2003)
[2] G.D. Morris et al., Phys. Rev. B 69, 214415 (2004)
[3] A. Ikeda et al., Phys. Soc. Jap. 70, 2248 (2001)

TT 42.2 Wed 15:00 P2/OG2

Search for superconductivity in $CeSb_2$ under chemical pressure — •Jan Weber, Kristin Kliemt, and Cornelius Krellner — Max-von-Laue Straße 1, 60438 Frankfurt am Main, Physikalisches Institut

Recently, an unconventional superconducting state was discovered at a pressure-induced magnetic quantum critical point in the Kondo-lattice system $CeSb_2$[1]. Under normal pressure CeSb2 crystallizes in the orthorombic $SmSb_2$ structure (Space group 64) [2]. At high pressures, the crystal structure changes and $CeSb_2$ adopts the $ZrSi_2$ - structure (Space group 63)[1]. This change in structure precedes the superconductivity around the magnetic quantum critical point. In this contribution, we present first attempts to replace the physical pressure using adequate substituents to reproduce the high-pressure structure at ambient pressure.

[1] O.P. Squire *et. al.*, arXiv:2211.00975 [cond-mat.str-el] (2022)
[2] R. Wang *et. al.*, Inorg. Chem. 6, 1685 (1967)

TT 42.3 Wed 15:00 P2/OG2

Searching for the critical endpoint in cobalt-doped $EuRh_2Si_2$ — •Franziska Walther, Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

The ternary europium-based intermetallic compounds with the $ThCr_2Si_2$-type structure show a variety of intriguing physical properties due to the coupling between lattice and electronic degrees of freedom. Eu ions can be present in a magnetic divalent or non-magnetic trivalent state. Under variation of temperature and pressure, it's possible to enforce a valence transition associated with a change of the unit cell volume [1]. At ambient pressure, $EuRh_2Si_2$ orders antiferromagnetically below T_N= 24 K in a stable divalent state [2], whereas the isoelectronic related compound $EuCo_2Si_2$ is nearly trivalent und indicates no magnetic ordering [1]. $EuRh_2Si_2$ undergoes a pressure-induced first order valence transition [3]. We expect the second order critical endpoint in the pressure range from 1.7 to 2.1 GPa, where the first-order phase transition terminates and critical elasticity may occur. We want to approach the critical endpoint by applying chemical pressure through substituting Rh in $EuRh_2Si_2$ with Co. We report on the growth of samples of the $Eu(Rh_{1-x}Co_x)_2Si_2$ -system and the characterization of their physical and chemical properties.

[1] Y. Onuki et al., J. Phys. Soc. Japan **89**, 102001 (2020)
[2] S. Seiro, C. Geibel, J. Phys.: Condens. Matter **26**, 046002, (2014)
[3] F. Honda *et al.*, J. Phys. Soc. Japan **85**, 063701 (2016)

TT 42.4 Wed 15:00 P2/OG2

Symmetry-broken low-temperature state in the Kondo system Ce_2Rh_2Ga — •Sajal Naduvile Thadathil[1,2], J Stirnat[1,2], P Devi[1], M Baenitz[3], A Strydom[4], D Soholov[4], J Wosnitza[1,2], and T Helm[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany — [3]Max Planck Institute for Chemical Physics of Solid, Dresden, Germany — [4]University of Johannesburg, South Africa

Cerium-based heavy-fermion conductors often exhibit unconventional transport and thermodynamic properties related to $4f$-electron physics. Ce_2Rh_2Ga exhibits a structural phase transition around $T_p \approx 130\,K$ from an orthorhombic to monoclinic crystal structure accompanied by an extreme anisotropy in its electrical conduction. Recent nuclear quadrupole resonance studies on polycrystals found evidence for the emergence of two inequivalent Ce ions below 2 K with different electronic environments that may provide grounds for multi-ion Kondo physics [1]. Here, we present results from magnetotransport studies on micron-sized devices cut from single crystals. We investigated the anisotropy between 0.3 and 300 K in fields up to 16 T. Below 5 K, the angular dependence of the magnetoresistance exhibits a significant change in its rotational anisotropy, indicating a broken symmetry. These findings may provide further evidence for multi-ion Kondo physics in Ce_2Rh_2Ga.

[1] Sh. Yamamoto et al., Phys. Rev. B 106, 115125 (2022)

TT 42.5 Wed 15:00 P2/OG2

Spin excitations in the field-induced phase of Ce_2Bi — •Nikolai Pavlovskii[1], Anton Kulbakov[1], Aleksandr Sukhanov[1], Michael Smidman[2], Federico Mazza[3], and Dmytro Inosov[1] — [1]TU Dresden, Dresden, Germany — [2]Zhejiang University, Hangzhou, China — [3]Vienna University of Technology, Austria

The compound Ce_2Bi represents a rare example of the heavy fermion materials that exhibit the coexistence of an antiferromagnetic magnetic (AFM) order and a tricritical point (TCP) in their temperature-magnetic field phase diagram. This combination is unusual because the TCP typically occurs in the ferromagnetic (FM) heavy fermion materials. In AFMs, the magnetic order can in many cases be continuously suppressed to zero temperature at a quantum critical point (QCP) by tuning pressure, magnetic fields, or chemical substitution. In the case of FMs, the situation is usually different. There, a QCP is generally avoided by changing the character of the magnetic phase transition from the second order to the first order, which induces a TCP. Using neutron time-of-flight spectroscopy, we observed two weakly-dispersed magnetic excitations modes in Ce_2Bi below Neel temperature that seem to show a nontrivial response to the applied magnetic field.

TT 42.6 Wed 15:00 P2/OG2

Transverse-field susceptibility of spin freezing at the mesoscale quantum phase transitions in $LiHoF_4$ — •Michael Lampl, Andreas Wendl, Felix Rucker, and Christian Pfleiderer — Physik-Department, Technical University of Munich, 85748 Garching, Germany

The perhaps best understood example of a quantum critical point is the response of the dipolar Ising ferromagnet $LiHoF_4$ under a transverse field [1-3]. When tilting the magnetic field away from the hard axis such that the Ising symmetry is always broken, a line of well-defined phase transitions emerges from the transverse-field quantum critical point, characteristic of further symmetry breaking, and in stark contrast to a crossover expected microscopically [4]. Detailed theoretical modelling in excellent agreement with experiment identifies this line of phase transitions as mesoscale quantum criticality. We report an experimental study of the transverse-field susceptibility of this mesoscale quantum criticality into a regime of spin freezing under large field tilting angles. Our observations will be compared with the characteristics of spin freezing, kinetic arrest, and quantum annealing observed in heavily diluted $LiHo_xY_{1-x}F_4$.

[1] D. Bitko et al., Phys. Rev. Lett. **77**, 940 (1996)
[2] H. M. Ronnow et al., Science **308**, 389 (2005)
[3] P. B. Chakraborty et al., Phys. Rev. B **70**, 144411 (2004)
[4] A. Wendl et al., Nature **609**, 65 (2022)

TT 42.7 Wed 15:00 P2/OG2

Phase diagram study of the Falicov-Kimball model on the two-dimensional Kagome lattice — Younes Javanmard[1] and •Ammar Nejati[2] — [1]Leibniz Universität Hannover, Hannover, Germany — [2]Jülich Centre for Neutron Science (JCNS), Forschungszentrum Jülich

The Falicov-Kimball Model (FKM) is a relatively simple model of coupled quantum and classic degrees of freedom, in the middle of the spectrum between the Hubbard and the Anderson models. A number of studies have revealed its rich phase diagram in two-dimensional lattices, e.g. square and triangular lattices [1,2]. In a square lattice with half-filling, depending on the interaction strength and temperature, FKM exhibits a rich variety of phases: At sufficiently low temperatures, there is a charge density wave (CDW) phase; at high temperatures and weak interactions, a weakly localized phase appears which becomes an Anderson-localized phase in the thermodynamic limit; at high temperatures and strong interactions, a Mott insulating phase emerges [1]. In addition, there are two other phases called "quantum liquid" and "classical liquid" in triangular lattices and away from half-filling at sufficiently low temperatures and weak interactions [2].

We set up a Monte Carlo algorithm for the two-dimensional FKM away from the half-filling regime on a Kagome lattice to study this model's rich phase diagram, and to extend the previous studies regarding the consequences of geometry on the emegent quantum phases and the corresponding phase transitions.

[1] Phys. Rev. Lett. 117, 146601
[2] Phys. Rev. Lett. 122, 197601

TT 42.8 Wed 15:00 P2/OG2

Quantum-critical properties of random transverse-field Ising models extracted by quantum Monte Carlo methods — •Calvin Krämer, Anja Langheld, Jan Koziol, Max Hörmann, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

The transverse-field Ising model with quenched disorder is studied in one and two dimensions at zero temperature by stochastic series expansion quantum Monte Carlo simulations. Using a sample-replication method we are able to determine distributions of pseudo-critical points, from which critical shift and width exponents $\nu_{s/w}$ are extracted by finite-size scaling. The scaling of the averaged magnetisation at the critical points is used further to determine the order-parameter critical exponent β. The dynamical scaling in the Griffiths phase is investigated by measuring the local susceptibility in the disordered phase and the critical exponent z' is extracted.

TT 42.9 Wed 15:00 P2/OG2

Numerical investigation of the Ising model in a light-induced quantized transverse field — •Anja Langheld and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We investigate the Ising model in a light-induced quantized transverse field [1] with a particular focus on antiferromagnetic, potentially frustrated Ising interactions. Using exact diagonalization, we provide data for the antiferromagnetic chain in a longitudinal field that is inconsistent with earlier results coming from mean-field considerations [2]. In order to study the model on frustrated, two-dimensional lattice geometries, we extend the mean-field calculation and develop a quantum Monte Carlo update based on the recently introduced wormhole update [3], for which the photons are integrated out. By this means, the photons induce a retarded spin-spin interaction in imaginary time that is also non-local in space in contrast to the Ising interaction inherent to the model.

[1] J. Rohn et al., Phys. Rev. Research 2, 023131 (2020)
[2] Y. Zhang et al., Sci. Rep. 4, 4083 (2014)
[3] M. Weber et al., Phys. Rev. Lett. 119, 097401 (2017)

TT 42.10 Wed 15:00 P2/OG2

High-order series expansions and crystalline structures for Rydberg atom arrays — •Antonia Duft, Jan Koziol, Matthias Mühlhauser, Patick Adelhardt, and Kai Phillip Schmidt — Friedrich-Alexander-Universität Erlangen-Nürnberg

We investigate a model of hardcore bosons on the links of a Kagome lattice subject to a long-range decaying van-der-Waals interaction. This model is known to be the relevant microscopic description of Rydberg atom arrays excited by a detuned laser field which has been realized in experiments recently. Particular interest lies on this system as it is an engineerable quantum platform which has been predicted to to host a topological phase. We investigate the quantum phase diagram for different limiting cases with a main focus on the low interaction-strength limit where we apply high-order linked cluster expansions.

TT 42.11 Wed 15:00 P2/OG2

Superexchange and spin-orbit coupling in the half-filled t_{2g} shell — •Marco Schönleber, Daniel Pranjic, and Maria Daghofer — Insitut für Funktionelle Materie und Quantentechnologien, Universität Stuttgart

Strongly correlated and spin-orbit coupled t_{2g} systems have been extensively investigated. By coupling orbital and spin angular momentum into one quantity, spin-orbit coupling (SOC) tends to reduce orbital degeneracy, e.g. for the widely studied case of one hole in the t_{2g} shell. However, the opposite has to be expected at half filling. Without spin-orbit coupling, all orbitals are half filled, no orbital degree of freedom is left and coupling to the lattice can be expected to be small. At dominant spin-orbit coupling, in contrast, one of the $j = 3/2$ states is empty and the system couples to the lattice. We investigate this issue. One finding is that the low-energy manifold evolves smoothly from the four $S = 3/2$ states in the absence of SOC to the four $j = 3/2$ states with dominant SOC. These fur states are always separated from other states by a robust gap. We then discuss relevant superexchange models.

TT 42.12 Wed 15:00 P2/OG2

From linear to circular polarized light - Floquet engineering in Kitaev-Heisenberg materials with Lissajous figures — •Pascal Strobel[1] and Maria Daghofer[1,2] — [1]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, 70550 Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Floquet engineering is a promising tool for tuning magnetic interactions in the candidate Kitaev material α-$RuCL_3$. Amplitude and frequency of the time periodic light field are able to modulate both sign and strength of Kitaev-, Heisenberg-, and Γ-interactions present in α-$RuCl_3$. This paves the way of possibly driving α-$RuCL_3$ into the sought after Kitaev spin-liquid phase.

We want to discuss possibilities of Floquet engineering with arbitrary polarized light in α-$RuCl_3$. In order to do so, we describe the influence of arbitrary polarization via an effective model including Lissajous figures. This model is derived via perturbation theory up to fourth order. Starting from linear and circular polarized light we bridge the gap between those two limiting cases. Moreover we study more complex Lissajous figures and general trends arising for them.

TT 42.13 Wed 15:00 P2/OG2

Complete field-induced spectral response of the spin-1/2 triangular-lattice antiferromagnet $CsYbSe_2$ — •Stanislav Nikitin[1], T. Xie[2], A. A. Eberharter[7], J. Xing[2], S. Nishimoto[3,4], M. Brando[5], P. Khanenko[5], J. Sichelschmidt[5], A. A. Turrini[1], D. G. Mazzone[1], P. G. Naumov[1], L. D. Sanjeewa[2], A. S. Sefat[2], B. Normand[1,6], A. M. Lauchli[1,6], and A. Podlesnyak[2] — [1]Paul Scherrer Institut, Switzerland — [2]Oak Ridge National Laboratory, USA — [3]TU Dresden, Germany — [4]IFW, Germany — [5]MPI CPfS, Germany — [6]EPFL, Switzerland — [7]Universitat Innsbruck, Austria

The spin 1/2 triangular lattice Heisenberg antiferromagnet remains on of the most attractive models to explore highly entangled quantum spin states in proximity to magnetic order. In my presentation I will discuss our recent results on $CsYbSe_2$. This materials exhibits strong two-dimensional magnetic behavior in absence of exchange and structural disorder and its spin Hamiltonian is well described by J_1–J_2 AFM Heisenberg model. We performed comprehensive INS measurements over the whole field scale starting from zero field up to the saturation and observed that corresponding excitation spectra evolve from continuum-like to relatively sharp spin-wave modes in the up-up-down phase, then back to continua and back to spin waves. We further support our observation by cylinder MPS calculation, which reproduce all observed features with semi-quantitative accuracy. Thus our comprehensive experimental and theoretical analysis of the field-induced spin excitations in the $CsYbSe_2$ provides valuable insight into the dynamics of a broad class of quantum many-body systems.

TT 42.14 Wed 15:00 P2/OG2

Low energy, mobile excitations in herbertsmithite revealed by magnetothermal conductivity — •Ralf Claus, Jan Bruin, Yosuke Matsumoto, Jürgen Nuss, Masahiko Isobe, and Hidenori Takagi — Max Planck Institute for Solid State Research, Stuttgart, Germany

We report the magnetothermal conductivity k(B) of the Kagome quantum spin liquid candidate herbertsmithite ($ZnCu_3(OH)_6Cl_2$) in the temperature range from 100 mK to 70 K with applied magnetic fields up to 12 T for heat flow parallel and perpendicular to the Kagome planes. We identify both phonon and magnetic contributions to k and find that the latter is only present for heat flow within the Kagome planes. These 2D magnetic contributions persist down to at least 200 mK, consistent with the presence of low-lying quantum spin liquid excitations with a gapless excitation spectrum.

TT 42.15 Wed 15:00 P2/OG2

Field-tuned critical fluctuations in the triangular-lattice delafossite $NaYbO_2$ probed by ^{23}Na NMR — •S. Luther[1,2], K. M. Ranjith[3,4], D. Opherden[1], S. Khim[3], H. Yasuoka[3], J. Wosnitza[1,2], M. Baenitz[3], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]MPI-CPfS, Dresden — [4]IFW Dresden

The frustrated triangular-lattice delafossite $NaYbO_2$ is a promising candidate for realizing a quantum spin liquid (QSL) ground state. The combination of a strong spin-orbit coupling and crystalline-electric-field effects leads to a magnetic anisotropy and a pseudospin-1/2 state of the Yb^{3+} ions at low temperatures. The absence of magnetic order and emergence of pronounced low-energy spin fluctuations have been shown by several experimental techniques, such as specific heat, inelastic neutron scattering, and muon spin relaxation. We present ^{23}Na NMR investigations of the low-temperature spin correlations by means of spectroscopy and $1/T_1$ measurements of polycrystalline $NaYbO_2$. At small magnetic fields and low temperatures, a strongly increased $1/T_1$ rate, as well as the absence of significant spectral line broadening suggest the presence of a QSL ground state with critical fluctuations at the verge of a magnetic instability. Above about 1 T, a crossover regime with persistent strong spin fluctuations and an onset of static magnetic ordering is observed. For fields above about 2 T, the formation of field-induced long-range magnetic order yields a strongly suppressed $1/T_1$ rate and an inhomogeneously broadened spectral lineshape.

TT 42.16 Wed 15:00 P2/OG2

Disorder effects in spiral spin liquids — •Pedro Monteiro Cônsoli and Matthias Vojta — Institut für Theoretische Physik, TU Dresden

Spiral spin liquids are a special kind of paramagnetic state that features a subextensive classical ground-state degeneracy related to a family of spin spirals whose ordering wave vectors form a submanifold of momentum space. As the number of their theoretical and experimental realizations grows, there is cumulative evidence that, under additional perturbations, spiral spin liquids constitute a promising platform for the emergence of exotic phases of matter and excitations, including quantum spin liquids, multiple-q states, and skyrmions. However, little is known about their response to quenched disorder. In this poster, we investigate how various types of defects affect the classical ground-state manifold of a spiral spin liquid on the honeycomb lattice. Among our results, we describe how different order-by-disorder mechanisms can arise, compete among themselves, and lead to spin-glass physics in these systems.

TT 42.17 Wed 15:00 P2/OG2

Second-harmonic generation in the Kitaev model — •Olesia Krupnitska[1,2] and Wolfram Brenig[1] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitskii Street, Lviv, 79011, Ukraine

Optical spectroscopies are important probes for elementary excitations of quantum magnets. In the present study, we investigate second-harmonic generation in the hexagonal Kitaev model induced by external electric fields. The prime interest is to identify fingerprints of fractionalization as has been shown to exist in this model in terms of Majorana particles and gauge excitations. For that purpose second order response functions are calculated within the equation of motion approach. Analytical results for the spectrum will be presented in the homogeneous gauge sector and exchange anisotropy and temperatures of Majorana fermions will be analyzed. The impact of gauge flux excitation will be speculated upon.

TT 42.18 Wed 15:00 P2/OG2

Magnetostriction in frustrated planar quantum magnets — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Using the numerical linked cluster expansion (NLCE) focussing on the single-site representation, we study the field-induced thermodynamic and magnetoelastic properties of paradigmatic frustrated planar spin models. Results are presented for the energy, the specific heat and the magnetization. Employing simple magnetoelastic modelling we calculate the linear magnetostriction coefficient versus temperature and external magnetic field. In particular we consider magnetostriction at field-induced quantum phase transitions. Results obtained for the generalized Kitaev honeycomb model are extended to include findings on the anisotropic triangular Heisenberg antiferromagnet.

TT 42.19 Wed 15:00 P2/OG2

Continuous similarity transformation for critical phenomena: bilayer antiferromagnetic Heisenberg-model and J_1-J_2-model — •Matthias R. Walther[1], Dag-Björn Hering[2], Götz S. Uhrig[2], and Kai P. Schmidt[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen — [2]Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund

We apply continuous similarity transformations (CSTs) to the bilayer antiferromagnetic Heisenberg model and the antiferromagnetic J_1-J_2 model on the square lattice. The bilayer Heisenberg model features a well studied, continuous phase transition in the O(3) universality class between a gapless Néel phase and a gapped paramagnetic dimer phase (valence bond solid). The J_1-J_2 features a gapless Néel phase for $J_1 \gg J_2$, a gapless columnar phase for $J_2 \gg J_1$ and an intermediate phase whose nature is still under debate. We start in both models from the magnetically ordered, collinear phases and approach the quantum phase transitions indicating the breakdown of these long-range ordered phases. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with $d \leq 2$ are taken into account. We determine critical points by studying the breakdown of the ordered phases and try to determine critical exponents from the flow of the couplings, the ground-state magnetization and the ground-state energy.

TT 42.20 Wed 15:00 P2/OG2

Continuous similarity transformation for critical phenomena: easy-axis antiferromagnetic XXZ model — •Dag-Björn Hering[1], Matthias R. Walther[2], Kai P. Schmidt[2], and Götz S. Uhrig[1] — [1]Technische Universität Dortmund, Department of Physics, Condensed Matter Theory, Otto-Hahn-Str. 4, 44227 Dortmund — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Institut für Theoretische Physik I, Staudtstraße 7, 91058 Erlangen

We apply continuous similarity transformations (CSTs) to the easy-axis antiferromagnetic XXZ-model on the square lattice. The CST flow equations are truncated in momentum space by the scaling dimension d so that all contributions with $d \leq 2$ are taken into account. The resulting quartic magnon-conserving effective Hamiltonian is analyzed in the zero-, one-, and two-magnon sector. In this way, a quantitative description of the ground-state energy, the one-magnon dispersion and its gap as well as of two-magnon bound states is gained for anisotropies ranging from the gapped Ising model to the gapless Heisenberg model. We discuss the critical properties of the gap closing as well as the evolution of the one-magnon roton mininum. The excitation energies of two-magnon bound states are calculated and their decay into the two-magnon continuum is determined via the inverse participation ratio.

TT 42.21 Wed 15:00 P2/OG2

Quantum criticality of the frustrated transverse-field Ising model on a triangular lattic using enhanced perturbative continous unitary transformations — •Lukas Schamriss[1], Matthias R. Walther[1], Dag-Björn Hering[2], and Kai P. Schmidt[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany

Ising models in a transverse field are paradigmatic models for quantum phase transitions of various universality classes which occur depending on the lattice geometry and the choice of antiferromagnetic of ferromagnetic coupling. We investigate the quantum phase diagram of the bilayer antiferromagnetic transverse field Ising model on a triangular lattice with an Ising-type interlayer coupling. Without a field, the model is known to host a classically disordered ground state, and in the limit of decoupled layers it exhibits the 3dXY transition of the corresponding single layer model. Our starting point for the unknown parts of the phase diagram is a high-order perturbative calculation from the limit of isolated dimers. Enhanced perturbative continuous unitary transformations (epCUTs) are used to derive series expansions for the ground state and the energy gap. These are refined by directly evaluated epCUTs (deepCUTs) which provide estimates which coincide with the perturbative series up to its respective order and add a non-perturbative correction. These allow to draw conclusions about the nature of occurring phase transitions.

TT 42.22 Wed 15:00 P2/OG2

Quantum simulation of transverse field Ising model using numerical linked cluster expansions with variational quantum eigensolver — •Sumeet Sumeet, Max Hörmann, and Kai P. Schmidt — Institut für Theoretische Physik I Friedrich-Alexander-Universität Erlangen-Nürnberg

With the advancements in quantum technologies it has become inevitable to investigate the potential existence of quantum advantage for the paradigmatic models of quantum-many body physics. One of the very basic models is the transverse field Ising model that can be simulated on a quantum computer to compute properties such as the ground-state energy of a spin system. This problem, when tackled on a classical computer, leads to an exponential surge in the cost of computation with increasing system size. The advent of classical-quantum hybrid algorithms has shifted the focus to investigate the solution to this problem with algorithms such as the variational quantum eigensolver (VQE) which is considered reasonably good for obtaining the ground-state energies of quantum many-body systems in the NISQ era. In this work, we exploit the Hamiltonian variational ansatz for calculating the ground-state energy and fidelity of the transverse-field Ising model on one- and two-dimensional geometries. We devise strategies to compute the ground-state energy in the thermodynamic limit on quantum computers. In that regard, we apply numerical linked cluster expansions (NLCE) to VQE in order to simulate infinite spin systems using calculations on finite graphs. Further, we extend this approach to geometrically frustrated systems.

TT 43: Poster: Correlated Electrons II

Time: Wednesday 15:00–18:00 Location: P2/OG3

TT 43.1 Wed 15:00 P2/OG3

Interplay between order-by-disorder and long-range interactions — •Jan Alexander Koziol and Kai Phillip Schmidt — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We study the ground-state properties of the antiferromagnetic long-range transverse-field Ising model in the limit of small transverse fields. We present degenerate perturbation theory calculations on the extensively degenerate nearest-neighbour ground-state space for finite systems, treating the long-range interaction and the transverse field perturbatively. The long-range interaction breaks the degeneracy and stabilises a gapped six-fold degenerate plain stripe phase in the absence of a transverse field. An infinitessimal transverse-field leads to an order-by-disorder emergent six-fold degenerate gapped clock-ordered phase in the nearest-neighbour case. We demonstrate a level crossing transition between the plain stripe phase and clock ordered phase for finite transverse fields and long-range interactions.

TT 43.2 Wed 15:00 P2/OG3

Magnetic dilution of a frustrated triangular-lattice spin system — •Florian Bärtl[1,2], Ellen Häussler[3], Thomas Doert[3], Jörg Sichelschmidt[4], Sven Luther[1,2], Tommy Kotte[1], Jochen Wosnitza[1,2], Michael Baenitz[4], and Hannes Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]Fakultät für Chemie und Lebensmittelchemie, TU Dresden — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

Among the Yb-based triangular-lattice magnets, the delafossite $NaYbS_2$ is one of the promising candidates for realizing a quantum-spin-liquid (QSL) ground state. The magnetic phase diagram was probed by several experimental methods, such as specific-heat, magnetization, and NMR measurements. The proposed QSL ground state of $NaYbS_2$ is suppressed at fields of several tesla, and long-range order with various spin configurations is manifested. As a next step, we investigated possible changes to this phenomenology by diluting the magnetic lattice of $NaYbS_2$ by means of Lu substitution. A series of $NaYb_{1-x}Lu_xS_2$ single crystals, with $0 \le x \le 1$, were synthesized and characterized by various probes, including ESR spectroscopy. The ESR data reveal a systematic reduction of the Weiss temperature as x is increased. Further, we present recent specific-heat measurements for samples with $x \le 0.5$, which reveal a systematic suppression of the transition temperatures to long-range order in magnetic fields with increasing Lu substitution.

We acknowledge the support of the SFB 1143.

TT 43.3 Wed 15:00 P2/OG3

Dynamic flash method for probing heat transport of quantum magnets — •Maximilian Schiffer[1], Xiaochen Hong[1], Martin Valldor[2], Christian Hess[1,3], and Bernd Büchner[3] — [1]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Centre for Materials Science and Nanotechnology (SMN), Department of Chemistry, University of Oslo, P.O. Box 1033 Blindern, N-0315 Oslo, Norway — [3]Leibniz-Institute for Solid State and Materials Research (IFW-Dresden), 01069 Dresden, Germany

Transport experiments in principle provide access to the investigation of exotic entropy carrying quasiparticles in quantum magnets, such as spinons in spin chains, triplons in spin ladders and Majorana fermions and visons in spin liquids. Generally, the thermal conductivity of an insulating, magnetic compound consists of phononic and magnetic contributions: $\kappa_{xx} = \kappa_{xx,ph} + \kappa_{xx,mag}$. Thus, measurement of κ_{xx} can offer a fine grasp of the above mentioned quasiparticles, which are currently under hot debate in the field of solid state physics.
Here we address heat transport experiments at elevated temperature which becomes important in materials with sizeable exchange interactions $J/k_B \gtrsim 100$ K. It is well known that standard steady state heat transport measurements are difficult for $T \geq 200$ K due to inevitable radiation losses. We present Laser Flash Analysis as a method for avoiding this problem. The method will be introduced, and initial results on various quantum materials will be discussed.

TT 43.4 Wed 15:00 P2/OG3

Modified nanoparticles of Prussian Blue metal organic frameworks — •Sascha A. Bräuninger and Hermann Seifert — Institute of General Radiology and Medical Physics, University of Veterinary Medicine Foundation, Hannover, Germany

Prussian Blue compounds (PBC), e.g. soluble $AFe^{3+}[Fe^{2+}(CN)_6]{\cdot}xH_2O$ ($A = K, Na, NH_4$), have shown a huge potential of applications in physics, chemistry, medicine and radioecology, e.g., PBC acting as efficient ion exchanger extracting the radioistope ^{137}Cs in solutions. For potassium, proposed ferromagnetism by superexchange is discussed between Fe(III) with $S = 5/2$ and an effective magnetic moment of $\mu_{\text{eff}} \approx 5.98\mu_B$ consistent with a spin-only value of Fe(III) high-spin. Powder neutron diffraction studies showed a Curie temperature $T_C \approx 5.6$ K consistent with susceptibility measurements. Here, we are presenting the synthesis and low-energy investigation of modified magnetic Prussion-blue nanoparticles protected by PVP (polyvinylpyrrolidene).

TT 43.5 Wed 15:00 P2/OG3

Experimental studies of phase diagram of compound $Ni(2aepy)_2Cl(H_2O)]Cl{\cdot}H_2O$ - a spin-1 antiferromagnetic chain — •Mariia Holub[1], Slavomíra Šterbinská[2], Marc Uhlarz[3], Juraj Černák[2], and Erik Čižmár[1] — [1]Institute of Physics, Faculty of Science, P.J. Šafárik University, Park Angelinum 9, Košice, Slovakia — [2]Institute of Chemistry, Faculty of Science, P.J. Šafárik University, Moyzesova 11, Košice, Slovakia — [3]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße, Dresden, Germany

We present the study of compound $Ni(2aepy)_2Cl(H_2O)]Cl{\cdot}H_2O$ (2aepy = 2-aminoethylpyridine) identified as a spin-1 antiferromagnetic chain with ratio of D/J=1.14 (D is the single-ion anisotropy, J is the intrachain exchange interaction). It represents a unique experimental example of a system close to the quantum critical point (QCP), which is a topological phase transition that separates Haldane and Large-D gapped phases for spin-1 chains. In this work, we observed the presence of field-induced crossover into the gapless Tomonaga-Luttinger liquid phase using low-temperature specific heat measurements. A very low first critical field is in good agreement with the small energy gap predicted close to QCP. Estimation of saturation field (second critical field) using D and J parameters was confirmed by high-field magnetic measurements at ≈12.5 T.

This work was supported by APVV-18-0016, APVV-18-0197, and HLD-HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 43.6 Wed 15:00 P2/OG3

Electrical and thermal transport properties of delafossite oxide $CuCr_{1-x}FexO_2$ — •Mithun Kumar Majee[1], Ratnamala Chatterjee[1], and Preeti Bhobe[2] — [1]Department of Physics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016, India — [2]Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Simrol, Indore-453552, India

In order to improve the thermoelectric property of a material the effect of phonon/magnon drag, and spin fluctuations are other central parameters apart from carrier concentration, and lower thermal conductivity. It is known from the literature that $CuCrO_2$ has a large Seebeck value of around 350 μV/K at room temperature, but its electronic concentration is low, hence the thermoelectric figure-of-merit (ZT) turns out to be quite poor. Hence to better its ZT, we attempt to replace some Cr ions with Fe in the series, $CuCr_{1-x}Fe_xO_2$ (0<x<1) and study its electrical and thermal conductivity, heat capacity, and Seebeck coefficient. Our results exhibit a large and complex Seebeck coefficient in 20 K<T<380 K. The low-temperature electrical conduction is observed to obey 3D variable range hopping mechanism. Unlike, nonmagnetic Cu-based Delafossites, we show that the thermal conductivity is strongly affected by spin-phonon scattering in $CuCr_{1-x}FexO_2$ compositions. The heat capacity measurements identify the Debye temperature and effects due to magnetic ordering temperatures. Out of the different contributed processes, the role of the phonon drag effect and complexity in temperature dependence is observed in the Cr-rich compositions.

TT 43.7 Wed 15:00 P2/OG3

Influence of lattice strain on the electronic and magnetic properties of $SrRuO_3/SrTiO_3$ heterostructures — •Robin Heumann, Robert Gruhl, and Philipp Gegenwart — Experimentalphysik VI, Universität Augsburg, 86159 Augsburg, Germany

Layered ruthenate Sr_2RuO4, consisting of strontium- and ruthenium-oxide stacks along the c-axis, is a prototype unconventional superconductor and continues to attract strong interest. Artificial heterostructures composed of layers of $SrRuO_3$ (SRO) and $SrTiO_3$ (STO) were recently considered by band-structure calculations [1,2]. It is predicted that SRO_1/STO_1 bilayers show a variety of emergent quantum states tunable by lattice strain, including ferro- and checkerboard-type antiferromagnetism, spin-density waves [1] and even unconventional superconductivity [2].

Utilizing metal-organic aerosol deposition $[SRO_n/STO_n]_m$ epitaxial heterostructures were grown. The superlattices show sharp interfaces and an atomically smooth surface morphology. Different substrates were used to study the effect of tensile and compressive lattice strain. Besides structural studies by x-ray diffraction, reciprocal space mapping and TEM imaging we utilized Hall- and magnetoresistance as well as magnetization measurements to investigate the electronic and magnetic properties.

[1] M. Kim *et al.*, Phys. Rev. B **106** (2022) L201103.
[2] B. Kim *et al.*, Phys. Rev. B **101** (2020) 220502(R).

TT 43.8 Wed 15:00 P2/OG3

Manipulating the metal-insulator transition in ultrathin oxide films by strain engineering — •Sizhao Huang, Philipp Scheiderer, Judith Gabel, Michael Sing, and Ralph Claessen — Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

The relationship between metal-insulator transition (MIT) and strain relaxation in films of strongly correlated perovskite oxides has been intensively studied. The oxide films can emerge numerous phenomena when the film thickness is reduced towards the 2D limit, such as SrVO3 (SVO). In our previous studies on SrTiO3 (STO) capped SVO films, a transition from the Mott insulating state at 6 u.c. to metallic behaviour at 10 u.c. film thickness has been found. In order to further explore the relationship between MIT transition and orbital occupation, we have grown coherently strained SVO thin films on various substrates with different lattice constants by pulsed laser deposition (PLD) in an Ar gas background. Using x-ray photoelectron spectroscopy and transport measurements, we have found that the MIT in SVO thin films can be fine-tuned by both film thickness and strain.

TT 43.9 Wed 15:00 P2/OG3

Towards noise spectroscopy at the Mott critical endpoint — •Tim Thyzel[1], Harald Schubert[1], Michael Lang[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-Universität Frankfurt, Frankfurt (Main), Germany — [2]Institute of Materials Research, Tohoku University, Sendai, Japan

Quasi-two-dimensional organic charge-transfer salts are ideal model systems for studying strongly correlated electrons due to their chemical variability, good physical tunability and rich phase diagrams.

Of special interest has been the family of Mott-Insulators κ-$(ET)_2Cu[N(CN)_2]Z$ where Z is Br or Cl, which exhibit superconductivity and an insulator-to-metal transition in an easily accessible temperature-pressure window. In particular, we focus on the critical endpoint of the Mott transition, where a breakdown of Hooke's law of elasticity has been observed [1], as well as indications of ergodicity breaking [2].

We employ resistance noise spectroscopy as a powerful method to detect slow dynamics in charge transport near the Mott endpoint, which we access in a cryogenic hydrostatic gas pressure setup. Using this technique, we search for a slowing-down of carrier dynamics, as well as the appearance of non-stationary fluctuations hinting at critical behaviour. Details on the experimental setup will be presented, as well as initial spectroscopy scans of the phase diagram.

[1] E. Gati, Sci. Adv. 2, e1601646 (2016)
[2] B. Hartmann, Phys. Rev. Lett. 114, 216403 (2015)

TT 43.10 Wed 15:00 P2/OG3

Thermal-history-dependent electronic properties of κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ close to the Mott metal-insulator transition — •Florian Kollmannsberger[1,2], Shamil Erkenov[1,2], Natalia Kushch[1], Toni Helm[3], Werner Biberacher[1], and Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, 85748 Garching, Germany — [2]Technische Universität München Fakultät Physik, 85748 Garching, Germany — [3]Hochfeld-Magnetlabor Dresden, HZDR, 01328 Dresden, Germany

The partially deuterated organic charge-transfer salt κ-$(BEDT\text{-}TTF)_2Cu[N(CN)_2]Br$ (shortly, κ-Br) can be tuned over the Mott-metal-insulator transition (MIT) by rapid cooling through the temperature interval around $T_g \simeq 75$ K where a glassy ordering of the BEDT-TTF ethylene endgroups occurs. It was suggested [1,2] that this tuning happens due to a change of the conduction bandwidth, an effect similar to that induced by hydrostatic pressure. We investigated the influence of the ethylene group ordering in purely hydrogenated κ-Br. To this end, we have studied the resistance as a function of temperature and magnetic field for samples cooled through the glass transition at different rates. In particular, we have studied the variation in the behavior of magnetoresistance quantum oscillations. This allows us to trace the change in the Hubbard model parameter U/t extracted from the renormalized effective cyclotron mass.

[1] B. Hartmann et al., Phys. Rev. B **90**, 195150(2014).
[2] D. Guterding et al., Phys. Rev. B **92**, 081109(R) (2015).

TT 43.11 Wed 15:00 P2/OG3

Tetragonal CuO : Suppression of nearest-neighbour correlations in a strongly correlated material — •Benjamin Bacq-Labreuil[1], Max Bramberger[2], Martin Grundner[2], Silke Biermann[3], Ulrich Schollwöck[2], Sebastian Paeckel[2], and Benjamin Lenz[4] — [1]Institut Quantique, Université de Sherbrooke, Sherbrooke, Canada — [2]Arnold Sommerfeld Center of Theoretical Physics, University of Munich, Munich, Germany — [3]CPHT, Ecole Polytechnique, Palaiseau, France — [4]IMPMC, Sorbonne Université, Paris, France

Since tetragonal CuO (t-CuO) is composed of well separated 2D CuO planes, it appears as an ideal candidate to connect model calculations with real materials in the quest of understanding the nature of high-temperature superconductivity. In this work [1], we investigate the low-energy electronic properties of t-CuO by means of Cellular Dynamical Mean Field Theory (CDMFT) using a 2D Hubbard model.

From experiment it was proposed that single layers of t-CuO can be viewed as two weakly interconnected sublattices. Our calculations support this assumption: we find a suppression of the nearest-neighbour (NN) correlations for the benefit of the next-nearest neighbour (NNN) ones. The calculated spectral function is in remarkable agreement with photoemission experiments, showing that a one-band model is sufficient to capture the low-energy physics of t-CuO. Finally, we study the transition from the paramagnetic to antiferromagnetic phase at finite temperature and elucidate the nature of the insulating regime in both phases.

[1] M. Bramberger *et al.*, arXiv:2203.07880 (2022)

TT 43.12 Wed 15:00 P2/OG3

Thermal expansion measurements at low temperatures of a valence fluctuating system close to a critical endpoint. — •Arif Ata, Bernd Wolf, Jan Zimmermann, Marius Peters, Kristin Kliemt, Cornelius Krellner, and Michael Lang — PI, SFB/TRR288, Goethe Univ., Frankfurt/M., Germany

Thermodynamic investigations of highly correlated electron systems at low-temperatures are of general interest. Especially strong-coupling effects between lattice- and electronic degrees of freedom, which are expected around second-order critical endpoints [1], have become topics of current interest. These include phenomena such as critical softening and deviations from Hooks law of elasticity [1]. The intermetallic compound $EuPd_2Si_2$ and its Ge-doped variants, which show different kinds of phase transitions such as valance- and magnetic- transitions, are promising target materials for such investigations [2]. Of particular interest is the possibility to approach the critical regime by the combination of chemical pressure (Ge-doping) and He-gas pressure. In this work we present results of thermal expansion measurements on single crystalline $EuPd_2(Si_{1-x}Ge_x)$ as a function of temperature for 4.2 K $\leq$ T $\leq$ 300 K and He-gas pressure P $\leq$ 12 kbar The data have been obtained by using a strain gauge, enabling measurements of thermal expansion and compressibility to be performed at high pressure, i.e., in P-T parameter ranges where He is in its solid phase.

[1] E. Gati *et al.*, Sci. Adv. **2**, e1601646 (2016).
[2] Y. Onuki *et al.*, Philosophical Magazine **97**, 3399 (2017).

TT 43.13 Wed 15:00 P2/OG3

Probing the electron-lattice coupling near the valence transition in $YbLn_{1-x}Ag_xCu_4$ — •Jan Zimmermann, Bernd Wolf, Michelle Ocker, Kristin Kliemt, Cornelius Krellner, and Michael Lang — PI, SFB/TRR288, Goethe Univ., Frankfurt/M,. Deutschland

The recently proposed phenomenon of *critical elasticity* is linked to a non-perturbatively strong coupling between lattice- and critical electronic degrees of freedom [1]. Intermetallic compounds that show various types of phase transitions such as valence- or structural instabilities that make it possible to study such collective phenomena, are currently a field of high interest. It has been shown that doping can be used in $EuPd_2(Si_{1-x}Ge_x)_2$ to generate chemical pressure which may open up the possibility to experimentally access directly the area around the critical endpoint [2]. It is expected to find similar effects for the valence transition in the doped intermetallic compound $YbLn_{1-x}Ag_xCu_4$ [3]. We are investigating the elasticity of $YbLn_{1-x}Ag_xCu_4$ using ultrasound-wave-propagation. In addition to measurements performed under variable temperature, we have developed a new setup that allows ultrasonic measurements to be performed under variable He-gas pressure. We will discuss first results on the elasticity, in comparison with data on the magnetic susceptibility, and highlight the additional experimental possibilities the new setup offers.

[1] E. Gati *et al.*, Sci. Adv. **2**, e1601646 (2016)
[2] B. Wolf *et al.*, arXiv:2210.12227, (2022)
[3] S. Zherlitsyn *et al.*, Phys. Rev. B, **60**, 5, (1999)

TT 43.14 Wed 15:00 P2/OG3

Order from disorder phenomena in $BaCoS_2$ — •Benjamin Lenz[1], Michele Fabrizio[2], and Michele Casula[1] — [1]IMPMC, Sorbonne Université, CNRS, MNHN, 4 Place Jussieu, 75005 Paris, France — [2]International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

We investigate different nematic and orbital ordered instabilities in the antiferromagnetic insulating phase of $BaCoS_2$, which shows a Néel transition at a surprisingly high temperature of $T_N \sim 300$ K. Based on *ab initio* simulations, we discuss several competing orders in terms of magnetic order, orbital composition and structural distortions to identify a set of nematic and orbital ordered states as possible candidates for the ground state. From these considerations we derive an effective spin model of $J_1 - J_2 - J_3$ type and discuss the consequences of the most probable, orbital ordered ground state for its parametrization. We finally identify a driving mechanism which allows to explain the high Néel temperature by C_4-symmetry breaking through orbital order and draw parallels to other quasi-2D materials such as pnictides.

TT 43.15 Wed 15:00 P2/OG3

Basis dependence of the Mott transition in Ba_2IrO_4 within Dynamical Mean Field Theory — •Francesco Cassol[1], Léo Gaspard[2], Cyril Martins[2], Michele Casula[1], and Benjamin Lenz[1] — [1]L'Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC) , Sorbonne Université, Paris, France — [2]Laboratoire de Chimie et Physique Quantiques, Université Toulouse III Paul Sabatier, Toulouse, France

Among strongly correlated materials Sr_2IrO_4 is often presented as a paradigmatic system for the complex competition that takes place between ligand field, spin-orbit coupling (SOC), Coulomb correlation and structural distortion. Ba_2IrO_4 has recently attracted some interest being simpler in view of the absence of structural distortion and being isostructural to La_2CuO_4. Normally, the physics of iridates has been described within a $j_{eff} = \frac{1}{2}$ basis representation solved by means of Dynamical Mean Field Theory (DMFT). This picture however, while it partially alleviates the sign problem of Quantum Monte Carlo solver, often goes in hands with some approximation that prevent the application of a fully Ab initio DFT+DMFT scheme. In this work, we will go beyond standard approximation comparing the usual schemes to the orbital picture.

TT 43.16 Wed 15:00 P2/OG3

Calculating moments for many-electrons systems — •Elaheh Adibi and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a technique for computing the moments $\langle E^M \rangle = \mathrm{Tr}\, H^M$ of the many-electron spectrum. Taking the trace over a basis of Slater determinants $|I\rangle$ and expressing the Hamiltonian in the same orbital basis, matrix elements $\langle I|H^M|I\rangle$ can only be non-zero when the orbital indices of the creation operators are a permutation of those of the annihilation operators. Writing the permutations in cycle notation and realizing that the trace over a cycle with different orbital indices only depends on the number of descends, we can write the trace as a sum over products of Eulerian numbers times binomial factors involving the number of orbitals and electrons.

TT 43.17 Wed 15:00 P2/OG3

Exact diagonalization with twisted boundary conditions — •Benjamin Heinrich — Institut für funktionelle Materie und Quantentechnologie, Universität Stuttgart

When using exact diagonalization, using twisted instead of periodic boundary conditions gives access to additional momentum points. We investigate here in detail flavour-specific twisted boundary conditions, where each spin and /or orbital can have different boundary conditions. One goal is to assess whether and to which extent this improves estimates of observables (e.g. the ground-state energy). As increased momentum resolution is of particular interest in excitation spectra, a second aim is to estimate the quality of these additional data. We investigate the method for one- and two-dimensional one- and two-band Hubbard models. First results suggest that the additional momenta work well where the relevant physics is to a large extent captured by one quasiparticle (e.g. the magnon in case of magnetic spectra), but are less reliable in more complex scenarios (e.g. two spinons).

TT 43.18 Wed 15:00 P2/OG3

Symmetries and independent parameters of Coulomb matrix elements — •Coraline Letouzé, Guillaume Radtke, Benjamin Lenz, and Christian Brouder — Sorbonne Université, Muséum National d'Histoire Naturelle, UMR CNRS 7590, IRD, Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie, IMPMC, 75005 Paris, France

In realistic (DFT+DMFT) calculations of correlated materials, the matrix of the partially-screened electron-electron Coulomb interaction is usually approximated in spherical symmetry and parameterized by Slater integrals (or, equivalently, Racah parameters). Few works have considered the real point-group symmetry of the Coulomb matrix. We suggest parameterizing the Coulomb matrix by its eigenvalues on the irreducible representations of the point group: this respects the point-group symmetry of the system and, compared to other approaches, is completely basis-independent. The permutation symmetry of the 1-electron states in the Coulomb matrix is also taken into account in the two cases of real and complex wavefunctions, to further reduce the number of independent parameters. Finally we apply this method to 3d-transition-metal monoxides.

TT 43.19 Wed 15:00 P2/OG3

Phase diagram of the SU(3) Fermi-Hubbard model with next-neighbor interactions — •Arturo Pérez Romero[1,2], Jereson Silva Valencia[2], and Roberto Franco Peñaloza[2] — [1]Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Departamento de Física, Universidad Nacional de Colombia, A. A. 5997 Bogotá, Colombia.

We explore the zero-temperature phase diagram of a one-dimensional gas composed of three-color fermions, which interact locally and with their next neighbors. Using the density matrix renormalization group method and considering one-third filling, we characterize the ground state for several values of the parameters, finding diverse phases, namely: phase separation, spin density wave, pairing phase, a metallic phase, two different charge-density waves, and a non-separable state with modulation of charge. We show that the von Neumann block entropy and the fidelity susceptibility are useful for estimating the borders between the phases.

TT 43.20 Wed 15:00 P2/OG3

Spatiotemporal dynamics of classical and quantum density profiles in low-dimensional spin systems — Tjark Heitmann[1], Jonas Richter[2], Fengping Jin[3], Kristel Michielsen[3], Hans De Raedt[4], and •Robin Steinigeweg[1] — [1]University of Osnabrück, DE — [2]University College London, UK — [3]FZ Jülich, DE — [4]University of Groningen, NL

We provide a detailed comparison between the dynamics of high-temperature spatiotemporal correlation functions in quantum and classical spin models. In the quantum case, our large-scale numerics are based on the concept of quantum typicality, which exploits the fact that random pure quantum states can faithfully approximate ensemble averages, allowing the simulation of up to 40 spin-1/2 spins. Due to the exponentially growing Hilbert space, we find that for such system sizes even a single random state is sufficient to yield results with extremely low noise. In contrast, a classical analog of typicality is missing. In particular, in order to obtain data with a similar level of noise in the classical case, extensive averaging over classical trajectories is required, no matter how large the system size. Focusing on (quasi-)one-dimensional spin chains and ladders, we find a remarkably good agreement between quantum and classical dynamics. Comparing space-time profiles of the spin and energy correlation functions, the agreement is found to hold not only in the bulk but also in the tails of the resulting density distribution. The mean-squared displacement of the density profiles is found to exhibit similar scaling for quantum and classical models.

TT 43.21 Wed 15:00 P2/OG3

Probing real-time broadening of nonequilibrium density profiles via a local coupling to a Lindblad bath — •Tjark Heitmann[1], Jonas Richter[2], Jacek Herbrych[3], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrück, Germany — [2]University College London, UK — [3]Wroclaw University of Science and Technology, Poland

The Lindblad master equation is one of the main approaches to open quantum systems. While it has been widely applied in the context of condensed matter systems to study properties of steady states in the limit of long times, the actual route to such steady states has attracted less attention yet. Here, we investigate the nonequilibrium dynamics of spin chains with a local coupling to a single Lindblad bath and analyze the transport properties of the induced magnetization. Combining typicality and equilibration arguments with stochastic unraveling, we unveil for the case of weak driving that the dynamics in the open system can be constructed on the basis of correlation functions in the closed system, which establishes a connection between the Lindblad approach and linear response theory at finite times. In this way, we provide a particular example where closed and open approaches to quantum transport have to agree strictly. We demonstrate this fact numerically for the spin-1/2 XXZ chain at the isotropic point and in the easy-axis regime, where superdiffusive and diffusive scaling is observed, respectively.

TT 43.22 Wed 15:00 P2/OG3

Configuration interaction based nonequilibrium steady state impurity solver for the Anderson-Holstein model — •Daniel Werner and Enrico Arrigoni — ITPCP, Graz, Austria

Recently we developed a non-equilibrium impurity solver based on the Auxiliary Master Equation Approach using Configuration Interaction (CI). This allowed us to treat a larger auxiliary system, which can more accurately model physical environments with more challenging hybridization functions, as compared to ED. Due to the promising results we obtained, we extended the solver to include phonons, since this gives access to interesting physical phenomena. In particular we are investigating the vibrational steps in the differential conductance in the Kondo regime. We limited ourselves to a single phonon mode, i.e. Holstein phonons, which we again treated with CI to keep the increase of the state space low. Preliminary results, as well as possible extensions for a more complicated treatment of phonons are being discussed.

TT 43.23 Wed 15:00 P2/OG3

Hilbert space fragmentation in open quantum systems — •Yahui Li, Pablo Sala, and Frank Pollmann — Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Several mechanisms have been identified that can lead to a breakdown of thermalization in closed quantum systems-including integrability and many-body localization. Recently, a novel mechanism for ergodicity breaking has been discovered in systems with certain dynamical constraints, where the Hilbert space fragments into exponentially many disconnected subspaces. An open question is how such systems evolve when they are coupled to a dissipative bath.

We find that the Hilbert space fragmentation can be utilized to preserve coherence in the presence of dissipation. We study a quantum fragmented model, which fragments in an entangled basis due to unconventional non-Abelian symmetries. We investigate the Lindblad dynamics under two different couplings, which either preserves or destroys the quantum fragmentation structure. At sufficiently large couplings, the operator space entanglement is suppressed, which allows for an efficient numerical simulation using tensor networks. Surprisingly, under the structure-preserving noise, we observe finite Renyi negativity, indicating non-vanishing quantum correlations. Using an analytic approach, we derive the stationary states under both couplings, which explains the long-time behaviors observed in numerical simulations.

TT 43.24 Wed 15:00 P2/OG3

Floquet engineering in tilted lattices — •Melissa Will[1], Pablo Sala[2,3], and Frank Pollmann[1] — [1]Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]Department of Physics and Institute for Quantum Information and Matter, California Institute of Technology, Pasadena, California 91125, USA — [3]Walter Burke Institute for Theoretical Physics, California Institute of Technology, Pasadena, California 91125, USA

Quantum many-body systems out of equilibrium can exhibit very rich and exciting phenomena. A particularly important question is whether and how a quantum system thermalizes under unitary evolution. In this context three classes of systems have been identified: ergodic, localized and an intermediate regime exhibiting so called quantum many-body scars. In this talk we discuss whether a time-periodic, local drive can induce thermalization of a localized system. We consider interacting hard-core bosons in an one dimensional, tilted system with periodic driving. We find that the system becomes ergodic for resonant driving frequencies. In contrast, if the tilt is not close to a multiple of driving frequency, the system stays localized. This observation can theoretically be understood by deriving an effective Hamiltonian using a Magnus expansion. Using large scale numerical methods, we explore entanglement entropy and imbalance over time. Our theoretical predictions are in good agreement with numerics.

TT 43.25 Wed 15:00 P2/OG3

Impact of decoherence on the route to equilibrium — •Jiaozi Wang and Jochen Gemmer — University of Osnabrück, Osnabrück, Germany

We study the time evolution of a small quantum system when coupling to a quantum chaotic bath, within the framework of projection operator techniques. We study this problem by employing a different approach which also take the so called pure-dephasing term as a part of the unperturbed Hamiltonian. With this method, a new formula of the relaxation rate is derived analytically in a random matrix model, which is also confirmed by numerical results. We find that, the relaxation process is slowed down by decoherence, which is in consistent with the quantum zeno effect.

TT 43.26 Wed 15:00 P2/OG3

Nonequilibrium steady-states in photodoped Mott insulators — •Fabian Künzel — Universität Hamburg, Hamburg, Germany

Photodoped states in Mott insulators are peculiar states which simultaneously host strongly correlated electron and hole-like carriers, and can show instabilities into various non-thermal orders. Here we stabilize a stationary photodoped state in a Mott insulator using Dynamical-Mean-Field-Theory (DMFT) in the nonequilibrium steady-state formalism. This formalism provides a description of the longtime dynamics of microscopic models with well separated timescales. The photodoping can be established by coupling the Hubbard model with external baths that pump holon and doublon excitations in the Hubbard bands. In particular, we develop an algorithm to stabilize DMFT solutions with a prescribed nonthermal distribution function in the local Green's functions. This formulation may allow for a nonperturbative solution of the DMFT impurity model, using methods like Quantum Monte Carlo, and it opens the possibility to study the dynamics of photodoped states using a Quantum Boltzmann equation.

TT 43.27 Wed 15:00 P2/OG3

Quantum oscillations beyond the Onsager relation in a doped Mott insulator — •Valentin Leeb[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, Germany; TUM School of Natural Sciences, Department of Physics, TQM — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The kinetic energy of electrons in a magnetic field is quenched resulting in a discrete set of highly degenerate Landau levels (LL). This gives rise to fascinating phenomena like quantum oscillations or the integer and fractional quantum Hall effect. The latter is a result of interactions partially lifting the degeneracy within a given LL while inter-LL interactions are usually assumed to be unimportant. Here, we study the LL spectrum of the Hatsugai–Kohmoto model, a Hubbard-like model which is exactly soluble on account of infinite range interactions. For the doped Mott insulator phase in a magnetic field we find that the degeneracy of LLs is preserved but inter-LL interactions are important leading to a non-monotonous reconstruction of the spectrum. As a result, strong interactions lead to aperiodic quantum oscillations of the metallic phase in contrast to Onsager's famous relation connecting oscillation frequencies with the Fermi surface areas at zero field. In addition, we find unconventional temperature dependencies of quantum oscillations and effective mass renormalizations. We discuss the general importance of inter-LL interactions for understanding doped Mott insulators in magnetic fields.

TT 43.28 Wed 15:00 P2/OG3

Magnetism of graphene beyond half filling using a mean-field approach — •Maxime Lucas, Andreas Honecker, and Guy Trambly de Laissardière — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France

The discovery of correlations between electronic flat-band states due to a Moiré pattern in twisted bilayers of graphene [1] or other 2D materials has recently stimulated studies of their magnetic properties. It is shown experimentally and theoretically that the filling of the flat bands is an essential parameter for understanding their properties. However, the behavior of a simple graphene layer is still unclear. Indeed, its half-filled case is well known and it has been studied by various theoretical approaches (mean-field theories (MFT), Monte Carlo) [2], but beyond half filling its magnetic properties are still unknown. Here, we present a detailed study of graphene magnetism using a combination of the Hubbard model and MFT. We focus on non half-filling cases, taking into account non-collinear magnetic moments.

[1] Y. Cao *et al.*, Nature **556**, 43 (2018); Nature **556**, 80 (2018)
[2] M. Raczkowski, R. Peters, T.T. Phùng, N. Takemori, F. F. Assaad, A. Honecker, J. Vahedi, Phys. Rev. B **101**, 125103 (2020), and references therein

TT 43.29 Wed 15:00 P2/OG3

Spectral densities of quantum magnets with quenched disorder using the coherent potential approximation and perturbative continuous unitary transformations — •Max Hörmann and Kai Phillip Schmidt — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

We combine perturbation theory by means of perturbative continuous transformations together with the coherent potential approximation to derive approximations for the averaged spectral density of the antiferromagnetic dimer-diluted Heisenberg bilayer model and the spin-diluted transverse-field Ising model on the square latttice. To this end, we calculate a dilution dependent series for the real and imaginary part of the one quasi-particle self-energy. While the real part shifts the extremal energy of the spectral density for fixed momentum the imaginary part reflects the finite-lifetime of momentum modes. Using extrapolations we study the applicability of this approach to critical behaviour and derive approximations for averaged spectral densities in non-perturbative regimes.

TT 43.30 Wed 15:00 P2/OG3

The influence of continuous electric bias fields on the dielectric loss of atomic tunneling systems — •Jan Blickberndt, Christian Ständer, Lukas Münch, Marcel Haas, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg, Germany

The low temperature properties of amorphous solids are dominated by atomic tunneling systems (TSs), which are known to act as a major source of noise and decoherence in superconducting quantum devices. We investigate the non-equilibrium dielectric loss of atomic tunneling systems under the influence of continuous electric bias fields at very low temperatures. The dielectric loss of an amorphous sample is obtained by measuring the quality factor of a micro-fabricated superconducting resonator. Simultaneously, an electric bias field can be applied via a cover electrode, which allows us to sweep TSs through the resonance frequency by modulating their energy splitting. Experimentally, we found that for slow changing bias fields, TSs are saturated by the driving field leading to a constant loss. For faster bias rates, more and more TSs are swept through resonance and therefore contribute to an increasing loss. In the limit of fast continuous bias sweeps, relaxation in between consecutive crossings diminishes and multiple coherent Landau-Zener transitions are possible, reducing the loss back to the saturation limit. We are able to verify these experimental results with a Monte Carlo based numerical simulation that shows good qualitative agreement.

TT 43.31 Wed 15:00 P2/OG3

Electrically and acoustically biased resonators for investigations of dielectric low temperature properties of amorphous solids — •Christian Ständer, Jan Blickberndt, Joyce Glass, Benedikt Frey, Andreas Reifenberger, 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 tunnelling systems, which can be described as two-level systems (TLS) with a distribution of their energy splitting E, as assumed by the phenomenological standard tunnelling model. Recent interest in these systems due to their deteriorative effects on the performance of superconducting quantum devices lead to novel experimental investigations of atomic tunnelling systems driven by novel measurement techniques.

We use newly designed microfabricated superconducting LC-resonators to study the dielectric rf-response of the amorphous sample in the presence of an electric bias field. A novel method of applying this electrical bias field was introduced to the resonators. Compared to previous experiments, the bias field is applied via an electrode placed above the resonator chip. We present first results of this new way of introducing a bias, which modifies the energy splitting E of a TLS.

In addition we tried to achieve a similar effect as with the electrical bias field with a mechanical strain field. To induce such a strain field, the amorphous substrate of the resonator chip was flexed by a piezo-actuator.

TT 43.32 Wed 15:00 P2/OG3

Investigating the Non-Equilibrium Dynamics of Two-Level Systems at Low Temperatures — •Marcel Haas, Mareike Dinger, Lukas Münch, Jan Blickberndt, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg, Germany

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), which are broadly distributed 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 decoherence time 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. The setup shows a unique property when two off-resonant pump tones are applied symmetrically. In this limit, the resonator is emitting at the intermediate frequency of the driving fields. The underlying mechanism can therefore be explained by a nonlinear interaction of the rf-field with the TLSs and the resonator which is creating additional lines in the frequency spectrum. We present measurements and a phenomenological describtion of the effect for a frequency of 1 GHz.

TT 43.33 Wed 15:00 P2/OG3

Machine learning stochastic dynamics of order parameters — •Francesco Carnazza[1], Federico Carollo[1], Igor Lesanovsky[1], Georg Martius[2], Sabine Andergassen[1], and Miriam Klopotek[3] — [1]University of Tuebingen — [2]Max Planck Institute for Intelligent Systems — [3]University of Stuttgart

The dynamics of coarse-grained observables, or of order-parameters, in many-body systems is usually rather intricate due to emergent nonlinearities and collective effects. In fact, except for few exactly solvable models, it is typically not possible to find the form of the differential equation describing the dynamics of these observables. Here, we address this problem exploiting a machine learning approach. We consider single trajectories of the thermal dynamics of a two-dimensional Ising model and feed these to a neural network. These trajectories, simulated by Monte Carlo methods, are intrinsically stochastic. Their dynamics can be approximated by a stochastic differential equation parametrised by a smooth term, the drift, and one multiplied by the differential of a Wiener process, that is, the diffusion.

In [1] a neural solver for stochastic differential equation was introduced, by means of which the drift and diffusion terms are approximated by neural networks. A classical integration method, e.g., Euler-Maruyama, is then adopted to recover full trajectories. We adopt this method to learn the drift and diffusion terms and infer the properties of the Ising model.

[1] Li et al., PMLR 108:3870-3882,2020.

TT 44: Focus Session: Superconducting Nickelates I

The discovery of superconductivity in hole-doped infinite-layer nickelates in 2019 has brought a breath of fresh air to the research on unconventional superconducting materials. These nickel oxides structurally closely resemble high-T_c cuprates and show a formally analogous nickel $d^{9-\delta}$ electronic configuration. Other striking similarities with cuprates have been recently reported, such as a dome-like doping dependence of the superconducting phase, sizeable antiferromagnetic exchange couplings, and a charge order instability in the underdoped region of the phase diagram. Likewise, a number of studies identified clear differences, e.g. concerning selected transport behavior as well as magnetic properties, and with regard to the relevance of oxygen-2p states. It is precisely this combination of strong similarities and specific differences that promises new, game-changing insights into the origin of high-temperature superconductivity. The goal of this focus seesion is to bring together the latest results for low-valence nickelates from studies of structure, electronic structure, magnetism, charge density waves and superconductivity, and thus setting the stage for a coherent picture of these complex quantum materials.

Organizers: Eva Benckiser (Max-Planck-Institute for Solid State Research, Stuttgart) and Frank Lechermann (Ruhr-Universität Bochum)

Time: Thursday 9:30–13:00 Location: HSZ 03

Invited Talk TT 44.1 Thu 9:30 HSZ 03

Atomic-scale insights to lattice and electronic structure in superconducting nickelates — •Berit Goodge — School of Applied and Engineering Physics, Cornell University — Kavli Institute at Cornell for Nanoscale Science, Cornell University — Max Planck Institute for Chemical Physics of Solids

Although the synthesis of superconducting nickelates [1,2] remains notoriously challenging [3,4], many materials realities including epitaxial strain, extended defects, impurities, and secondary phases are largely undiscussed in the context of understanding their measured properties. As direct probes of lattice and electronic structure down to the atomic scale, scanning transmission electron microscopy (STEM) and electron energy loss spectroscopy (EELS) offer unique insights to build a holistic understanding of both the intrinsic physical properties in these materials as well as more extrinsic features and their consequences, many of which arise from their multistep synthesis. Here, we discuss how quantitative lattice-scale measurements can disentangle many of these effects, revealing, for example, multi-band hole interactions [5], nontrivial interface reconstruction [6], and the impact of epitaxial strain [2, 7].

[1] Li et al., Nature 572, 624 (2019)
[2] Lee et al., arXiv:2203.02580 (2022)
[3] Lee et al., APL Mat. 8:4, 041107 (2020)
[4] Pan et al., Nat. Mat. 21, 160 (2022)
[5] Goodge et al., PNAS 118:2, (2021)
[6] Goodge et al., arXiv:2201.03613 (2022)
[7] Segedin et al., under review (2022)

Invited Talk TT 44.2 Thu 10:00 HSZ 03

Nickelate and cuprate superconductors: Similar yet different — •Vamshi Mohan Katukuri — Max Planck Institute for Solid State Research, Stuttgart, Germany

The discovery of superconductivity in hole-doped infinite-layer $NdNiO_2$ – a transition metal oxide that is both isostructural and isoelectronic to cuprate superconductors – has lead to renewed enthusiasm in the hope of understanding the origin of unconventional superconductivity. In this talk, I will present and discuss the similarities and differences in the electronic structure of nickelates and cuprates from the perspective of *ab initio* many body wavefunction analysis derived from state-of-the-art quantum chemistry calculations. After highlighting the main differences in the parent (undoped) infinite-layered $NdNiO_2$ and $CaCuO_2$ compounds, I will discuss the character of the doped hole by analyzing the electron-removal (which mimics hole-doping) states in the two compounds. In the end, I will discuss the evolution of the electronic structure of nickelates under pressure.

Invited Talk TT 44.3 Thu 10:30 HSZ 03

Superconducting instabilities in strongly-correlated infinite-layer nickelates — •Andreas Kreisel — Niels Bohr Institute, University of Copenhagen, Denmark

Unconventional superconductivity is often referred to as originating from a pairing mechanism different from electron-phonon interactions and connected to an anisotropic superconducting order parameter with sign change of the Cooper pair wavefunction. In this talk, I will start from a discussion of the mechanism of spin-fluctuation mediated pairing that can lead to d-wave states as evidenced in the cuprate superconductors, but also the sign-changing $s_\pm$ state that seems to be realized in Fe-based superconductors. The discovery of superconductivity in infinite-layer nickelates has immediately posed the question about the pairing mechanism and the pairing symmetry in this system and sparked proposals of analogs towards well studied families of materials in the class of unconventional superconductors. To connect to this open question, the leading superconducting instability is computed from magnetic fluctuations relevant for infinite-layer nickelates incorporating the strongly correlated multi-orbital nature of the low-energy electronic degrees of freedom. Observing the interplay between the Ni $d_{x^2-y^2}$ and d_{z^2} orbitals as well as the self-doping band, a transition from d-wave pairing symmetry to nodal $s_\pm$ superconductivity is uncovered. This is driven by strong fluctuations in the d_{z^2}-dominated orbital states. As probe of the detailed superconducting gap structure, we discuss the properties of the resulting superconducting condensate in light of tunneling and penetration depth experiments.

15 min. break

Invited Talk TT 44.4 Thu 11:15 HSZ 03

Infinite-layer nickelate thin films: From synthesis to spectroscopy — •Daniele Preziosi — Université de Strasbourg, CNRS, IPCMS UMR 7504, F-67034 Strasbourg, France

In the last three decades, special efforts were devoted to the realization of nickelates mimicking the electronic structure of cuprates. These efforts led to the realization of infinite-layer nickelates characterized by a stable $Ni-3d^9$ configuration and reduced dimensionality. A superconducting state below 15 K was reported for $Nd_{0.8}Sr_{0.2}NiO_2$ thin films deposited onto (001) $SrTiO_3$ (STO). Soon after this discovery, x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) experiments on undoped ($LaNiO_2$, $NdNiO_2$) and doped ($Nd_{1-x}Sr_xNiO_2$) samples showed that infinite-layer nickelates show some important differences compared to layered cuprates, in particular a larger charge transfer energy and an important Nd 5d-Ni 3d hybridization. In this talk, after introducing our efforts to stabilize the infinite-layer phase, I will show that some of those aforementioned differences depend also on the presence/absence of a STO-capping-layer. A robust charge order is observed in undoped capping-free thin films, while strong magnetic excitations around 200 meV energy-loss characterize capped samples. Polarization-resolved RIXS measurements unambiguously demonstrated that also the low-energy excitations for uncapped samples are magnetic in nature, but largely damped. The 'altered' doping effect as observed from the enlarging of the XAS feature at the NiL_3-edge combined to a strong $Ni3d-Nd5d$ hybridization for uncapped samples, may speak in favor of this extra softening.

Invited Talk TT 44.5 Thu 11:45 HSZ 03

Superconducting layered square-planar nickelates: Synthesis, properties, and progress — •Grace Pan[1], Dan Ferenc Segedin[1], Harrison LaBollita[2], Qi Song[1], Berit Goodge[3], Lena Kourkoutis[3], Charles Brooks[1], Antia Botana[2], and Julia Mundy[1] — [1]Harvard University, Cambridge, MA, USA — [2]Arizona State University, Tempe, AZ, USA — [3]Cornell University, Ithaca, NY, USA

Since the discovery of high-T_c superconductivity in the cuprates, there have been sustained efforts to both understand the origins of this phase and discover new cuprate-like superconductors. One prime materials platform has been the rare-earth nickelates; indeed, superconductivity was discovered in the doped compound $Nd_{0.8}Sr_{0.2}NiO_2$ in 2019. Undoped $NdNiO_2$ belongs to a series of layered square-planar nickelates with chemical formula $Nd_{n+1}Ni_nO_{2n+2}$ and is known as the infinite-layer (n=∞) nickelate. Here, we describe the synthesis of the quintuple-layer (n=5) member, $Nd_6Ni_5O_{12}$, in which optimal cuprate-like electron filling ($d^{8.8}$) is achieved without chemical doping. We observe a superconducting transition beginning at $\sim$13 K. Electronic structure calculations fortified with experiments suggest that $Nd_6Ni_5O_{12}$ interpolates between cuprate-like and infinite-layer nickelate-like behaviour. By engineering a distinct superconducting nickelate, we identify the square-planar nickelates as a new family of superconductors that can be tuned via both doping and dimensionality. In this talk, I will further discuss ongoing experimental progress on the synthesis and characterization of these layered nickelates.

TT 44.6 Thu 12:15 HSZ 03

Nickelate superconductors: One-band Hubbard model plus decoupled A pocket picture — •Karsten Held[1], Motoharu Kitatani[2], Liang Si[1,3], and Paul Worm[1] — [1]Institute for Solid State Physics, TU Wien, Austria — [2]University of Hyogo , Japan — [3]Northwest University, Xi'an, China

At first glance, nickelate superconductors appear to be more complicated than their cuprate peers. Based on density functional theory (DFT) plus dynamical mean-field theory (DMFT) we however arrived at a picture that the physics of nickleate superconductors is dominated by the Ni $d_{x^2-y^2}$-band and the pockets are, in many respects, merely passive bystanders [1]. Other groups have argued instead for the importance of the Ni d_{z^2}-band based, e.g., on self-interaction corrected (sic)DFT+DMFT [2].

Taken the premise of a $d_{x^2-y^2}$-band Hubbard model description, we have predicted the phase diagram, superconducting critical temperature T_c vs. doping x [1]. Later experiments synthesizing high-quality films are in excellent qualitative and even quantitative agreement [3], as is the resonant inelastic x-ray (RIXS) spectrum. Also the pentalayer nickelate superconductor which has no pockets in DFT+DMFT and the increase T_c with pressure nicely match this picture [4].

[1] M. Kitatani *et al.*, npj Quantum Materials 5, 59 (2020)
[2] F. Lechermann, Phys. Rev. B 101, 081110 (2020);
A. Kreisel *et al.*, Phys. Rev. Lett. 129, 077002 (2022)
[3] K. Lee *et al.*, arXiv:2203.02580
[4] P. Worm *et al.*, Phys. Rev. Mater. 6, L091801 (2022)

TT 44.7 Thu 12:30 HSZ 03

Single-layer T' nickelates — Kerstin Wissel[1], Fabio Bernardini[2], Heesu Oh[2], Sami Vasala[3], Björn Blaschkowski[2], Pieter Glatzel[3], Matthias Bauer[4], Olivier Clemens[1], and •Andrés Cano[5] — [1]University of Stuttgart, Stuttgart, Germany — [2]University of Cagliari, Cagliari, Italy — [3]ESRF, Grenoble, France — [4]Padeborn University, Padeborn, Germany — [5]Institut NEEL, CNRS, Grenoble, France

The discovery of superconductivity in the infinite-layer nickelates has renewed the interest in these potential analogs of the high-Tc cuprates motivating the search for additional materials in this class [1]. In the talk, I will introduce the recently synthesised single-layer T' nickelates [2,3] and discuss their structural and electronic properties in relation to previous nickelates and cuprates.

[1] See e.g. A. Botana, F. Bernardini and A. Cano, JETP 159, 711 (2021) for a review.
[2] K. Wissel et al., Chem. Mater. 32, 3160 (2020)
[3] K. Wissel et al., Chem. Mater. 34, 7201 (2022)

TT 44.8 Thu 12:45 HSZ 03

Synthesis and physical properties of perovskite and infinite-layer nickelate crystals — •Pascal Puphal[1], Vignesh Sundaramurthy[1], Valentin Zimmermann[1], Björn Wehinger[2], Gaston Garbarino[2], Kathrin Küster[1], Ulrich Starke[1], Jürgen Nuss[1], Bernhard Keimer[1], Masahiko Isobe[1], and Matthias Hepting[1] — [1]Max Planck Institute for Solid State Research — [2]European Synchrotron Radiation Facility

Infinite-layer (IL) nickelates are an emerging family of superconductors whose synthesis in thin film form is an established process by now, whereas the growth of their bulk counterparts remains a formidable challenge. In a previous study, we achieved the reduction of perovskite La1-xCaxNiO3 single-crystals grown by a flux method under high external pressure to the IL phase $La_{1-x}Ca_xNiO_2$ [1]. The typical lateral dimension of these crystals was 150 μm. As an advanced approach, we recently accomplished the reduction of millimeter-sized $LaNiO_3$ crystals obtained by optical floating zone growth under high oxygen gas pressure to the IL phase $LaNiO_2$ [2]. We will present our characterization of the crystalline, magnetic, and electronic properties of the $LaNiO_2$ crystals, and give an outlook on the synthesis of millimeter-sized crystals of pure $LaNiO_3$ and $PrNiO_3$ as well as ones with hole- and electron doping.

[1] P. Puphal *et al.*, Sci. Adv. 7, eabl8091 (2021)
[2] P. Puphal *et al.*, arXiv:2209.12787 (2022)

TT 45: Correlated Electrons: 1D Theory

Time: Thursday 9:30–12:15 Location: HSZ 103

TT 45.1 Thu 9:30 HSZ 103

On the alternating spin chain with continuous spectrum of scaling dimensions — Mouhcine Azhari and •Andreas Klümper — Universität Wuppertal

We investigate the low-lying spectrum of an integrable staggered Heisenberg spin-1/2 chain possessing in the large length (L) limit a CFT structure with logarithmic corrections ($1/(\log L)^2$). This realizes a continuous spectrum of conformal weights similar to that of for instance the $SL(2,R)/U(1)$ black hole sigma model.

The quantum spin chain is exactly "solvable" by Bethe ansatz and other techniques from the theory of integrability. However, the analysis of the resulting Bethe Ansatz equations is challenging and manageable by numerical techniques only for relatively small sizes L. Integral equations for the distribution functions of the Bethe roots suffer from singularities of the kernel functions.

Due these phenomena and challenges the model attracted interest by several groups of authors (Ikhlef, Jacobsen, Saleur 08, 12; Frahm, Martins 12; Candu, Ikhlef 13; Frahm, Seel 14; Bazhanov, Kotousov, Koval, Lukyanov 20).

In our contribution we report on recent progress allowing us to rewrite already existing non-linear integral equations (NLIE) with a singular, i.e. long-ranged kernel in a novel form without such problems. We present results for the lowest lying excitations for system sizes $L = 10, 10^2, 10^3, ..., 10^9, ...$

TT 45.2 Thu 9:45 HSZ 103

Electron spin resonance as a direct probe of spinon interactions in a $S = 1/2$ chain — •Kirill Povarov[1,2], Timofei Soldatov[3], Ren-Bo Wang[4], Andrey Zheludev[1], Alexander Smirnov[3], and Oleg Starykh[4] — [1]Laboratory for Solid State Physics, ETH Zürich — [2]Dresden High Magnetic Field Laboratory (HLD), Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [3]P.L. Kaptiza Institute for Physical Problems RAS — [4]Department of Physics and Astronomy, University of Utah

The presence of well-hidden backscattering between the fractionalized spinon excitations was known to be a somewhat exotic part of the $S = 1/2$ chain physics. However, its dramatic consequences for the dynamics were realized recently [1]. They are challenging for observation, as applied field and nonzero momenta are simultaneously required. We have succeeded in the experimental verification of these effects using electron spin resonance as probe [2]. Our observations are enabled by the specific pattern of Dzyaloshinskii–Moriya interactions in our target material $K_2CuSO_4Br_2$. Description of the observed spectrum requires accounting for the backscattering on a qualitative level. Quantitative analysis allows us to estimate the backscattering constant as $2.4J$ (intrachain exchange), in agreement with the renormalization group predictions. This work has been supported by SNSF Division II (ETHZ), the NSF CMMT grant DMR-1928919 (U. Utah), and the RSF Grant 17-12-01505 (IPP).

[1] A. Keselman *et al.*, PRL **125**, 187201 (2020)
[2] K. Povarov *et al.*, PRL **128**, 187202 (2022) *Editor's Suggestion*

TT 45.3 Thu 10:00 HSZ 103

Dominant superconducting correlations in a Luttinger liquid induced by spin fluctuations — •Niels Henrik Aase and Asle Sudbø — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

In the last decades, heterostructures of magnetic materials and various conductors have received much attention. Several studies have focused on the emergent interfacial phenomena and their possible application in spintronic devices. Motivated by this, we study the simplest equivalent heterostructure in one dimension: an interacting metallic chain coupled to a spin chain. Confining interacting electrons to one dimension causes the breakdown of Fermi liquid theory, so our study provides insight into how spin fluctuations can induce superconductivity in a strongly correlated non-Fermi liquid with repulsive electronic interactions only.

Treating the system using bosonization, we calculate the correlation functions of the electrons in the metal. Based on the non-universal power-law decay of different order parameters, we outline the electron phase diagram as a function of the interchain coupling and the interactions in the metal. The coupling favors triplet pairing, suggesting that the metal chain can sustain a spin-polarized supercurrent. In some parameter regimes, the superconducting triplet correlations persist in the case of repulsive interactions in the metal. The spin chain is thus an essential ingredient for overcoming electron repulsion in a Luttinger liquid.

TT 45.4 Thu 10:15 HSZ 103

The role of electron-electron interactions in electron emission from arrays of nanotubes — •Naira Grigoryan[1] and Piotr Chudzinski[1,2] — [1]Institute of Fundamental Technological Research, Polish Academy of Sciences, Adolfa Pawinskiego 5b, 02-106 Warsaw, Poland — [2]School of Mathematics and Physics, Queen's University Belfast, University Road, Belfast, NI BT7 1NN, United Kingdom

Nanotubes and nanorods have been recently established as very good materials to build electron sources in the cold emission process. These are 1D materials where electron-electron interactions are known to play a crucial role in their physics. The interactions in 1D systems lead to a collective modes' physics that is usually described using Tomonaga-Luttinger liquid (TLL) formalism. The advantage is that within this method all correlation functions are known and can be expressed in terms of power laws with non-universal, interaction dependent, exponents. To capture this situation we generalize a canonical Fowler-Northeim theory of field emission to solve the case of a barrier described by any power-law potential. With this generalization, expressed in terms of a confluent hypergeometric function, we are able to compute currents from arrays of carbon nanotubes. We shall present results showing an influence of various interaction terms, as encoded in varying TLL parameters, as well as effects of a finite temperature.

TT 45.5 Thu 10:30 HSZ 103

Delta-T noise for weak tunneling in one-dimensional systems: interactions versus quantum statistics — Gu Zhang[1], Igor V. Gornyi[2], and •Christian Spanslatt[3] — [1]Beijing Academy of Quantum Information Sciences, 100193 Beijing, China — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, S-412 96 Göteborg, Sweden

Delta-T noise - excess charge noise at zero charge current but due to a finite temperature bias - has recently emerged as a novel transport spectroscopy tool for mesoscopic systems. In this talk, I present recent work [1] on delta-T noise for weak tunneling in one-dimensional, interacting systems. We show that the sign of the delta-T noise is generically determined by the scaling dimensions of the dominating tunneling process. Importantly, we clarify how this sign can be related to the quantum exchange statistics of the tunneling quasiparticles.

In systems with interacting and chiral channels, we find that when the delta-T noise is negative, the tunneling particles are boson-like, revealing their tendency towards bunching. Thus, one might expect that negative delta-T noise is a smoking gun for detecting "intrinsic anyons". Here, we find that this is not the case, since boson-like particles do not necessarily produce negative delta-T noise. Our findings clarify how delta-T noise can be used to probe the nature of collective excitations in interacting one-dimensional systems.

[1] G. Zhang, I. V. Gornyi, C. Spånslätt, PRB 105, 195423 (2022)

TT 45.6 Thu 10:45 HSZ 103

Terminable transitions in a topological fermion ladder — Yuchi He[1,2], Dante Kennes[2,3], Christoph Karrasch[4], and •Roman Rausch[4] — [1]Rudolf Peierls Centre for Theoretical Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom — [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]Technische Universität Braunschweig, Institut für Mathematische Physik, Mendelssohnstraße 3, 38106 Braunschweig, Germany

Interacting fermion ladders are important platforms to study quantum phases of matter including various Mott-insulators with different symmetry properties, such as the D-Mott and S-Mott phase. The latter hold pre-formed electron pairs and become paired liquids (d-wave and s-wave) upon doping. We show that the D-Mott and S-Mott phases are in fact two facets of the same topological phase and that the transition between them is terminable. With this, we provide a quantum analog of the well-known terminable liquid-gas transition. However, the phenomenology we uncover is even richer, as in contrast to the liquid-gas transition, the order of the transition can be tuned by the interaction and bears relevance for the topological properties of the system. The numerical results are obtained using the variational uniform matrix-product state (VUMPS) formalism, and are complemented by analytical field-theoretical explanations.

15 min. break

TT 45.7 Thu 11:15 HSZ 103

Critical and topological phases of a dimerized Kitaev chain in the presence of a quasiperiodic potential — •Saurabh Basu[1], Sk Noor Nabi[2], and Shilpi Roy[1] — [1]Department of Physics, Indian Institute of Technology Guwahati-Guwahati, 781039 Assam, India — [2]Department of Physics, Indian Institute of Technology Kharagpur, Kharagpur - 721302, West Bengal, India

We investigate the localization and topological properties of a dimerized Kitaev chain with p-wave superconducting correlations and a quasiperiodically modulated chemical potential. In the localization studies, we illustrate the existence of distinct phases, such as, the extended phase, the critical (intermediate) phase, and the localized phase that arise due to the competition between the dimerization and the onsite quasiperiodic potential. Most interestingly, the critical phase comprises of two distinct phase transitions that are found to exist between the extended to the localized phase, and between the critical (multifractal) and localized phases. Furthermore, we study the topological properties of the zero-energy edge modes via computing the real-space winding number and number of the Majorana zero modes present in the system. We specifically demonstrate that our model undergoes a phase transition from a topologically trivial to a non-trivial phase (topological Anderson phase) beyond a critical dimerization strength under the influence of the quasiperiodic potential strength. Finally, in presence of a large potential, we demonstrate that the system undergoes yet another transition from the topologically non-trivial to an Anderson localized phase.

TT 45.8 Thu 11:30 HSZ 103

Statistics induced phase transitions in the extended bosonic anyon Hubbard model — •Imke Schneider[1], Kevin Jägering[1], Martin Bonkhoff[1], Shijie Hu[2], Axel Pelster[1], and Sebastian Eggert[1] — [1]Department of Physics and Research Center Optimas, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Beijing Computational Science Research Center, Beijing 100193, China

We study a 1D extended Hubbard model of anyons with statistical exchange phases ranging from bosons to pseudo-fermions. The model can be realized in optical lattice experiments implementing occupation-dependent hopping amplitudes. We enforce a two-body hard-core constraint and numerically determine the full phase diagram including attractive on-site interactions. Surprisingly, the symmetry protected topological Haldane phase remains robust up to large statistical angles close to the pseudo-fermionic limit. However, for a critical angle the phase diagram qualitatively changes involving a dimer phase while the Haldane phase disappears. This behavior is analytically described by an adapted bosonization approach.

TT 45.9 Thu 11:45 HSZ 103

Fractonic Luttinger liquids and supersolids in a constrained Bose-Hubbard model — •Philip Zechmann[1,2], Ehud Altman[3], Michael Knap[1,2], and Johannes Feldmeier[1,2,4] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MC-QST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, University of California, Berkeley, CA 94720 — [4]Department of Physics, Harvard University, Cambridge, MA 02138, USA

Quantum many-body systems with fracton constraints are widely conjectured to exhibit unconventional low-energy phases of matter. In this work, we demonstrate the existence of a variety of such exotic quantum phases in the ground states of a dipole-moment conserving Bose-Hubbard model in one dimension. For integer boson fillings, we perform a mapping of the system to a model of microscopic local dipoles, which are composites of fractons. We apply a combination of low-energy field theory and large-scale tensor network simulations to demonstrate the emergence of a novel dipole Luttinger liquid phase. At non-integer fillings our numerical approach shows an intriguing compressible state described by a quantum Lifshitz model in which charge density-wave order coexists with dipole long-range order and superfluidity - a 'dipole supersolid'. While this supersolid state may eventually be unstable against lattice effects in the thermodynamic limit, its numerical robustness is remarkable. We discuss potential experimental implications of our results.

TT 45.10 Thu 12:00 HSZ 103

Phase diagram detection via Gaussian fitting of number probability distribution — Daniele Contessi[1,2,3], Alessio Recati[1], and •Matteo Rizzi[2,3] — [1]Università di Trento & INO-CNR Pitaevskii BEC Center, Povo, Italy — [2]Peter-Grünberg-Institut 8, FZ Jülich, Germany — [3]Institute for Theoretical Physics, University of Cologne, Germany

In recent years, methods for automatic recognition of phase diagrams of quantum systems have gained large interest in the community: Among others, machine learning analysis of the entanglement spectrum has proven to be a promising route. Here, we discuss the possibility of using an experimentally readily accessible proxy, namely the number probability distribution that characterizes sub-portions of a quantum many-body system with globally conserved number of particles. We put forward a linear fitting protocol capable of mapping out the ground-state phase diagram of the rich one-dimensional extended Bose-Hubbard model: The results are quantitatively comparable with more sophisticated traditional numerical and machine learning techniques. We argue that the studied quantity should be considered among the most informative and accessible bipartite properties.

[1] D. Contessi, A. Recati, M. Rizzi, arXiv:2207.01478

TT 46: Frustrated Magnets: Spin Liquids

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

TT 46.1 Thu 9:30 HSZ 201

Magnetic and elastic properties of spin ice materials in high magnetic fields — •Nan Tang[1,2], Masaki Gen[3], Mingxuan Fu[2], Huiyuan Man[4], Akira Matsuo[5], Koichi Kindo[5], Akihiko Ikeda[5,6], Yasuhiro H. Matsuda[5], Kazuyuki Matsuhira[7], Yoshimitsu Kohama[5], and Satoru Nakatsuji[2,5] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Department of Physics, University of Tokyo, Tokyo, Japan — [3]Riken Center for Emergent Matter Science, Saitama, Japan — [4]Geballe Laboratory for Advanced Materials, Stanford University, California, U.S.A. — [5]ISSP, University of Tokyo, Chiba, Japan — [6]Department of Engineering Science, University of Electro-Communications, Tokyo, Japan — [7]Department of Engineering, Kyushu Institute of Technology, Fukuoka, Japan

Spin ice is a prototypical state of frustrated magnets, in which Ising spins form a short-range "2-in, 2-out" correlation instead of a long-range order due to geometrical frustrations of pyrochlore lattice. Local Ising anisotropy induced by the competition between crystal electric field (CEF) effect and magnetic interactions play important roles to stabilize such spin-ice correlations. Generally, frustrated magnets show characteristic magnetostrictive responses and in this study, we measured both magnetization and magnetostriction of classical spin ice $Ho_2Ti_2O_7$ and quantum spin ice $Pr_2Zr_2O_7$ under high magnetic fields to explore the regime beyond the Ising limit. In the talk, we will discuss the influences of CEF splitting and exchange-striction on the magnetostrictive responses in the two spin ice materials.

TT 46.2 Thu 9:45 HSZ 201

XMCD studies of honeycomb lattice compound $RuBr_3$ — •Sahana Roessler[1], X. Wang[1], S. Agrestini[2], Z. Hu[1], C. Guillemard[3], J. Herrero-Martin[3], U. Schwarz[1], M. W. Haverkort[4], and L. H. Tjeng[1] — [1]Max-Planck Institute for Chemical Physics of Solids, Dresden Germany — [2]Diamond Light Source, Oxfordshire, United Kingdom — [3]ALBA Synchrotron Light source, Barcelona, Spain — [4]Institute of theoretical physics, Heidelberg University, Germany.

The high-pressure phase of $RuBr_3$ consisting of a honeycomb lattice [1] is structurally essentially isotypic to the Kitaev quantum spin liquid candidate α-$RuCl_3$. As in α-$RuCl_3$, Ru^{3+} ion in $RuBr_3$ is in $4d^5$ electronic configuration and expected to be in a spin-orbit coupled J_{eff} =1/2 doublet ground state. Here, we will present the results of X-ray magnetic circular dichroism (XMCD) measurements on $RuBr_3$ performed at the Ru $L_{2,3}$ absorption edges. The spin and orbital moments were determined using the sum rule analysis. In addition, the XMCD spectra were simulated using the full atomic-multiplet cluster calculations within the configuration interaction approach. By comparing the experimental spectra with the theoretical simulations, we determined the ratio of spin to orbital moments along with the values of the crystal field splitting and the spin-orbit coupling in $RuBr_3$. Our results indicated the $J_{\text{eff}} = 1/2$ ground state for $RuBr_3$, which is one of the requisites for the Kitaev quantum spin-liquid behavior. [1] Imai et al., Phys. Rev. B 105, L041112 (2022).

TT 46.3 Thu 10:00 HSZ 201

Structural transition in single crystals of Kagome compound $Y_3Cu_9(OH)_{19}Cl_8$ — •Katharina M. Zoch[1], Pascal Puphal[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Kagome systems serve as the ideal candidates to obtain an experimental realization of a quantum spin liquid, a class of matter where the spins strongly fluctuate down to lowest temperatures, thus preventing order. $Y_3Cu_9(OH)_{19}Cl_8$ presents a distorted Kagome lattice with a rich magnetic phase diagram [1]. The improved synthesis of phase-pure single crystals crystals via an external gradient method lead to the evidence of subtle structural instabilities at 33 K and 13 K in thermodynamic measurements while preserving the magnetic model of the system. The compound shows a magnetic phase transition at 2.2 K with persistent spin dynamics below the ordered state in powder samples [2]. We present the single crystal growth as well as thermodynamic and magnetic measurements of this compound.

[1] M. Hering et al., npj Comput. Mater. 8, 10 (2022)
[2] Q. Barthelemy et al., Phys. Rev. Mater. 3, 074401 (2019)

TT 46.4 Thu 10:15 HSZ 201

Thermodynamics of the spin liquid candidate $KYbS_2$ — •Franziska Grussler[1], Sebastian Bachus[1], Noah Winterhalter-Stocker[1], Mamoun Hemmida[2], Hans-Albrecht Krug von Nidda[2], Yurii Skourski[3], Philipp Gegenwart[1], and Alexander Tsirlin[4] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg — [3]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf — [4]Felix Bloch Institute for Solid-State Physics, University of Leipzig

Triangular antiferromagnets with competing nearest-neighbor and next-nearest-neighbor interactions offer a promising playground for realizing quantum spin liquid behavior. However, detailed nature of this state and its manifestations in real materials remain heavily debated. Here, we show that a quantum disordered, potentially spin liquid state can be realized in the disorder-free triangular antiferromagnet $KYbS_2$ and report its temperature-field phase diagram using heat capacity, dilatometry, magnetocaloric and magnetization measurements down to below 0.1 K. The phase diagram reveals an additional phase between the up-up-down and putative spin liquid phases, so far not observed in other members of the same structural family. Following a systematic analysis of the nuclear contribution and its evolution in the applied field, we conclude that at zero field the magnetic specific heat shows quadratic behavior in the low-T limit in accordance with the expectations for a gapless Dirac spin liquid.

TT 46.5 Thu 10:30 HSZ 201

Anisotropic phonon-spin scattering in the quantum spin liquid canidate $NaYbS_2$ — •Matthias Gillig[1,2], Xiaochen Hong[1,3], Ellen Häussler[2], Philipp Schlender[2], Thomas Doert[2], Bernd Büchner[1,2], and Christian Hess[1,3] — [1]IFW Dresden — [2]TU Dresden — [3]Bergische Universität Wuppertal

A perfect triangular spin lattice and absence of long-range magnetic order down to T = 260 mK make the delafossite material $NaYbS_2$ a prime candidate to host a quantum spin liquid ground state. We present the results of heat transport experiments on $NaYbS_2$ in the low-temperature limit ($T <$ 1 K), where the in-plane thermal conductivity κ_{ab} shows a peculiar temperature dependence mimicking a potential residual linear term that decays below 500 mK. Application of in-plane magnetic field drastically enhances the thermal conductivity until it saturates in the field polarized limit. This behavior hints at phonon dominated heat transport with very strong magnetic phonon scattering where magnetic field suppresses the phonon scattering off spin fluctuations and the phonon thermal conductivity recovers at high field. In the field-dependence of κ broad features appear that indicate possible field-induced phase transitions in the magnetic system. Within this framework no clear evidence for magnetic heat transport due to spin excitations is observed. The investigation of the anisotropy of κ reveals that the phonon-spin scattering is strongly anisotropic and the out-of-plane coupling of phonons to spin excitations is weakened.

TT 46.6 Thu 10:45 HSZ 201

Thermodynamics studies on RE_3BWO_9 (RE = Nd and Pr) spin-liquid candidate systems — •Ahmed Elghandour[1], P Khuntia[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]Department of Physics, IIT Madras, Chennai 600036, India

Boratotungstates exhibit a distorted Kagome structure of rare-earth ions (RE), thereby providing a platform to unveil the pure Kagome physics fully dominated by magnetic frustration of RE moments while avoiding the influence of conduction electrons. We report the thermodynamic properties of poly crystals of RE_3BWO_9 (RE = Nd and Pr) by means of means of DC magnetometry (0.4 - 350 K) and heat capacity studies (0.4 - 270 K). In Nd_3BWO_9, our dc magnetization and c_p data indicate a possible transition at $T = 1\ K$ while there is no evidence of long-range order at higher temperatures. This yields $\frac{\theta}{T_N} = 45$. Isotherm magnetization measured at $T = 400\ mK$, demonstrates saturation up to 7 T at half of the expected saturation magnetization, which we attribute to crystal-field effects. In addition, there are two low field anomalies at $\frac{1}{4}$ and $\frac{1}{8}$ of the theoretical saturation field. In contrast, Pr_3BWO_9 does not signal long-range order down to $T = 90\ mK$ [5] (i.e., $\frac{\theta}{T_N} > 300$) and M vs B only shows smooth right bending at $T = 400\ mK$ again with reduced saturation moment (0.8 μ_B/Pr at $B = 7\ T$). The data are discussed in terms of an unconventional persistent fluctuating paramagnetic ground state as suggested by recent NMR data [1].

[1] Zeng et al., PRB 104, 155150 (2021)

TT 46.7 Thu 11:00 HSZ 201

Low temperature phase diagram of $PbCuTe_2O_6$ for magnetic fields B || (110) — •Paul Eibisch[1], Christian Thurn[1], Ulrich Tutsch[1], Arif Ata[1], Abanoub R. N. Hanna[2], A. T. M. Nazmul Islam[2], Shravani Chillal[2], Bella Lake[2], Bernd Wolf[1], and Michael Lang[1] — [1]PI Goethe-University Frankfurt — [2]HZ Berlin

The quantum-spin-liquid (QSL) state shows interesting phenomena such as fractional spin excitations and spin entanglement. Here we investigate the spin-liquid-candidate system $PbCuTe_2O_6$ where antiferromagnetic interactions among $s = 1/2$ spins lead to a 3D network of triangles similar to the hyper-Kagome lattice. While first experiments on polycrystalline samples, were found to be consistent with the QSL state [1], a recent study on single crystals showed a far more complex scenario including a ferroelectric transition at $T = 1\,\mathrm{K}$ with strong lattice distortions and a quantum critical behaviour close to $B = 0\,\mathrm{T}$ [2]. For the present study we combine thermodynamic, dielectric and magnetic experiments to investigate the field- and temperature phase diagram of $PbCuTe_2O_6$ for fields up to $B = 14.5\,\mathrm{T}$ parallel to the [110] direction. In addition to the ferroelectric state we find a structurally distorted phase which coincides with the ferroelectric state at low fields but splits above $B = 6\,\mathrm{T}$ as well as a long-range magnetically ordered phase for fields $B > 11\,\mathrm{T}$. Based on our experimental results we discuss how the elastic, dielectric and magnetic degrees of freedom are coupled.

[1] S. Chillal *et al.*, Nat. Commun. **11**, 2348 (2020)
[2] C. Thurn *et al.*, npj Quantum Materials 6:95 (2021)

15 min. break

TT 46.8 Thu 11:30 HSZ 201

Delafossite magnet $AgCrSe_2$: frustration, short range correlations, and field-tuned anisotropic order — •Michael Baenitz[1], S. Luther[2,3], M. Piva[1], J. Sichelschmidt[1], M. Nicklas[1], H. Zhang[1], B. Schmidt[1], H. Rosner[1], D. Khalyavin[4], P. Manuel[4], J. Wosnitza[2,3], H. Kuehne[2], and M. Schmidt[1] — [1]MPI for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, 01062 Dresden Germany — [4]ISIS Neutron and Muon Source, Rutherford Appelton Laboratory, Chilton, Didcot OX11 OQX, United Kingdom

In contrast to Cr based oxy delafossites (DFs) with predominant antiferromagnetic (afm) nearest neighbor (nn) interaction in the Heisenberg triangular lattice, $AgCrSe_2$ as a non oxy DFs member is characterized by competing interactions (ferromagnetic nn- vs afm third neighbor interaction). Due to this, the magnetism, can be tuned by relatively small magnetic fields, allowing us to probe the H-T phase diagram in great detail. Large single crystals are grown by chemical vapor transport and studied by magnetization, specific heat, and thermal expansion and Cr-electron spin resonance and neutron diffraction as local probes. An anisotropic cycloidal ordering with unusual extended two-dimensional fluctuations is found [1]. The impact of antisymmetric interactions (Dzyaloshinskii-Moriya) due to the noncentrosymmetric polar space group (R3m) is discussed.

[1] M. Baenitz et al. PRB 104, 134410 (2021)

TT 46.9 Thu 11:45 HSZ 201

Dynamical signatures of symmetry broken and liquid phases in an $S = 1/2$ Heisenberg antiferromagnet on the triangular lattice — •Markus Drescher[1], Laurens Vanderstraeten[2], Roderich Moessner[3], and Frank Pollmann[1,4] — [1]TU München, 85748 Garching, Germany — [2]University of Ghent, 9000 Gent, Belgium — [3]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [4]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

We present the dynamical spin structure factor of the antiferromagnetic spin-$\frac{1}{2}$ $J_1 - J_2$ Heisenberg model on a triangular lattice obtained from large-scale matrix-product state simulations. The high frustration due to the combination of antiferromagnetic nearest and next-to-nearest neighbour interactions yields a rich phase diagram. We resolve the low-energy excitations both in the 120°-ordered phase and in the putative spin liquid phase at $J_2/J_1 = 0.125$. In the ordered phase, we observe an avoided decay of the lowest magnon-branch, demonstrating the robustness of this phenomenon in the presence of gapless excitations. Our findings in the spin-liquid phase chime with the field-theoretical predictions for a gapless Dirac spin liquid, in particular the picture of low-lying monopole excitations at the corners of the Brillouin zone. We comment on possible practical difficulties of distinguishing proximate liquid and solid phases based on the dynamical structure factor.

TT 46.10 Thu 12:00 HSZ 201

Generic interplay of magnetism and structural dimerization in pressured Kitaev materials — •Bin Shen[1], Franziska Breitner[1], Angel M. Arevalo-Lopez[2], Danil Prishchenko[3], Maximilian Seidler[1], Friedrich Freund[1], Anton Jesche[1], Philipp Gegenwart[1], and Alexander A. Tsirlin[1,4] — [1]EP VI, EKM, University of Augsburg, Germany — [2]University of Lille, France — [3]Yekaterinburg, Russia — [4]Felix Bloch Institute, University of Leipzig, Germany

Quantum spin liquids in the Kitaev honeycomb model feature quantum entanglement and exotic fractionalized spin excitations, thus attracting tremendous attention. However, experimental realization of Kitaev quantum spin liquid phases in real materials has been proven difficult due to the presence of competing interactions beyond Kitaev exchange. Almost all known structurally ordered Kitaev candidate materials host a magnetically ordered ground state. Suppression of the order by various tuning parameters is currently subject of extensive investigations. We explore the possibility of suppressing magnetic order by high-pressure magnetization measurements on several Kitaev materials under hydrostatic pressure and reveal a generic interplay of magnetism and structural dimerization: Upon applying hydrostatic pressure, structural dimerization emerges and becomes visible as step in the temperature dependence of the magnetic susceptibility that shifts to higher temperatures upon further compression. We also investigate how magnetic order disappears once dimerization emerges.

TT 46.11 Thu 12:15 HSZ 201

Variational States for the S=3/2 Kitaev spin liquids — •Willian Massashi Hisano Natori[1,2], Hui-Ke Jin[3], Frank Pollmann[3,4], and Johannes Knolle[2,3,4] — [1]Institut Laue-Langevin — [2]Imperial College London — [3]Technische Universität München — [4]Munich Center for Quantum Technology and Science

The lack of a mapping to free fermion models has for a long time prevented the analytical characterization of Kitaev spin liquids (KSLs) for general values of S. The most complicated of these spin liquids was the S=3/2 KSL, which defied both analytical and numerical techniques. This problem importance increased thanks to recent studies pointing out the relevance of Kitaev interactions on chromium-based van der Waals magnets.

We recently uncovered the ground state of the S=3/2 KHM perturbed by a single-ion anisotropy (SIA) using an SO(6) parton mean-field theory that displayed a remarkable quantitative agreement with DMRG simulations (Nat. Comm. 13, 3813). In this follow-up work, we uncover similarities between the S=3/2 KSL and the Majorana quantum spin-orbital liquids that emerge as ground states of exactly solvable Kugel-Khomskii models. We show that expectation values of several observables can be exactly calculated over a set of parton wavefunctions without Gutzwiller-projection, including the own KHM, quadrupolar parameters and correlation functions. The S=3/2 KSLs are then identified to the Gutzwiller projection of the state in this set minimizing the energy.

TT 46.12 Thu 12:30 HSZ 201

Linked-cluster expansions of perturbed topological phases — •Viktor Kott, Matthias Mühlhauser, and Kai Phillip Schmidt — FAU, Erlangen-Nürnberg, Deutschland

We investigate the robustness of Kitaev's toric code in a uniform magnetic field on the square and honeycomb lattice by perturbative linked cluster expansions using a full graph decomposition. In particular, the full graph decomposition allows to correctly take into account the non-trivial mutual exchange statistics of the elementary anyonic excitations. This allows us to calculate the ground-state energy and excitation energies of the topological phase which are then used to study the quantum phase transitions out of the topologically ordered phase as a function of the field direction.

TT 46.13 Thu 12:45 HSZ 201

Spin-Peierls instability of the U(1) Dirac spin liquid — •Josef Willsher[1], Urban Seifert[2], and Johannes Knolle[1,3,4] — [1]TU Munich, Germany — [2]Kavli Institute, University of California, Santa Barbara, USA — [3]MCQST, Munich, Germany — [4]Imperial College London, UK

Quantum spin liquids are tantalising phases of quantum matter, but experimental evidence of their existence has remained elusive. Recent theoretical and numerical studies have provided evidence that triangular-lattice Heisenberg magnets may host a U(1) Dirac spin liquid (DSL): a state of matter whose low-energy description is given by compact quantum electrodynamics in 2+1 dimensions coupled to four Dirac fermions, which is believed to flow to a strongly interacting conformal fixed point. Monopole operators constitute a strongly relevant perturbation to this fixed point, driving the spin liquid into magnetically ordered or VBS states, but are forbidden by the microscopic (UV) symmetries on the triangular lattice. However, in this work we show that a coupling between certain monopoles and phonons is symmetry-allowed and produces a 2+1-dimensional analog of the spin-Peierls instability for a spin liquid. We study monopole-phonon interactions within a conformal field theory framework and show that the DSL state is generically unstable to a static deformation, precipitating VBS ordering. Finally, we discuss implications for experimental realisations and signatures of the DSL in real 2D materials by addressing a full dynamical quantum model of phonons; here we predict a weak-coupling regime within which the spin-liquid phase remains stable.

TT 47: Quantum-Critical Phenomena

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

TT 47.1 Thu 9:30 HSZ 204

The mystery of the missing heavy-fermion weight — •Chia-Jung Yang[1], Oliver Stockert[2], Hilbert v. Löhneysen[3], Shovon Pal[1,4], Johann Kroha[5], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]KIT Karlsruhe, Germany — [4]School of Physical Science, NISER Bhubaneshwar, India — [5]University of Bonn, Germany

The fermionic quasiparticle weight is one of the keys to understanding the quantum critical scenarios across a quantum phase transition (QPT). In heavy-fermion compounds, $CeCu_{6-x}Au_x$ (CCA), Cu substitution by Au expands the lattice, thereby inducing a QPT at x = 0.1 from a paramagnetic Fermi-liquid state to an antiferromagnetically-ordered ground state. Recently, the evolution of spectral weight has been revealed in CCA at x = 0, 0.1, and 1.0 via terahertz (THz) time-domain spectroscopy [1,2]. Here, we further investigate the spectral weight within the RKKY-dominated region where x = 0.2 and 0.3. In both samples, we find that the spectral weight increases slightly with decreasing temperature (T), but settles at a strongly suppressed, T-independent value already at and below 100 K, about two orders of magnitude above the Néel temperature [3]. This indicates that across QPT in CCA, the Kondo singlet formation is suppressed by the T-independent RKKY interaction, not by the critical magnetic fluctuations, in agreement with theoretical predictions [4].

[1] Nat. Phys. **14**, 1103 (2018)
[2] PRR **2**, 033296 (2020)
[3] Eur. Phys. J. B **5**, 447 (1998)
[4] PRL **118**, 117204 (2017)

TT 47.2 Thu 9:45 HSZ 204

Phonon softening close to a structural instability at zero temperature — T. Gruner[1,2], S. Lucas[1], C. Geibel[1], K. Kaneko[3], S. Tsutsui[4,5], K. Schmalzl[6], and •O. Stockert[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom — [3]Materials Sciences Research Center, Japan Atomic Energy Agency, Tokai, Naka, Ibaraki 319-1195, Japan — [4]Japan Synchrotron Radiation Research Institute, SPring-8, Sayo, Hyogo 679-5198, Japan — [5]Institute of Quantum Beam Science, Graduate School of Science and Engineering, Ibaraki University, Hitachi, Ibaraki 316-8511, Japan — [6]Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at ILL, 38042 Grenoble, France

The structural transition in $LuPt_2In$ is interesting since it can be tuned to zero temperature upon substituting Pd for Pt in $Lu(Pt_{1-x}Pd_x)_2In$. Of particular interest is the appearance of a superconducting dome around the structural quantum criticality. We combined inelastic neutron and x-ray scattering measurements and studied in detail this structural transition in $Lu(Pt_{1-x}Pd_x)_2In$. As a result we determined the low-energy phonon dispersions and clearly identified the relevant phonon branch becoming soft at the transition. In general, the theoretical calculations broadly agree with the measured dispersion. However, large tails of the superstructure intensity above the structural transition clearly point to a non-mean-field behavior, which might be related to quantum criticality and/or the superconducting dome.

TT 47.3 Thu 10:00 HSZ 204

Search for ferromagnetic quantum phase transitions in CePt — Marc Seifert[1], •Florian Kübelbäck[1], Pau Jorba[1], Michael Schulz[2], Georg Benka[1], Andreas Bauer[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technical University of Munich, D-85748 Garching, Germany — [2]MLZ, Technical University of Munich, D-85748 Garching, Germany

We report an investigation of the ferromagnetic properties and the putative existence of quantum phase transitions in CePt. Tracking the neutron depolarization of polycrystalline samples under pressure by means of bespoke diamond anvil cell and focussing neutron guides [1], we confirm the presence of a ferromagnetic to paramagnetic quantum phase transition at 13 GPa as inferred previously from the resistivity [2]. An additional drop in the depolarization deep in the ferromagnetic state for pressures up to 5 GPa suggests an additional small moment to large moment transition. We explore the nature and possible existence of a second quantum phase transition in the ferromagnetic state of single-crystal CePt grown under ultra-high vacuum compatible conditions. The pressure versus temperature phase diagram of CePt and its magnetic properties will be compared with the emergence of a Kondo cluster glass in the isostructural sibling CePd of CePt when suppressing ferromagnetic order by substitutional Rh doping [3].

[1] P. Jorba et al., Phys. Stat. Solidi b, 2100623 (2022)
[2] J. Larrea et al., Phys. Rev. B, **72**, 035129 (2005)
[3] M. Seifert et al., Phys. Rev. Res. **4**, 043029 (2022)

TT 47.4 Thu 10:15 HSZ 204

Quantum criticality on a compressible lattice — Saheli Sarkar, •Lars Franke, Nikolas Grivas, and Markus Garst — Institut für Theoretische Festkörperphysik, Karlsruhe, Germany

It is a long standing result in the theory of classical criticality that a second order phase transition when coupled to a compressible lattice will become first order if the Larkin-Pikin criterion[1] is satisfied. More recently the extension of these results to quantum criticality has sparked the interest of the community[2,3]. However, until now a detailed analysis of a microscopic theory describing a quantum phase transition on a compressible lattice and its implications for the nature of the phase transition as well as the consequences for the lattice has been missing. Here we provide this calculation for a Lorentz-invariant ϕ^4-theory with quadratic coupling to strain and analyse it using renormalization group (RG) methods to one-loop order. We find that both critical and phonon velocity flow with RG leading to an additional fixed point where the phonons have a renormalized dynamical exponent. Furthermore, our results show that the quantum version of the Larkin-Pikin criterion[2] holds, but even when the criterion is not satisfied a structural instability can still occur, if the coupling is large enough.

[1] A. Larkin and S. Pikin, Sov. Phys. JETP 29, 891 (1969)
[2] P. Chandra, P. Coleman, M. A. Continentino, and G. G. Lonzarich, Phys. Rev. Res. 2, 043440 (2020)
[3] A. Samanta, E. Shimshoni, and D. Podolsky, Phys. Rev. B 106, 035154 (2022)

TT 47.5 Thu 10:30 HSZ 204

Marginal Fermi liquid at a magnetic quantum critical point

from dimensional confinement — •Bernhard Frank[1], Zi Hong Liu[2], Fakher F. Assaad[2], Matthias Vojta[1], and Lukas Janssen[1] — [1]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

Metallic quantum criticality is frequently discussed as a source for non-Fermi liquid behavior, but controlled theoretical treatments are scarce. Here, we identify and study a novel magnetic quantum critical point in a two-dimensional antiferromagnet coupled to a three-dimensional environment of conduction electrons. By combining an effective field theory analysis and sign-problem-free quantum Monte Carlo simulations, we demonstrate that the quantum critical point exhibits marginal Fermi liquid behavior. In particular, we compute the electrical resistivity for transport across the magnetic layer, which is shown to display a linear temperature dependence at criticality. Experimental realizations in Kondo heterostructures are discussed.

TT 47.6 Thu 10:45 HSZ 204

Transverse-field quantum phase transitions in $CoNb_2O_6$ — •Alexander Engelhardt[1], Andreas Wendl[1], Andreas Bauer[1], Andreas Erb[2], Matthias Vojta[3], and Christian Pfleiderer[1] — [1]Physik-Department, Technical University of Munich, D-85748 Garching, Germany — [2]Walther-Meißner-Institut, D-85748 Garching, Germany — [3]Institut for Theoretical Physics, Technical University of Dresden, D-85748 Garching, Germany

The ferromagnetic Ising chain in a transverse magnetic field displays the perhaps best understood theoretical example of a quantum phase transition. One of the closest realizations has been reported in the columbite compound $CoNb_2O_6$ [1,2,3], in which, however, weak interchain couplings result in incommensurate antiferromagnetism as a function of decreasing temperature, followed by a transition to commensurate antiferromagnetic order. We have grown high-quality single-crystal $CoNb_2O_6$ by means of optical float-zoning. Measuring the transverse magnetic ac susceptibility of a spherical sample down to 90 mK under arbitrary field orientations, we have mapped out the emergence of the quantum phase transitions associated with the incommensurate and commensurate antiferromagnetic order under transverse field, as well as the evolution of the magnetic phase diagram when systematically tilting the magnetic field away from the hard magnetic axis.

[1] R. Coldea et al., Science **327**, 177 (2010)
[2] M. Fava et al., PNAS **117**, 25219 (2020)
[3] C. M. Morris et al., Nat. Phys. **17**, 852 (2021)

TT 47.7 Thu 11:00 HSZ 204

Non-Fermi liquid behavior at flat hot spots at the onset of density wave order in two-dimensional metals — •Lukas Debbeler and Walter Metzner — Max Planck Institute for Solid State Research, Stuttgart, Germany

We analyze the quantum critical point (QCP) at the transition towards incommensurate charge or spin density wave order with a $2k_F$ wave vector that connects a single pair of hot spots on the Fermi surface. From a theoretical point of view the fate of this QCP is debated. Strong fluctuations might lead to a discontinuously opening gap and therefore a first order transition [1]. On the other hand a fluctuation driven flattening at the hot spots of the Fermi surface has been found [2,3], which could protect the QCP. Hence, we investigate the effect of quantum critical fluctuations for a flat Fermi surface at the nesting points. We report non-Fermi liquid properties and provide numerical values for anomalous exponents.

[1] B. L. Altshuler et al., Phys. Rev. B 52, 5563 (1995)
[2] J. Sýkora et al., Phys. Rev. B 97, 155159 (2018)
[3] J. Halbinger et al., Phys. Rev. B 99, 195102 (2019)

15 min. break

TT 47.8 Thu 11:30 HSZ 204

Frozen deconfined quantum criticality — •Vira Shyta[1,2], Jeroen van den Brink[1,3], and Flavio Nogueira[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Kyiv Academic University, 36 Vernadsky blvd., Kyiv 03142, Ukraine — [3]Institute for Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01069 Dresden, Germany

There is a number of contradictory findings with regard to whether the theory describing easy-plane quantum antiferromagnets undergoes a second-order phase transition. The traditional Landau-Ginzburg-Wilson approach suggests a first-order phase transition, as there are two different competing order parameters. On the other hand, it is known that the theory has the property of self-duality which has been connected to the existence of a deconfined quantum critical point (DQCP). The latter regime suggests that order parameters are not the elementary building blocks of the theory, but rather consist of fractionalized particles that are confined in both phases of the transition and only appear at the critical point. Here we establish from exact lattice duality transformations and renormalization group analysis that the easy-plane CP1 antiferromagnet does feature a DQCP. We uncover the criticality starting from a regime analogous to the zero temperature limit of a certain classical statistical mechanics system which we therefore dub frozen. At criticality our bosonic theory is dual to a fermionic one with two massless Dirac fermions, which thus undergoes a second-order phase transition as well.

TT 47.9 Thu 11:45 HSZ 204

Finite temperature entanglement negativity of fermionic topological phases and quantum critical points — •Wonjune Choi[1,2], Frank Pollmann[1,2], and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

In condensed matter physics, topology is vital in describing quantum phases of matter beyond the Ginzburg-Landau paradigm. Two symmetry-preserving quantum states may not be adiabatically connected if the topological structure encoded in the many-body entanglements is distinct. Hence, this talk presents how quantum entanglements can be quantified to unveil the underlying topological nature of the gapped topological phases and the quantum critical points. We demonstrate that the logarithmic negativity between spatially separated disjoint intervals can sharply count the topologically protected edge modes. Notably, the quantized values of the negativity could reveal the topological indices of the gapless quantum states described by the conformal field theories having the same central charge. At finite temperatures, the entanglement negativity for the disjoint intervals is no longer quantized. However, the negativity for the two adjacent intervals leaves the structure similar to the quantum critical fan, which signals the highly entangled ground state even at a finite temperature window.

TT 47.10 Thu 12:00 HSZ 204

Symmetry enriched topological quantum phase transition in projected entangled pair states — •Lukas Haller, Yu-Jie Liu, Wen-Tao Xu, and Frank Pollmann — Department of Physics, Technical University of Munich, 85748 Garching, Germany

Phase transitions between topologically ordered phases can exhibit a rich structure and are generically challenging to study. In this context, we consider the 2D toric code decorated with 1D symmetry protected topological states and construct a family of parametrized projected entangled pair states (PEPS), which describes the ground states of time-reversal (TR) symmetric Hamiltonians. The system can exhibit three distinct phases of matter: (i) A trivial phase; (ii) the toric code phase, where TR symmetry is not fractionalized; (iii) a symmetry enriched topological (SET) phase, where TR symmetry can be fractionalized on anyons. We characterize different phases using topological entanglement entropy and membrane order parameters. By mapping the PEPS to the partition functions of 2D classical models, we show that the trivial phase is separated from the toric code and the SET phases by critical points described by an Ising conformal field theory (CFT) with central charge $c = 1/2$, while the phase transition between the toric code and the SET phase is described by a compactified free-boson CFT with $c = 1$. The model realizes a direct phase transition between the toric code and the SET phases at a microscopic level.

TT 47.11 Thu 12:15 HSZ 204

Antiferromagnetic Weyl quantum criticality in three-dimensional Luttinger semimetals — •David Jonas Moser and Lukas Janssen — Technische Universität Dresden, Dresden, Deutschland

Luttinger semimetals are three-dimensional strongly-spin-orbit-coupled systems, in which valence and conduction bands touch quadratically at the Fermi level. They provide a rich playground for highly unconventional physics and serve as a parent state to a number of exotic states of matter, such as Weyl semimetals, topological insulators, or spin ice. Here, we discuss a quantum critical point between Luttinger and antiferromagnetic Weyl semimetals using a renormalization group approach. Our results are relevant for the low-temperature behavior of rare-earth pyrochlore iridates, such as $Pr_2Ir_2O_7$ or $Nd_2Ir_2O_7$.

TT 47.12 Thu 12:30 HSZ 204

Renormalization group flow of the Yukawa-SYK model — •Niklas Cichutek and Peter Kopietz — Goethe University Frankfurt

We use the functional renormalization group to calculate the global renormalization group flow of the Yukawa-SYK model describing N fermions on a quantum dot which are coupled to M phonons by a disorder-induced Yukawa coupling in the large N and M limit for an arbitrary ratio $\frac{N}{M}$. By determining the fixed-point structure we identify the different phases as well as the quantum critical point and their corresponding anomalous dimensions. The stability analysis of the fixed points sheds light on the self-tuning to criticality of the Yukawa-SYK model.

TT 47.13 Thu 12:45 HSZ 204

Quantum criticality of Heisenberg systems with long-range interactions — •Patrick Adelhardt and Kai Phillip Schmidt — Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

The majority of numerical approaches investigating long-range quantum systems is restricted to one-dimensional systems and systems in two dimensions with quickly decaying long-range interactions. While models with discrete symmetries like the long-range transverse-field Ising model have been studied thoroughly, much less is known about long-range models with continuous symmetries where long-range interactions can cricumvent the Hohenberg-Mermin-Wagner theorem in one dimension allowing the spontaneous breaking of continuous symmetries or can give rise to massive excitations violating Goldstone's theorem. We study the breakdown of the rung-singlet phase in the quasi one-dimensional Heisenberg ladders as well as two-dimensional Heisenberg bilayer systems with algebraically decaying long-range interactions. To this end we use the method of perturbative continuous unitary transformations (pCUT) as a white graph expansion with classical Monte Carlo simulations yielding high-order series in the thermodynamic limit about the limit of isolated dimers. This allows us to determine the critical point as well as critical exponents as a function of the decay exponent.

TT 48: Topological Superconductors

Time: Thursday 9:30–11:15 Location: HSZ 304

TT 48.1 Thu 9:30 HSZ 304

Superconductivity mediated by topological phonons — •Alessio Zaccone — Department of Physics, University of Milan, 20133 Milano, Italy

Topological phononic insulators are the counterpart of three-dimensional quantum spin Hall insulators in phononic systems and, as such, their phononic topological surfaces are characterized by Dirac cone-shaped gapless edge states arising as a consequence of a bulk-boundary correspondence. We proposed [1] a theoretical framework for the possible superconductivity in these materials, where the attractive interaction between electrons is mediated by topological phonons in nontrivial boundary modes. Within the BCS limit, we developed a self-consistent two-band gap equation, whose solutions show that the superconducting T_c has a nonmonotonic behavior with respect to the phononic frequency in the Kramers-like point. This remarkable behavior is produced by a resonance that occurs when electrons and phonons on the topological surfaces have the same energy: this effectively increases the electron-phonon interaction and hence the Cooper pair binding energy, thus establishing an optimal condition for the superconducting phase. With this mechanism, the T_c can be increased by well over a factor 2, and the maximum enhancement occurs in the degenerate phononic flat-band limit.
[1] D. Di Miceli, C. Setty, A. Zaccone, Phys. Rev. B 106, 054502 (2022)

TT 48.2 Thu 9:45 HSZ 304

Topological superconductivity on the honeycomb lattice: Effect of normal state topology and disorder — •Stephan Rachel — School of Physics, University of Melbourne, Australia

The search for topological superconductors is one of the most pressing and challenging questions in condensed-matter and material research. Despite some early suggestions that doping a topological insulator might be a successful recipe to find topological superconductors, to date there is no general understanding of the relationship of the topology of the superconductor and the topology of its underlying normal state system. Here we present an analysis of doped insulators - topological and trivial. Our approach allows us to study and compare superconducting instabilities of different normal state systems and present rigorous results about the influence of the normal state system's topology. If time permits we will also discuss the influence of disorder on topological superconductivity on the honeycomb lattice.

TT 48.3 Thu 10:00 HSZ 304

Ground state topology of a multiterminal superconducting double quantum dot — •Lev Teshler, Hannes Weisbrich, and Wolfgang Belzig — Universität Konstanz, Konstanz, Germany

Multiterminal Josephson junctions can provide topological Andreev bound states in the space of the superconducting phases [1]. The topology of the Andreev bound states manifests itself in a quantized transconductance when applying voltages to two terminals. Such systems are candidates to realise higher-dimensional topology and non-Abelian Berry phases using their synthetic dimensions [2]. For practical purposes a linear arrangement of quantum dots coupled to superconductors might be beneficial and was shown to exhibit nontrivial topology [3]. In this work, we study a double quantum dot in which each dot is coupled to two superconductors. This system that depends on three superconducting phase differences already displays non-trivial topology in terms of the first Chern number and is an example that allows to study the fundamental properties of this class of systems. We will study the ground state and the respective topological phase diagram for different sets of parameters of the double quantum dot. Furthermore, we will also discuss the influence of Coulomb interaction and Zeeman splitting on the topological properties of the ground state.
[1] R.-P. Riwar et al., Nat. Commun. 7, 1 (2016)
[2] H. Weisbrich et al., PRX Quantum 2, 010310 (2021)
[3] R. Klees et al., Phys Rev B 103, 014516 (2021)

TT 48.4 Thu 10:15 HSZ 304

Fractional transconductance via non-adiabatic topological Cooper pair pumping — •Hannes Weisbrich[1], Raffael L. Klees[2], Oded Zilberberg[1], and Wolfgang Belzig[1] — [1]Universität Konstanz — [2]Universität Würzburg

Many robust physical phenomena in quantum physics are based on topological invariants, which are intriguing geometrical properties of quantum states. A prime example is the 2D quantum Hall effect with its quantized quantum Hall conductance in units of $\frac{e^2}{h}$ protected by the respective 2D topology. A comparable effect in superconducting systems is the appearance of a quantized transconductance in units of $\frac{4e^2}{h}$ for topological Andreev bound states in multiterminal Josephson junctions.

In this work, we theoretically demonstrate how fractional quantized plateaus in the transconductance can be observed as a result of topological Cooper pair pumping in a chain of Josephson junctions. The fractional plateaus in the transconductance are stabilized by non-adiabatic Landau-Zener transitions which even allow for a robustness to disorder in the chain.

TT 48.5 Thu 10:30 HSZ 304

Magnetic-domain mediated topological superconductivity in a Josephson Junction — •Ignacio Sardinero[1], Rubén Seoane Souto[2,3], and Pablo Burset[1] — [1]Department of Theoretical Condensed Matter Physics, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Division of Solid State Physics and NanoLund, Lund University, S-221 00 Lund, Sweden — [3]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

Topological superconductors are appealing building blocks for robust and reliable quantum information processing. Most platforms for engineering topological superconductivity rely on a combination of materials with intrinsic spin-orbit coupling and external magnetic fields, which are usually challenging to manipulate. We propose and describe a setup without spin-orbit or magnetic fields where a conventional Josephson junction is linked by a narrow ferromagnetic insulator with multi-domain structure along the interface. Our calculations show that sequences of magnetic domains preserving the net magnetization's rotation direction are sufficient for generating topological superconductivity in a wide range of parameters and degrees of disorder. We find that the topological phase transition strongly depends on the magnitude and period of the net magnetization. Interestingly, a phase bias across the junction can control and tune the formation and localization of a pair of Majorana zero-energy modes along the junction interface, with an observable effect on the current-phase relation.

TT 48.6 Thu 10:45 HSZ 304

Symmetry enriched entanglement properties of chiral Skyrme insulators — •Joe Winter[1,2,3], Bernd Braunecker[3], and Ashley Cook[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nothnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Straße 38, 01187 Dresden, Germany — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, North Haugh, St. Andrews KY16 9SS, UK

The expectation value of an observable $\mathcal{O}$ may be computed with a density matrix ρ as $\mathrm{Tr}\,(\rho\mathcal{O})$. In this work, we introduce the symmetry-enriched partial trace operation for density matrices, $\tilde{\rho}_{\mathcal{T}} = \tilde{\mathrm{Tr}}_{\bar{\mathcal{T}}}\,(\rho)$, a partial trace performed over $\bar{\mathcal{T}}$ degrees of freedom on a density matrix as part of partial computation of an expectation value for an observable $\mathcal{O}$. That is, for representation of observable $\mathcal{O}$ after tracing out $\bar{\mathcal{T}}$ being $\mathcal{O}_{\mathcal{T}}$, $\tilde{\rho}_{\mathcal{T}}$ satisfies $\mathrm{Tr}\,(\rho\mathcal{O}) = \langle\mathcal{O}\rangle = \langle\mathcal{O}_{\mathcal{T}}\rangle = \mathrm{Tr}\,(\tilde{\rho}_{\mathcal{T}}\mathcal{O}_{\mathcal{T}})$, with symmetry-enrichment deriving from differences in symmetry between $\mathcal{O}$ and $\mathcal{O}_{\mathcal{T}}$. We use this to characterize bulk-boundary correspondence of topological skyrmion phases, by computing the symmetry-enriched reduced density matrix in the 2D bulk of a topological skyrmion phase, and for slab geometries with open boundary conditions in one direction. We show winding of this reduced density matrix matches winding of the spin expectation value vector in the bulk, and the entanglement spectrum of the reduced density matrix for the slab geometry reveals $\mathcal{Q}$ topologically-protected, chiral edge modes for skyrmion number $\mathcal{Q}$ characterizing the bulk topological skyrmion phase.

TT 48.7 Thu 11:00 HSZ 304

Non-Hermitian dimerized interacting Kitaev chain — •Sharareh Sayyad[1] and Jose Lado[2] — [1]MPI for the sicence of light, Erlangen, Germany — [2]Aalto University, Espoo, Finland

Non-Hermitian models have risen as a new paradigm to manipulate and interpret various emergent quantum phenomena. While numerous studies have been focused on exploring (effective) non-Hermitian non-interacting models. The role of interactions in modifying the non-interacting non-Hermitian physics still needs to be well-explored. In this talk, I will present how incorporating many-body interactions can enrich non-interacting physics. To be more precise, combining our exact analytical results and tensor- network numerical calculations, I will discuss the phase diagram of the non-Hermitian dimerized interacting Kitaev chain. Here, the non-Hermiticty is due to the complex-valued nearest-neighbor density-density interaction strength. I will show that the ground state degeneracy of this system may be fourfold, twofold, or nondegenerate, depending on the parameter regimes. I will further discuss how these degeneracies are lifted in the presence of non-Hermiticity. Elaborating on this behavior clarifies the role of non-Hermiticity in washing out multiple phases in the phase diagram of the Hermitian interacting model.

TT 49: Quantum Coherence and Quantum Information Systems I

Time: Thursday 11:30–13:00 Location: HSZ 304

TT 49.1 Thu 11:30 HSZ 304

Inter-lab quantum microwave teleportation — •Michael Renger[1,2], Simon Gandorfer[1,2], Wun Kwan Yam[1,2], Florian Fesquet[1,2], Kedar Honasoge[1,2], Fabian Kronowetter[1,2,3], Yuki Nojiri[1,2], Achim Marx[1], Rudolf Gross[1,2,4], and Kirill G. Fedorov[1,2] — [1]Walther-Meißner-Institut, BadW, 85748 Garching, Germany — [2]TUM School of Natural Sciences, Technische Universität München, Garching, Germany — [3]Rohde & Schwarz GmbH & Co. KG, 81671 Munich, Germany — [4]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Quantum communication enables secure and efficient information exchange among different quantum nodes. To avoid inefficient frequency conversion for data transfer between superconducting quantum processors, we implement our quantum communication protocols with propagating quantum microwave states, directly in the microwave frequency regime which relies on ambient temperatures below 100 mK. To realize such a microwave quantum channel, we connect two dilution refrigerators over a distance of 6.5 m via a cryogenic link, operating at a base temperature of 52 mK. We employ our system to demonstrate inter-lab quantum teleportation of coherent microwave states, where we achieve the teleportation fidelity of 55%, exceeding the classical threshold. We discuss quantum advantage and security of this protocol and provide an outlook into the future of microwave quantum communication.

TT 49.2 Thu 11:45 HSZ 304

A co-design superconducting quantum circuit for quantum simulations — •Daria Gusenkova, Jayshankar Nath, Hsiang-Sheng Ku, Julia Lamprich, Nicola Wurz, Stefan Pogorzalek, Florian Vigneau, Ping Yang, Frank Deppe, Antti Vepsäläinen, Alessandro Landra, Vladimir Milchakov, Caspar Ockeloen- Korppi, Wei Liu, Lan-Hsuan Lee, Seung-Goo Kim, Hermanni Heimonen, Manish Thapa, and Inés de Vega — IQM Germany GmbH, Nymphenburger Str. 86, 80335 Munich

The co-design concept of building application-specific quantum processors is a viable strategy for reaching quantum advantage with noisy intermediate-scale quantum computers. We consider many-body problems which map onto a Hamiltonian with all-to-all interacting qubits. Here, a prototypical example is the simulation of a nanoscale NMR system consisting of an NV center coupled to multiple nuclear spins. We discuss the implementation on a star-topology circuit developed in IQM. Compared to the general-purpose square-grid topology, the star reduces the number of SWAP gates in the algorithm implementation, and thus tolerates higher gate errors for a given computational precision [1]. In order to allow for hardware scaling, we use a distributed-element resonator as a center component in the circuit. To use this resonator as a computational element, we develop qubit-resonator SWAP and CZ gates. In this talk, we present the experimental progress towards digitally simulating the nanoscale NMR problem.

[1] M. G. Algaba et. al., Phys. Rev. Research 4, 043089 (2022)

TT 49.3 Thu 12:00 HSZ 304

Showcasing the effective direct interaction between a readout resonator and a strongly coupled junction defect mediated by a transmon qubit — •Alexander K. Händel, Alexander Bilmes, Alexey V. Ustinov, and Jürgen Lisenfeld — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Decoherence from material defects constitutes a principal problem on the way to improve superconducting quantum bits. Strongly coupled defects residing in the Josephson junction pose a particular challenge, demonstrating coupling strengths of multiple MHz. This strong coupling leads to avoided level crossings when qubit and defect come into resonance, and spoils qubit performance. In this work, we reveal an additional decoherence channel that occurs due to the resonant interaction between defects in the qubit's Josephson junction with the qubit's readout resonator, through an interaction mediated by the qubit. We investigate this effect using multi-photon spectroscopy and QuTiP simulations of the tripartite energy level spectrum.

TT 49.4 Thu 12:15 HSZ 304

Modular flip-chip architecture for generalized flux qubits — •Soeren Ihssen[1], Simon Geisert[1], Martin Spiecker[2], Patrick Winkel[2], Wolfgang Wernsdorfer[1,2], and Ioan M. Pop[1,2] —

[1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Germany — [2]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

Superconducting circuits are a promising and widely-used platform to implement quantum information processing hardware. However, scaling up to more sophisticated devices requires major engineering efforts due to the complexity of the mandatory coupling, readout and control circuitry. To investigate innovative coupling and scaling strategies, we developed a modular flip-chip architecture, in which the various circuit elements reside on dedicated chips that are capacitively coupled. A unit cell of our architecture consists of a qubit chip that is flipped above a control chip. The qubit chip contains a single generalized flux qubit (GFQ) and a harmonic readout mode, through which dispersive readout is possible. The control chip is used to excite, read out and flux bias the qubit. We tested our architecture by characterizing the GFQs in all conventional flux qubit regimes by modifying the qubit loop inductance as well as the shunt capacitance and the Josephson energy of the alpha junction. This resulted in qubit frequencies between 150 MHz and 7.5 GHz, and dispersive shifts of 60 kHz to 6 MHz. Coupling between unit cells may be achieved through coupler chips, so that our unit cell can be used as a basic building block of a scalable qubit array.

TT 49.5 Thu 12:30 HSZ 304

Improving Fabrication Methods for Highly Coherent Superconducting Qubits — •Niklas Bruckmoser[1,2,3], Leon Koch[1,2,3], David Bunch[1,2,3], Tammo Sievers[1,2,3], Kedar E. Honasoge[1,2,3], Thomas Luschmann[1,2,3], and Stefan Filipp[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Superconducting qubits and resonators with long coherence times pave the way towards useful quantum processors. Significant improvements in coherence time have already been made over the last years. However, the fidelity is still limited by decoherence due to noise and losses arising in the local environment of the qubit. It is thus an integral endeavor of fabrication efforts to mitigate these effects. Here, we demonstrate that qubit lifetimes well beyond 0.1 ms can be achieved by a combination of substrate cleaning, etching optimization and post-process sample cleaning. By improving on these processes we reach quality factors above 4×10^6 for thin-film niobium coplanar waveguide resonators in the single photon regime and qubit lifetimes of more than 0.2 ms for niobium based transmons.

TT 49.6 Thu 12:45 HSZ 304

Dynamics of superconducting qubit coherence times due to fluctuations of two-level systems — •Ivan Tsitsilin[1,2] and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

Recent studies have shown that the stability of coherence times is strongly affected by two-level systems (TLSs). This is caused by chaotic frequency fluctuations of TLSs, which, when in proximity to the qubit resonance, significantly reduce its T_1 times. Understanding and mitigating this behavior is crucial to realize functional quantum processing devices based on superconducting qubits. In this work, we perform a long-time stability analysis of the qubit T_1 times as a function of qubit frequency utilizing the AC-Stark shifting technique[1]. We present an extensive analysis of the TLS distributions and their impact on T_1 times for different qubit sample materials and RF line configurations. Furthermore, our results provide insight into the effect of the noise spectrum on the behavior and density of TLSs.

[1] Carroll et al., arXiv:2105.15201

TT 50: Focus Session: Superconducting Nickelates II

Time: Thursday 15:00–17:00 Location: HSZ 03

TT 50.1 Thu 15:00 HSZ 03

Fermi liquid on the verge of antiferromagnetism: Nonlocal correlations in bulk $LaNiO_3$ as seen by SX-ARPES — •Johannes Falke[1], Cheng-En Liu[1,2,3], Keng-Yung Lin[1,4], Chang-Yang Kuo[1,2,3], Hanjie Guo[1], Alexander Komarek[1], Chun-Fu Chang[1], Philipp Hansmann[5], and Liu Hao Tjeng[1] — [1]MPI CPfS, Dresden, Germany — [2]NYCU, Hsinchu, Taiwan — [3]NSRRC, Hsinchu, Taiwan — [4]NTU, Taipei, Taiwan — [5]FAU, Erlangen, Germany

Soft X-ray ARPES measurements were performed on large single crystals of the metallic oxide $LaNiO_3$ along high symmetry directions, revealing the bulk electronic structure of the full valence band. The experimental Fermi surface is accurately reproduced by conventional band theories, whereas the nonzero frequency part of the spectra shows k-dependent renormalizations that cannot be explained by DFT even accounting for octahedral rotations and require true many-body methods to accurately explain.

TT 50.2 Thu 15:15 HSZ 03

Insights into the electronic structure of oxygen reduced and doped nickelates from core-level spectroscopy — •Rebecca Pons — Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — Stewart Blusson Quantum Matter Institute, UBC Vancouver, Canada

With the observation of superconductivity in Sr-doped infinite-layer nickelate $Nd_{0.8}Sr_{0.2}NiO_2$ research interest in this material class intensified. We used ozone assisted molecular beam epitaxy to grow RNiO$_3$ thin films (R=La,Pr) and investigated the subsequent topotactic soft-chemistry reaction, needed to synthesize the square-planar phase, at different stages of reduction by x-ray absorption spectroscopy. We observe the evolution of the Ni oxidation state and that the process is laterally homogeneous down to length scales of 50 nm. To reach the superconducting phase hole doping of the infinite-layer nickelates is required with an optimal doping level around x=0.2. This can be achieved by self-doping in quintuple-layer Ruddlesden-Popper nickelates or alkaline-earth doping, Ca or Sr, in infinite-layer films. Using angle-resolved photoemission spectroscopy (ARPES) we studied changes in the Fermi surface upon alkaline-earth doping in (La,Ca)NiO_3.

TT 50.3 Thu 15:30 HSZ 03

Thickness-dependent interface polarity in infinite-layer nickelate superlattices — •Chao Yang[1], Roberto A. Ortiz[1], Yi Wang[2], Wilfried Sigle[1], Hongguang Wang[1], Eva Benckiser[1], Bernhard Keimer[1], and Peter A. van Aken[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, 70569, Germany — [2]Center for Microscopy and Analysis, Nanjing University of Aeronautics and Astronautics, Nanjing, 210016, P.R. China

The interface polarity plays a vital role in the physical properties of oxide hetero-interfaces, since it can enforce a reconstruction of the electronic and atomic structure. In the recently discovered superconducting nickelate thin films, interfacial effects could play an important role. This motivated our investigation of the electronic and atomic structure at the atomic scale at interfaces of infinite-layer nickelate thin films. Using four-dimensional scanning transmission electron microscopy (4D-STEM) and electron energy-loss spectroscopy (EELS), we systematically studied the effects of oxygen distribution and site occupancy, polyhedral distortion, elemental intermixing, as well as dimensionality on interface properties of infinite-layer NdNiO2/SrTiO3 superlattices. The oxygen intensity and distribution maps show the local symmetry change from octahedral to square planar induced by the reduction process and a gradual change of the oxygen content in the nickelate layers. Remarkably, we demonstrate spatially controlled interface polarity with accompanying interface reconstructions. Our results provide insights to understand the effects of polarity and dimensionality on the interface properties of infinite-layer nickelates.

TT 50.4 Thu 15:45 HSZ 03

GW+EDMFT investigation of $Pr_{1-x}Sr_xNiO_2$ under pressure — •Viktor Christiansson, Francesco Petocchi, and Philipp Werner — University of Fribourg, Fribourg, Switzerland

The recent experimental observation of a large pressure effect on T_c

in $Pr_{1-x}Sr_xNiO_2$ opens up an interesting prospect for reaching even higher values of T_c in the nickelates. On the theoretical side, systematic changes with pressure also provides a new possibility for probing the single- versus multi-orbital nature of these systems. In this talk, we discuss the electronic structure of this system as a function of pressure and doping, based on numerical calculations using self-consistent GW+EDMFT. We show that the normal state properties demonstrate a non-trivial interplay between physical pressure and chemical doping, and we find small but systematic changes with increasing pressure. The proper treatment of correlation effects, beyond density functional theory, is shown to play an important role in revealing these trends. While the pressure dependent changes of the undoped compound suggest a more single-orbital-like behavior towards the high-pressure regime, a qualitatively different behavior is observed for the doped system with a multi-orbital nature manifesting itself also at high pressures.

TT 50.5 Thu 16:00 HSZ 03

Nature of magnetic coupling in bulk infinite-layer nickelates versus cuprates — •Armin Sahinovic, Benjamin Geisler, and Rossitza Pentcheva — Fakultät für Physik, Universität Duisburg-Essen

In contrast to cuprates, where the proximity of antiferromagnetism (AFM) and superconductivity is well established, first indications for AFM interactions in superconducting infinite-layer nickelates [1] were only recently obtained [2,3]. Here, we explore, based on first-principles simulations, the nature of the magnetic coupling in $NdNiO_2$ as a function of the on-site Coulomb and exchange interaction, varying the explicit hole doping and the treatment of the Nd $4f$ electrons. The U-J phase diagrams for undoped nickelates and cuprates indicate G-type ordering, yet show different U dependency. By either Sr hole doping or explicit treatment of the Nd $4f$ electrons, we find a transition to a Ni C-type AFM ground state. We trace this back to a distinct response of the Ni vs. Cu e_g orbitals to the hole doping. The interaction between Nd $4f$ and Ni $3d$ spin stabilizes C-type AFM order on both sublattices. Though spin-orbit interactions induce a band splitting near the Fermi energy, the bad-metal state is retained under epitaxial strain. The magnetocrystalline anisotropy features an in-plane easy axis, related to the planar NiO_2 coordination. These results establish the nickelates as a unique platform to study unconventional superconductivity.

[1] D. Li et al., Nature 572, 624 (2019)
[2] J. Fowlie et al., Nature Physics 18, 1043 (2022)
[3] H. Lu et al., Science 373, 213 (2021)

TT 50.6 Thu 16:15 HSZ 03

Magnetic interactions in $InNiO_3$ compared to RNiO$_3$ — •Alexander Yaresko, Graham McNally, Minu Kim, and Hidenori Takagi — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

RNiO$_3$ nikelates undergo with lowering temperature a metal-to-insulator (MIT) transition, accompanied by orthorhombic-to-monoclinic distortion of their crystal structure, and another transition at T_N to a magnetically ordered state with the ordering vector $\mathbf{q}=(1/2, 0, 1/2)$. Two Ni sites in the monoclinic unit cell are nonequivalent, with the average Ni_1–O distance being significantly larger than Ni_2–O. In compounds with the large radius of a R^{3+} ion the two transitions occur simultaneously. As the R size decreases, the crystal structure becomes more distorted. As a consequence, the MIT temperature increases while T_N decreases. Recently, a new $InNiO_3$ compound, in which an In^{3+} ion is even smaller than the smallest rare-earth Lu^{3+}, has been synthesized. We performed DFT(+U) calculations for $InNiO_3$ and compare the results to other nikelates. In order to quantify the effect of structural distortions on the magnetic properties we estimated exchange interactions between magnetic Ni_1 ions by mapping the energies of spin-spirals with different wave vectors $\mathbf{q}$ to an effective Heisenberg model. We found that the strongest interactions are those along Ni_1-O-Ni_2-O-Ni_1 bonds but their strength decreases with increasing lattice distortions. The experimental $\mathbf{q}=(1/2, 0, 1/2)$ order can only be reproduced if a sufficiently small value of Coulomb repulsion U is used for more covalent Ni_2 ion.

TT 50.7 Thu 16:30 HSZ 03

Transport properties of $Nd_{1-x}Sr_xNiO_2$ based on a realistic 3-band model — •Steffen Bötzel, Ilya Eremin, and Frank Lechermann — Institut für theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Here, we consider theoretically the quasiparticle transport in the superconducting nickelate $Nd_{1-x}Sr_xNiO_2$ based on a realistic 3-band low-energy model derived from a first-principle approach [1]. The transport properties are obtained from the standard Kubo formalism. They depend on the band structure near the Fermi surface and are consequently a probe of the hitherto poorly understood low-energy electronic structure. We find significant contributions from different orbitals and bands depending on temperature and doping. Their interplay gives rise to multi-band characteristics, which are in accordance to available experimental data. This observation is important for the ongoing debate whether the low-energy physics is single- or multi-band like and points towards multi-band physics in these compounds.

[1] F. Lechermann, Phys. Rev. X. 10, 041002 (2020)

TT 50.8 Thu 16:45 HSZ 03

High-pressure crystal growth and physical properties of Ruddlesden-Popper trilayer nickelates $La_4Ni_3O_{10}$ — •Ning Yuan, Kaustav Dey, Jan Arneth, Ahmed Elghandour, and Rüdiger Klingeler — Kirchhoff Institute for Physics, Heidelberg University, Germany

Single crystals of $La_4Ni_3O_{10}$ were successfully grown by the high-pressure optical floating-zone method under 20 bar oxygen pressure. We investigate the different growth and post-annealing processes leading to two different polymorphs, namely $P2_1/a$ (No.14) and $Bmab$ (No.64), respectively, and report high-resolution thermal expansion, specific heat and magnetometry data on both of them. Our thermodynamic studies show sharp anomalies associated with the reported Metal-to-Metal Transition (MMT) in $La_4Ni_3O_{10}$ and distinct anisotropy. For the $P2_1/a$ phase, the MMT transition is found at 134 K while it appears at 152 K for $Bmab$. Our thermal expansion data in particular confirm that the MMT transition is associated with strong lattice changes (cf. [1]) but is also reveals clear contradictions to the published XRD data [2].

[1] D. Rout *et al.*, Phys. Rev. B 102, 195144 (2020)
[2] J. Zhang *et al.*, Phys. Rev. M 4, 083402 (2020)

TT 51: Correlated Electrons: Charge Order

Time: Thursday 15:00–17:30 Location: HSZ 103

TT 51.1 Thu 15:00 HSZ 103

The zoo of magnetic states in the 2D Hubbard model — •Robin Scholle, Pietro Bonetti, Demetrio Vilardi, and Walter Metzner — MPI FKF Stuttgart

We use real-space Hartree-Fock theory to construct a magnetic phase diagram of the two-dimensional Hubbard model as a function of temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order without biasing the system towards one of them. For an intermediate interaction strength we predominatly find Néel order close to half-filling, stripe order for low temperatures or large doping, and an intermediate region of spiral order.

I will give a short summary of the method followed by a presentation of our current results and an outlook for possible further applications.

TT 51.2 Thu 15:15 HSZ 103

Effect of higher-order van Hove singularity on the formation of spin density waves — Alkistis Zervou[1], Garry Goldstein[2], Joseph Betouras[1], and •Dmitry Efremov[3] — [1]Department of Physics and Centre for the Science of Materials, Loughborough University, Loughborough LE11 3TU, UK. — [2]Physics Department, Boston University, Boston MA 02215, USA — [3]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany.

Van-Hove singularities in the density of states, which occur due to Lifshitz transitions in electronic band structures, affect different types of ordering in quantum materials. In addition to the usual Van Hove singularities, there are higher-order Van Hove singularities (HOVHS) with DOS divergence according to the power law. We find that the spin wave density and charge density of the phase formation can be enhanced by the presence of a singularity depending on the strength of certain interactions, with the critical temperature increasing by orders of magnitude. We discuss the application of our findings to various experimental systems such as Sr3Ru2O7.

15 min. break

TT 51.3 Thu 15:45 HSZ 103

Kinetic theory of charge-density waves — •Viktor Hahn and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We present a theoretical study of the dynamics of the collective amplitude and phase modes in the charge-density wave (CDW) state of the electronically quasi one-dimensional material $K_{0.3}MoO_3$ (blue bronze). For this purpose we formulate a kinetic theory using the method of expansion in connected equal-time correlations. Our kinetic equations for the CDW order parameter has the same form as the phenomenological equation of motion obtained within a time-dependent Ginzburg-Landau approach. From the numerical solution of our kinetic equations we extract the frequencies and the damping of the collective amplitude and phase modes in the CDW state. We find that the damping is strongly enhanced when the temperature approaches the critical temperature from below, in agreement with recent experiments.

TT 51.4 Thu 16:00 HSZ 103

Collective modes in the quasi one-dimensional charge-density wave material blue bronze — •Max Oberon Hansen — Goethe University, Frankfurt am Main, Germany

We calculate the spectrum of collective modes (amplitude, phase, phonon, and plasmon) in the charge-density wave state of the quasi-one dimensional metal $K_{0.3}MoO_3$, named blue bronze. Using a functional integral approach we derive effective actions for the different types of collective modes in Gaussian approximation and compare our results with experiments. Our approach emphasizes the role of acoustic phonons to guarantee that the phase mode remains gapless in the presence of long-range Coulomb interactions.

TT 51.5 Thu 16:15 HSZ 103

Lattice instability in charge-frustrated CsW_2O_6 — •Pascal Reiss[1], Peter Wochner[1], Armin Schulz[1], Jürgen Nuss[1], Masahiko Isobe[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, The University of Tokyo, Bunkyo, Tokyo, Japan

The transition metal compound CsW_2O_6 represents an intriguing example of a pyrochlore structure at quarter filling. Starting from a bad metal with a nominal $W^{5.5+}$ oxidation state, the system suffers a metal-to-insulator transition around $T_c \approx 215\,K$. Here, a breathing distortion leads to the formation of regular molecular W_3 trimers with 2 localised electrons each, and a remaining W^{6+} site devoid of $5d$ electrons [1]. However, the origin of the transition as well as the electronic nature of the low-temperature phase remain unclear [2].

To elucidate the origin of the 215 K transition, we will present our recent structural investigations and transport measurements on CsW_2O_6 conducted under high pressures, where we uncover another structural instability, distinct from the ambient pressure one.

[1] Y. Okamoto et al., Nat. Commun. 11 (2020)
[2] N. Nakai and C. Hotta, Nat. Commun. 13 (2022)

TT 51.6 Thu 16:30 HSZ 103

Pressure-induced stabilization mechanism of molecular orbital crystals in $IrTe_2$ — •Tobias Ritschel[1], Quirin Stahl[1], Maximilian Kusch[1], Gaston Garbarino[2], Volodymyr Svitlyk[2], Mohamed Mezouar[2], Junjie Yang[3], Sang-Wook Cheong[4], and Jochen Geck[1] — [1]Institute of Solid State and Materials Physics, TU Dresden, 01069 Dresden, Germany — [2]ESRF, Grenoble, France — [3]New Jersey Institute of Technology, Newark, New Jersey 01702, USA — [4]Rutgers, New Jersey, USA

Doped $IrTe_2$ is considered a platform for topological superconductivity and therefore receives currently a lot of interest. In addition, the superconductivity in these materials exists in close vicinity to electronic order and the formation of molecular orbital crystals, which we explore here by means of high-pressure single crystal x-ray diffraction in combination with density functional theory. Our crystallographic refinements provide detailed information about the structural evolution as a function of applied pressure up to 42 GPa. Using this structural information for density functional theory calculations, we show that the local multicenter bonding in $IrTe_2$ is driven by changes in the Ir-Te-Ir bond angle. When the electronic order sets in, this bond angle decreases drastically, leading to a stabilization of a multicenter molecular orbital bond. This unusual local mechanism of bond formation in an itinerant material provides a natural explanation for the different electronic orders in $IrTe_2$. It further illustrates the strong coupling of the electrons with the lattice and is most likely relevant for the superconductivity in this material.

TT 51.7 Thu 16:45 HSZ 103

Lifshitz transition at the onset of superconductivity from mismatched nesting in $TiSe_2$ — •Roemer Hinlopen[1], Owen Moulding[1,2], Felix Flicker[3], Charles Sayers[4], Enrico Da Como[4], Jasper van Wezel[5], and Sven Friedemann[1] — [1]University of Bristol, UK — [2]Institut Néel, Grenoble, France — [3]Cardiff University, UK — [4]University of Bath, UK — [5]University of Amsterdam, The Netherlands

Fermi surface reconstructions and topological (Lifshitz) transitions can have a profound effect on the electronic ground state of a metal. For example, re-entrant superconductivity (SC) in URhGe may be due to the appearance of a small pocket [1], whereas in Bechgaard salts [2] and doped $BaFe_2As_2$ [3] the appearance of large pockets from mismatched nesting may give rise to SC within the magnetic phase.

Here, we report quantum oscillation measurements and DFT calculations under pressure in the prototypical charge density wave (CDW) compound $TiSe_2$. We observe the emergence of new Fermi surface pockets at 2 GPa within the CDW arising as a result of mismatched nesting. This Lifshitz transition coincides with the emergence of superconductivity [4], suggesting an intimate link between SC and the presence of these Fermi pockets similar to $BaFe_2As_2$. This suggests that SC in $TiSe_2$ might be of extended $s^{\pm}$-wave character - the first such case in a CDW system.

[1] Yelland, Nat. Phys. 7, 890 (2011)
[2] Bourbonnais, C. R. Physique 12, 532 (2011)
[3] Liu, Nat. Phys. 6, 419 (2010)
[4] Kusmartseva, PRL 103, 236401 (2009)

TT 51.8 Thu 17:00 HSZ 103

Spin stripe fluctuations in antiferromagnetic $Pr_{2-x}Sr_xNiO_{4+\delta}$ — •Avishek Maity[1], Rajesh Dutta[2,3], and Werner Paulus[4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, 85747 Garching, Germany — [2]Institut für Kristallographie, RWTH Aachen Universität, 52066 Aachen, Germany — [3]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), 85747 Garching, Germany — [4]ICGM, Univ. Montpellier, CNRS, ENSCM, Montpellier, France

Spin and charge stripe correlations and their dynamics have been well explored in the ordered state of $RE-$based 214-nickelates for last 3 decades. In this regards, what remains less explored is the fluctuating state of the spin stripes from which the long-range spin stripes develop on cooling. In this talk, we present our recent inelastic neutron scattering study of the low energy spin stripe fluctuations in $Pr_{2-x}Sr_xNiO_{4+\delta}$ with magnetic incommensurability $\epsilon = 0.33$ above the spin stripe ordering temperature $T_{so} = 190$ K [1]. The spin stripe fluctuations measured at the at the incommensurate wave vector show a non-dispersive character with no detectable anisotropy persisting up to a maximum energy 10 meV, and strongly suppressed already below the charge stripe ordering temperature $T_{co} = 255$ K. Our results clearly indicate the presence of static charge stripe order is essential for the spin stripe fluctuations in 214-type nickealtes.

[1] A. Maity *et al.*, Phys. Rev. B 106, 024414 (2022)

TT 51.9 Thu 17:15 HSZ 103

Glass-like transitions in the frustrated charge system θ-(BEDT-TTF)$_2MM'$(SCN)$_4$ (MM' = CsZn, CsCo, and RbZn) revealed by thermal expansion measurements — •Yohei Saito[1], Tatjana Thomas[1], Yassine Agarmani[1], Tim Thyzel[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2,3], Jens Müller[1], and Michael Lang[1] — [1]Goethe University Frankfurt, Frankfurt (M), Germany — [2]University of Tokyo, Chiba, Japan — [3]Tohoku University, Sendai, Japan

Geometrical frustration causes degenerate states and a frustrated charge system is proposed in organic conductors. It is expected that charge order (CO) is suppressed and is possibly replaced by a charge glass state. In organic condutors, the CO transition accompanies a structural transition. Therefore, investigating their elastic properties is of fundamental interest. We performed thermal expansion measurements on θ-(BEDT-TTF)$_2MM'$(SCN)$_4$ (MM' = CsZn, CsCo, and RbZn) : whereas the CsZn and CsCo salts exhibit no CO transition, slowly-cooled RbZn salt shows the transition. The thermal expansion coefficient of no-CO salts exhibited a glassy transition at 90-100 K. This behavior is reminiscent of the freezing of the terminal ethylene end-groups on the BEDT-TTF molecules. For the RbZn salt we observe a CO transition at 210 K and also an ethylene-group related glass-like transition at 80-100 K. Therefore, the glass-like anomaly around 90 K appears as a common feature in θ-type salts regardless of whether long-range CO exists. These results point to the importance of the lattice degrees of freedom in the frustrated charge system.

TT 52: Frustrated Magnets: Strong Spin-Orbit Coupling

Time: Thursday 15:00–17:30 Location: HSZ 201

TT 52.1 Thu 15:00 HSZ 201

Finite temperature nonlinear optical response of the Kitaev magnet — •Wolfram Brenig[1] and Olesia Krupnitska[1,2] — [1]Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany — [2]Institute for Condensed Matter Physics, NASU, Svientsitskii Str. 1, 79011 Lviv, Ukraine

One of the key properties of a quantum spin liquid is fractionalization. In the spin liquid hosted by the Kitaev model, this occurs in terms of two types of quasiparticles, i.e., itinerant Majorana fermions and localized gapped Z_2 fluxes. A multitude of probes have been suggested to provide evidence for the response and spectral continua related to such fractionalization. Here we report results on the nonlinear optical response of a Kitaev magnet at finite temperature. 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 52.2 Thu 15:15 HSZ 201

Thermal decomposition of the Kitaev material α-$RuCl_3$ and its influence on the low-temperature properties — •Franziska Breitner[1], Anton Jesche[1], Vladimir Tsurkan[2], and Philipp Gegenwart[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

Thermally driven decomposition and reduction of honeycomb ruthenium-trichloride has been known long before the material attracted considerable interest as a Kitaev system [1,2]. We systematically explore the effect of heat treatment in argon atmosphere under various temperatures up to 500°C on single crystals by study of the mass loss, microprobe energy dispersive x-ray spectroscopy, powder x-ray diffraction, as well as low-temperature magnetic susceptibility and specific heat experiments. For annealing temperatures beyond 300°C we detect clear signatures of dechlorination and oxidation of Ru. The specific heat is consistently described by the sum of a major α-$RuCl_3$ and minor RuO_2 volume fraction, whose latter C∼T contribution dominates the total specific heat below 1 K. Comparison with measurements on unannealed crystals suggests that even therein a tiny RuO_2 metal fraction cannot be excluded, which could be relevant also for other physical properties.

[1] A.E. Newkirk and D.W. McKee, J. Catal. 11, 370 (1968)
[2] J.A. Sears et al., Phys. Rev. B 91, 144420 (2015)

TT 52.3 Thu 15:30 HSZ 201

Spin-phonon dynamics in α-$RuCl_3$ probed by ultrasound — •Andreas Hauspurg[1,2], S. Zherlitsyn[1], T. Helm[1], V. Tsurkan[3], K. Y. Choi[4], S. H. Do[5], W. Brenig[6], N. Perkins[7], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden, HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Institute of Physics, University of Augsburg, Germany — [4]Department of Physics, Sungkyunkwan University, Republic of Korea — [5]Oak Ridge National Lab, USA — [6]Institute for Theoretical Physics, TU Braunschweig, Germany — [7]School of Physics and Astronomy, University of Minnesota, USA

Among the most studied honeycomb-lattice materials predicted to host Kitaev interactions is the spin-orbit-coupled Mott insulator α-$RuCl_3$. Despite antiferromagnetic ordering at 7 K, α-$RuCl_3$ is considered proximate to the Kitaev quantum spin liquid (QSL) state, which features fractionalized quasiparticle excitations. A promising approach to study such excitations is to investigate the spin-phonon interaction in this material. Our studies of the elastic properties of α-$RuCl_3$ by means of ultrasound pulse-echo technique indicate unconventional physics of the debated QSL phase. Here, we present low-temperature results of the sound velocity and attenuation in external magnetic fields and discuss their behavior with respect to the quasiparticle excitations in α-$RuCl_3$. In our studies we observed a linear temperature dependence of the attenuation beyond the ordered state at 8 T that follows a characteristic C_6 symmetry. Anomalies in the acoustic properties shed new light on the H-T phase diagram.

TT 52.4 Thu 15:45 HSZ 201

Rethinking α-$RuCl_3$ again — •Marius Möller[1], Roser Valentí[1], and Alexander L. Chernyshev[2] — [1]Institute for Theoretical Physics, Goethe University Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany — [2]Department of Physics and Astronomy, University of California, Irvine, California 92697, USA

The honeycomb Kitaev material α-$RuCl_3$ is widely investigated due to its originally suspected proximity to a spin liquid state suggested by unusual neutron scattering results. The magnetic Hamiltonian was initially formulated as a generalized Kitaev model K_1-J_1-Γ_1-Γ_1'-J_3 in a cubic spin reference orientated along the Ru-Cl bonds. Recent studies, however, suggest that a crystallographic parametrization of the Hamiltonian in a spin-ice-like language $J(XY)$-Δ-$J_{\pm\pm}$-$J_{z\pm}$-J_3 could lead to significant reduction of the parameter space, hinting towards a potential minimal model of α-$RuCl_3$. We present the classical and quantum phase diagram of this $J(XY)$-$J_{z\pm}$-J_3 minimal model candidate obtained by Luttinger-Tisza method (LT), Exact Diagonalization (ED) and Density Matrix Renormalization Group (DMRG). Further, we present the phase diagrams of three interesting parameter regions with constrained anisotropic exchanges K_1,Γ_1,Γ_1' leading to effective J_1-J_3 models which possibly capture the relevant region to describe the essential physics of α-$RuCl_3$.

M.M. and R.V. gratefully acknowledge funding by the DFG(German Research Foundation): TRR 288 - 422213477; M.M. gratefully acknowledges funding by Studienwerk Villigst.

TT 52.5 Thu 16:00 HSZ 201

Evolution of electronic and magnetic properties of the Kitaev-type compound $Ru(Br_{1-x}I_x)_3$ — •Jihuan Gu[1], Tomohiro Takayama[1,2], Alexander Yaresko[1], and Hidenori Takagi[1,2] — [1]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]Institut für Funktionelle Materie und Quantentechnologien, University of Stuttgart, 70550 Stuttgart, Germany

Kitaev magnets like α-$RuCl_3$ have attracted great attention in the field of solid-state physics as a potential realization of exotic quantum spin-liquid state. If such Kitaev materials are turned into a metallic state, exotic electronic properties may be realized near the critical phase boundary, such as unconventional superconductivity. So far, carrier doping via intercalation or application of pressure has been attempted to induce a metal-insulator transition (MIT), but no metallic state has been obtained. Recently, the two honeycomb compounds $RuBr_3$ and RuI_3, which are isostructural to α-$RuCl_3$, have been reported. While $RuBr_3$ is a Mott insulator with a zigzag magnetic order, RuI_3 was reported to be a correlated semimetal, likely induced by the enhanced d-p hybridization. Hence, the MIT phase boundary should be expected between $RuBr_3$ and RuI_3. We thus synthesized $Ru(Br_{1-x}I_x)_3$ with various doping levels x. The successful substitution of Br with I was confirmed by the systematic change of lattice parameters. The MIT phase boundary seems to be at x around 0.7. We will discuss the evolution of electronic and magnetic properties in the series of $Ru(Br_{1-x}I_x)_3$ and a marginal metallic state near MIT.

15 min. break

TT 52.6 Thu 16:30 HSZ 201

Milli-Kelvin thermal conductivity of $YbAlO_3$, a quasi-one-dimensional quantum magnet — •Parisa Mokhtari[1,2,3], Ulrike Stockert[1], Stanislav Nikitin[4], Leonid Vasylechko[5], Manuel Brando[2], and Elena Hassinger[1] — [1]Institute of Solid State and Materials, Dresden, Germany — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [3]Physics Department, Technical University of Munich, Garching, Germany — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]Lviv Polytechnic National University, Lviv, Ukraine

In 2019, Wu *et al.* found the typical excitation spectrum of the fractionalised magnetic excitations, so-called spinons, in the Q-1D material $YbAlO_3$ via neutron scattering at 1 K. $YbAlO_3$ exhibits AFM (J_c=2.3 K) and FM (J_{ab}=0.8 K) exchange interaction along and perpendicular to the chain direction, respectively [1, 2]. In zero field (B), a 3D AFM order is established at 0.88 K. For $B \parallel a$, this order is suppressed and replaced by an incommensurate-AFM state, until the field-polarised state occurs for B >1.5 T.

In this work, we investigate the thermal conductivity (κ) of $YbAlO_3$ down to 30 mK in B up to 4 T, with a focus on the magnetic excitations' contribution in thermal transport within different phases and their interactions with lattice vibrations. Notably, our results are in agreement with the previous reports, as well as providing new anomalies compared to thermodynamics' probes and theoretical predictions.

[1] L. S. Wu *et al.*, Nat. Commun. 10, 698 (2019).
[2] L. S. Wu *et al.*, Phys. Rev. B 99, 195117 (2019).

TT 52.7 Thu 16:45 HSZ 201

Thermal expansion and magnetostriction as the probe of exotic magnetism in honeycomb $BaCo_2(AsO_4)_2$ — •Prashanta K. Mukharjee[1], Bin Shen[1], Anton Jesche[1], Julian Kaiser[1], Philipp Gegenwart[1], and Alexander Tsirlin[2] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Felix Bloch Institute for Solid-State Physics, University of Leipzig, 04103 Leipzig, Germany

The $3d^7$ Co-based honeycomb materials have received wide attention as a possible platform for the experimental realization of the celebrated Kitaev model. Here, we elucidate the thermodynamic properties of the candidate material $BaCo_2(AsO_4)_2$ using high-resolution thermal expansion and magnetostriction measurements. At 2 K, with an increase in field, the linear magnetostriction coefficient shows two well-separated anomalies around critical field $H_{c1} \sim 0.2$ T and $H_{c2} \sim 0.5$ T transition around H_{c1} is hysteretic, pointing towards a first-order type transition, whereas the transition at H_{c2} lacks hysteresis, reflecting the second-order nature. The linear thermal expansion coefficient shows a sharp positive peak in 0 T, which decreases, then changes its sign with the rise in the field and smears out entirely above H_{c2}. Below T_N, for H_{c1} « H « H_{c2}, our angle-dependent magnetization shows an apparent six-fold symmetry, whereas significant deviations have been observed below Hc1 and above H_{c2}. We draw the in-plane phase diagram from the above experiments and other complementary techniques and discuss the interplay of first and second-order transitions in this material.

TT 52.8 Thu 17:00 HSZ 201

Phononic-magnetic dichotomy of the thermal Hall effect in the Kitaev-Heisenberg candidate material $Na_2Co_2TeO_6$ — Matthias Gillig[1], Xiaochen Hong[2,1], Christoph Wellm[1], Vladislav Kataev[1], Weiliang Yao[3], Yuan Li[3], Bernd Büchner[1], and •Christian Hess[2,1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [3]International Center for Quantum Materials, School of Physics, Peking University, 100871 Beijing, China

We investigate the thermal Hall effect of the Kitaev quantum spin liquid candidate material $Na_2Co_2TeO_6$ in both the magnetically ordered and the paramagnetic phase, with a magnetic field perpendicular to the honeycomb layers of this material. The transversal heat conductivity κ_{xy} is sizeable, but remains at all temperatures investigated significantly smaller than one half of the thermal conductance quantum which has been predicted as fingerprint of topologically protected Majorana edge modes in a Kitaev quantum spin liquid. κ_{xy} is negative in the paramagnetic phase but becomes positive deep in the antiferromagnetically ordered phase suggesting a non-phononic origin. However, distinct similarities are present in κ_{xy} and the longitudinal thermal conductivity κ_{xx} concerning both their temperature and field dependences. Thus our findings imply an at least two-component, i.e. magnetic and phononic origin of the thermal Hall effect in $Na_2Co_2TeO_6$.

TT 52.9 Thu 17:15 HSZ 201

Triple-Q order in $Na_2Co_2TeO_6$ from proximity to hidden-SU(2)-symmetric point — •Wilhelm Krüger[1], Wenjie Chen[2], Xianghong Jin[2], Yuan Li[2,3], and Lukas Janssen[1] — [1]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany — [2]International Center for Quantum Materials, School of Physics, Peking University, Beijing 100871, China — [3]Collaborative Innovation Center of Quantum Matter, Beijing 100871, China

In extended Heisenberg-Kitaev-Gamma-type spin models, hidden-SU(2)-symmetric points are isolated points in parameter space that can be mapped to pure Heisenberg models via nontrivial duality transformations. Such points generically feature quantum degeneracy between conventional single-Q and exotic multi-Q states. We argue that recent single-crystal inelastic neutron scattering data place the honeycomb magnet $Na_2Co_2TeO_6$ in proximity to such a hidden-SU(2)-symmetric point. The low-temperature order is identified as a triple-Q state arising from the Néel antiferromagnet with staggered magnetization in the out-of-plane direction via a 4-sublattice duality transformation. This state naturally explains various distinctive features of the magnetic excitation spectrum, including its surprisingly high symmetry and the dispersive low-energy and flat high-energy bands. Our result demonstrates the importance of bond-dependent exchange interactions in cobaltates, and illustrates the intriguing magnetic behavior resulting from them.

TT 53: Graphene

Time: Thursday 15:00–17:45 Location: HSZ 204

TT 53.1 Thu 15:00 HSZ 204

Andreev and normal reflections processes in gated bilayer graphene — •Panch Ram[1], Detlef Beckmann[2], Romain Danneau[2], and Wolfgang Belzig[1] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany

We present our theoretical study of the Andreev and normal reflections processes in a bilayer graphene normal-superconductor junction where gate fields are applied (equal and opposite). Gating can induce a gap in the dispersion of the graphene layer. We employ the Dirac-Bogoliubov-de Gennes equation for the low-energy gated bilayer graphene Hamiltonian and calculate the Andreev and normal reflections probabilities using the scattering theory, and also obtain the differential conductance within the Blonder-Tinkham-Klapwijk formalism [1, 2]. We observe the Andreev retro-reflection (specular-reflection) below (above) the Fermi energy when the bias voltage is within the superconducting gap [3]. Interestingly, both retro-reflection as well as specular reflection are strongly modified in the presence of the gate field. For small gate field, they can be tuned to either specular or retro Andreev reflection by changing the Fermi energy. Moreover, we find double Andreev reflections and double normal reflections (specular and retro) when the gate field becomes comparable to the interlayer coupling strength.

[1] A. F. Andreev, Sov. Phys. JETP 19, 1228 (1964)
[2] G. E. Blonder et al., Phys. Rev. B 25, 4515 (1984)
[3] C. W. J. Beenakker, Phys. Rev. Lett. 97, 067007 (2006)

TT 53.2 Thu 15:15 HSZ 204

Graphene superlattice due to twisted hexagonal boron nitride monolayers — •Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

Stacking of two-dimensional (2D) materials of similar lattice structures on top of each other with a small twist angle leads to the so-called Moiré pattern due to the large-scale lattice inteference. When one of them is a conducting material such as graphene, the Moiré pattern serves as a large-scale periodic potential, turning the host conducting lattice into a superlattice, whose modified electronic properties can be seen in transport experiments and simulations. Graphene placed on a hexagonal boron nitride (hBN) layer is one of the best known graphene superlattices, while twisted bilayer graphene made of two monolayers of graphene is another example under intensive investigations during the past years. Twisted monolayers of hBN also form the Moiré pattern, yet its effect on transport properties of neighboring graphene is less known. Here, we consider graphene put on monolayers of twisted hBN (thBN), and perform quantum transport simulations considering the effect of the charge-polarized superlattice potential [1]. Due to the exceptionally long Moiré wavelength of the twisted hBN, multiple satellite Dirac points emerge in the transmission spectrum within the experimentally accessible range of the carrier density. Possible experiments confirming the model of graphene on thBN as well as further exploring novel transport behaviors due to the thBN will be discussed.

[1] C. R. Woods *et al.*, Nat. Commun. **12**, 347 (2021)

TT 53.3 Thu 15:30 HSZ 204

Transport signatures of Van Hove singularities in mesoscopic twisted bilayer graphene — •Aleksander Sanjuan Ciepielewski[1], Jakub Tworzydło[2], Timo Hyart[1,3], and Alexander Lau[1] — [1]MagTop, IF PAN, Warsaw, Poland — [2]University of Warsaw, Poland — [3]Aalto University, Finland

Magic-angle twisted bilayer graphene (TBG) exhibits quasiflat low-energy bands with Van Hove singularities (VHS) close to the Fermi level. These singularities play an important role in the exotic phenomena observed in this material, such as superconductivity and magnetism, by amplifying electronic correlation effects. In this work [1], we study the correspondence of four-terminal conductance and the Fermi surface topology as a function of the twist angle, pressure, and energy in mesoscopic, ballistic samples of small-angle TBG. We establish a correspondence between features in the wide-junction conductance and the presence of VHS in the density of states. Moreover, we identify additional transport features, such as a large, pressure-tunable minimal conductance, conductance peaks coinciding with nonsingular band crossings, and unusually large conductance oscillations as a function of the system size. Our results suggest that TBG close the magic angle is a unique system featuring simultaneously large conductance due to the quasiflat bands, strong quantum nonlinearity due to the VHS, and high sensitivity to external parameters, which could be utilized in high-frequency device applications and sensitive detectors.

[1] A. Sanjuan Ciepielewski, J. Tworzydło, T. Hyart, and A. Lau, Phys. Rev. Research 4, 043145 (2022)

TT 53.4 Thu 15:45 HSZ 204

Coulomb blockade effects in minimally twisted bilayer graphene — •Patrick Wittig[1], Fernando Dominguez[1], Christophe De Beule[2,3], and Patrik Recher[1,4] — [1]Institute for Mathematical Physics, TU Braunschweig, 38106 Braunschweig, Germany — [2]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg — [3]Department of Physics and Astronomy, University of Pennsylvania, Philadelphia PA19104 — [4]Laboratory of Emerging Nanometrology, 38106 Braunschweig, Germany

In the presence of a finite interlayer electric field, minimally twisted bilayer graphene displays a triangular network of chiral valley Hall states that propagate along the AB/BA interfaces and scatter at the metallic AA regions. Previous studies model the chiral network using a phenomenological scattering matrix approach based entirely on the symmetries of the system [1,3]. So far, the physics of the metallic AA scattering regions has been disregarded, although in the chiral network regime are also flat bands corresponding to a finite density of states in the AA region [2]. Therefore, we include in the phenomenological scattering matrix the AA regions in form of quantum dots: A set of discrete energy levels with Coulomb interaction, which we treat in mean field theory. We study the resulting network through the energy spectrum and magneto-conductance calculations.

[1] D. Efimkin, A. MacDonald, PRB 98, 035404 (2018)
[2] A. Ramires, J. Lado, PRL 121, 146801 (2018)
[3] C. De Beule, F. Dominguez, P. Recher, PRL 125, 096402, (2020)

TT 53.5 Thu 16:00 HSZ 204

Twisted bilayer graphene at charge neutrality: Spontaneous symmetry breaking of SU(4) Dirac electrons — •Nikolaos Parthenios and Laura Classen — Max-Planck Institute for Solid State Research, Stuttgart, Germany

We study possible patterns for spontaneous symmetry breaking in twisted bilayer graphene at charge neutrality. Starting from an effective Dirac Hamiltonian, we show how an SU(4) symmetry emerges that is composed of combined spin, valley and sublattice transformations. We construct the corresponding low-energy model that includes all symmetry-allowed four-fermion interactions and employ a renormalization group treatment to identify the critical points that describe transitions into the different ordered phases. The resulting phase diagram depends on the number of fermion flavours and we argue that for twisted bilayer graphene it is governed by a quantum Hall state or SU(4) manifolds of spin-valley orders with emergent Lorentz symmetry. Due to the large symmetry, small perturbations will determine the final symmetry breaking mechanism.

TT 53.6 Thu 16:15 HSZ 204

Analog gravity in twisted bilayer graphene — •Mireia Tolosa-Simeón[1], Stefan Floerchinger[2], and Michael Scherer[1] — [1]Institut für Theoretische Physik III, Ruhr-Universität Bochum — [2]Theoretisch-Physikalisches Institut, Friedrich-Schiller-Universität Jena

Condensed-matter systems can sometimes be used to emulate and study phenomena from a completely different field of physics, for example, from elementary particle physics or gravity. Such analog condensed-matter models may provide a novel perspective to approach difficult problems in the original systems, and can potentially be realized experimentally in a well-controlled environment.

In this contribution, we will address the problem of cosmological fermion production in expanding universes using twisted bilayer graphene as an analog model. In particular, we study twisted bilayer graphene's Dirac electrons near charge neutrality, which acquire a mass gap through a symmetry-breaking phase transition. Introducing a time-dependent Fermi velocity, we show the emergence of an analog of cosmological pair production. Our scenario could be scrutinized experimentally in the future.

15 min. break

TT 53.7 Thu 16:45 HSZ 204

Quantum transport simulation for graphene on transition-metal dichalcogenides — •Wun-Hao Kang and Ming-Hao Liu — Department of Physics, National Cheng Kung University, Tainan, Taiwan

The strength of spin-orbit coupling (SOC) in pristine graphene was found from first-principles calculations to be in the order of μeV [1], which gives nearly no effects in transport experiments. Subsequent studies showed that the SOC can be significantly enhanced to the order of meV by putting graphene on transition-metal dichalcogenides (TMDC) [2]. Very recently, Tiwari P. et al. reported that the enhanced SOC can be experimentally observed in graphene/WSe2 systems [3]. Here we perform quantum transport simulations for graphene on TMDCs based on real-space tight-binding models [4], considering the Fabry-Pérot interferometer by using a gate-induced potential barrier as the cavity.

[1] M. Gmitra et al., Phys. Rev. B **80**, 235431 (2009)
[2] M. Gmitra et al., Phys. Rev. B **93**, 155104 (2016)
[3] P. Tiwari et al., npj 2D Mater Appl. **6**, 68 (2022)
[4] M. Zubair et al., Phys. Rev. B **101**, 165436 (2020)

TT 53.8 Thu 17:00 HSZ 204

Theory of broken symmetry quantum Hall states in the $N = 1$ Landau level of Graphene — •Nikolaos Stefanidis[1] and Inti Sodemann[2,1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden 01187, Germany — [2]Institut für Theoretische Physik, Universität Leipzig, D-04103, Leipzig, Germany

We study many-body ground states for the partial integer fillings of the $N = 1$ Landau level in graphene, by constructing a model that accounts for the lattice scale corrections to the Coulomb interactions. Interestingly, in contrast to the $N = 0$ Landau level, this model contains not only pure delta function interactions but also some of its derivatives. Due to this we find several important differences with respect to the $N = 0$ Landau level. For example at quarter filling when only a single component is filled, there is a degeneracy lifting of the quantum hall ferromagnets and ground states with entangled spin and valley degrees of freedom can become favourable. Moreover at half-filling of the $N = 1$ Landau level, we have found a new phase that is absent in the $N = 0$ Landau level, that combines characteristics of the Kekulé state and an antiferromagnet. We also find that according to the parameters extracted in a recent experiment, at half-filling of the $N = 1$ Landau level graphene is expected to be in a delicate competition between an AF and a CDW state, but we also discuss why the models for these recent experiments might be missing some important terms.

TT 53.9 Thu 17:15 HSZ 204

Multi-layered atomic relaxation in van der Waals heterostructures — Dorri Halbertal[1], •Lennart Klebl[2], Valerie Hsieh[1], Jacob Cook[3], Stephen Carr[4], Guang Bian[3], Cory Dean[1], Dante M. Kennes[5,6], and Dmitri N. Basov[1] — [1]Department of Physics, Columbia University, United States — [2]1st Institute of Theoretical Physics, University of Hamburg, Germany — [3]Department of Physics and Astronomy, University of Missouri, United States — [4]Physics Department, Brown University, United States — [5]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [6]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

When two-dimensional van der Waals materials are stacked to build heterostructures, Moiré patterns emerge from twisted interfaces or from mismatch in lattice constant of individual layers. Relaxation of the atomic positions is a direct, generic consequence of the Moiré pattern, with many implications for the physical properties. Motivated by experimental findings in multi-layered van der Waals heterostructures, we develop a generic continuum approach to model (multi-layered) relaxation processes based on the generalized stacking fault energy functional. The continuum property of the approach enables us to access large scale regimes and achieve agreement with experimental findings. Furthermore, we study the impact of multi-layered relaxation on the local density of states of a twisted graphitic system. We identify measurable implications for the system, experimentally accessible by scanning tunneling microscopy.

TT 53.10 Thu 17:30 HSZ 204

Non-destructive low-temperature contacts to MoS_2 nanoribbon and nanotube quantum dots — •Robin T. K. Schock[1], Jonathan Neuwald[1], Konstantin D. Schneider[1], Matthias Kronseder[1], Luka Pirker[2], 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, Institute Jožef Stefan, 1000 Ljubljana, Slovenia

Planar TMDCs are at the center of manifold research efforts due to their intrinsic two dimensional nature. Despite detailed studies of their optical parameters, worldwide efforts to reach single level transport in lithographically designed quantum dots at low temperatures have so far been largely unsuccessful. This is due to the requirement for very small confinement potentials as well as disorder from dangling bonds at the edges of nanoflakes. Both issues can be circumvented by using as-grown MoS_2 nanotubes and nanoribbons. First Coulomb blockade measurements were recently performed on a MoS_2 nanotube[1], so far limited by disorder below the metallic scandium contacts.

Here, we present low temperature measurements on MoS_2 nanotubes and nanoribbons contacted with bismuth[2]. Our data clearly shows the non-destructive and transparent nature of these contacts to our quantum dots and indicates quantum confinement[3].

[1] S. Reinhardt *et al.*, pssRRL **13**, 1900251 (2019)
[2] P. C. Shen *et al.*, Nature **593**, 211 (2021)
[3] R. T. K. Schock *et al.*, arXiv:2209.15515 (2022).

TT 54: Quantum Coherence and Quantum Information Systems II

Time: Thursday 15:00–17:45 Location: HSZ 304

TT 54.1 Thu 15:00 HSZ 304

Dominant materials losses in superconducting circuits based on tantalum thin films — •Ritika Dhundhwal[1], Haoran Duan[2], Dirk Fuchs[1], Alexander Welle[3], Mahya Khorramshahi[1], Jasmin Aghassi-Hagmann[2], Ioan M. Pop[1], and Thomas Reisinger[1] — [1]Institut für Quantenmaterialien und technologien — [2]Institut für Nanotechnologie — [3]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie

Superconducting quantum circuits are a promising hardware platform in the fields of quantum computing and detection. To improve their performance, exploring new materials is highly relevant. One promising candidate material is tantalum (Ta), which was recently shown to improve transmon qubit lifetimes[1]. However, the understanding of the dominant loss mechanisms related to Ta is limited. Here, we present a study of losses in epitaxial Ta films deposited using magnetron sputtering, with the aim of relating basic material properties to loss mechanisms. A variation in the deposition parameters (mainly substrate temperature) leads to structurally different films. We characterized these using high-resolution X-ray diffraction, Time-of-Flight secondary-ion mass spectrometry, scanning electron microscopy and superconducting transition temperature measurements. We fabricated lumped element resonators from the films and measured their quality factors as a function of photon number and temperature. In addition, we vary the energy participation ratio of Ta metal-substrate interface to find the dominant loss mechanism.

[1] A. P. M. Place *et al.*, Nat. Commun. 12, 1779 (2021)

TT 54.2 Thu 15:15 HSZ 304

Many body localization of 2D transmon arrays with a quasi-periodic potential and perturbative Walsh-Hadamard coefficients — •Evangelos Varvelis and David DiVincenzo — JARA, Aachen, Germany

Recently it has been shown that transmon qubit architectures experience a phase transition between many body localized and quantum chaotic. It is crucial for quantum computation that the system remains in the localized regime, yet the most common way to achieve this relies on random disorder. Here we propose a quasi-periodic potential as a substitute for random disorder, with the purpose of localizing a 2D transmon array. We demonstrate, using the Walsh-Hadamard diagnostic, that the quasiperiodic potential is more effective at achieving localization. In order to study the localizing properties of our new potential for experimentally relevant system sizes, we develop a many-body perturbation theory whose computational cost scales only with the non-interacting system dimensions.

TT 54.3 Thu 15:30 HSZ 304

Linear response for pseudo-Hermitian Hamiltonian systems: Application to PT-symmetric qubits — •Mikhail V. Fistul, Leander Tetling, and Ilya M. Eremin — Ruhr-Universität Bochum, Bochum Germany

We develop the linear response theory formulation suitable for application to various *pseudo-Hermitian Hamiltonian* systems. The analytical expressions for the generalized temporal quantum-mechanical correlation function and the time-dependent dynamic susceptibility, $\chi(t)$, are derived [1].

We apply our results to two PT-symmetric non-Hermitian quantum systems: a single qubit and two unbiased/biased qubits coupled by the exchange interaction. For both systems we identify PT-symmetry unbroken and broken quantum phases and quantum phase transitions between them. The temporal oscillations of the dynamic susceptibility of the qubits polarization, $\chi(t)$, relate to *ac* induced transitions between different eigenstates, and we analyze the dependencies of the oscillations frequency and the amplitude on the gain/loss parameter γ and the interaction strength g.

Studying the time dependence of $\chi(t)$ we observe different types of oscillations, i.e., undamped, heavily damped and amplified ones, related to the transitions between eigenstates with broken (unbroken) PT-symmetry. These predictions can be verified in the microwave transmission experiments.

[1] L. Tetling, M. V. Fistul, and I. M. Eremin, Phys. Rev. B **106**, 134511 (2022).

TT 54.4 Thu 15:45 HSZ 304

High kinetic inductance microstrip networks for integrated quantum information devices — •Niklas Gaiser[1], Ciprian Padurariu[1], Björn Kubala[1,2], Nadav Katz[3], and Joachim Ankerhold[1] — [1]ICQ and IQST, University of Ulm, Ulm, Germany — [2]Institute of Quantum Technologies, German Aerospace Center (DLR), Ulm, Germany — [3]The Racah Institute of Physics, The Hebrew University of Jerusalem, Israel

Modern superconducting quantum information devices integrate qubits and readout resonators into complex microwave circuits. Efficient qubit operation and fast readout require relatively strong coupling. This, however, can compromise the qubit lifetime due to spontaneous emission through the resonator. An elegant solution is provided by a Purcell filter, an added circuit element that suppresses transmission at the qubit frequency.

Here, we present a theoretical proposal for circuit architectures that realize qubit readout with Purcell filters, utilizing the highly versatile platform of high-kinetic inductance microstrip networks experimentally realized in [1]. The strongly reduced phase velocities in such materials allow compact filter designs that can be integrated on-chip. We describe band-structure design techniques to build an efficient Purcell filter and provide quantitative estimations for the suppression of unwanted relaxation channels.

[1] S. Goldstein, G. Pardo, N. Kirsh, N. Gaiser, C. Padurariu, B. Kubala, J. Ankerhold, and N. Katz, New J. Phys. 24 023022 (2022)

TT 54.5 Thu 16:00 HSZ 304

Microwave radiation emitted by a phase qubit — •Surangana Sengupta[1], Ciprian Padurariu[1], Bjoern Kubala[1,2], and Joachim Ankerhold[1] — [1]ICQ and IQST, Ulm University, Germany — [2]German Aerospace Center (DLR), Ulm, Germany

Josephson photonics devices consist of a DC-biased Josephson junction in series with a superconducting microwave cavity and are promising sources of bright quantum states of microwave radiation. Such devices realize the regime of strong-coupling circuit quantum electrodynamics, when the effective fine structure constant of the circuit approaches unity. In this case, multi-photon downconversion processes, where one tunnelling Cooper pair emits k photons in the cavity ($k \leq 6$), have been observed [1].

Here, we propose a new regime for Josephson photonics devices, where both the inductive as well as the capacitive behavior of the Josephson junction is taken into account [2]. Thereby, the Josephson phase is treated as an electronic degree of freedom, characterized by the plasma frequency of the junction, that is independent of the photonic degree of freedom, described by the phase of the cavity. We present a preliminary study of the coupled photonic and electronic dynamics, discuss the nature of the coupling and present a detailed comparison to conventional Josephson photonics dynamics. As an example, we focus on the case when the Josephson junction is operated as a phase qubit and study the resulting statistics of radiation emitted in the cavity.

[1] G. C. Ménard *et al.*, Phys. Rev. X **12**, 021006 (2022)
[2] C. Yan *et al.*, Nat. Electron. **4**, 885-892 (2021)

15 min. break

TT 54.6 Thu 16:30 HSZ 304

Heat transport and rectification in an ultrastrongly-coupled qubit-resonator system — •Luca Magazzu[1], Milena Grifoni[1], and Elisabetta Paladino[2] — [1]Regensburg University — [2]University of Catania

Inspired by the recent experimental developments in the field of heat transport in the quantum regime, we consider a flux qubit coupled to a superconducting resonator as a composite open quantum system.

The two elements of this open quantum Rabi system interact with two heat baths held at different temperatures. At the steady state, a heat current is established which is the result of photon exchanges between the system and the baths. Due to the geometry of the setup, the coupling to the heat baths is asymmetric. In turn this entails the presence of a preferred direction for the heat current, to a degree quantified by the heat rectification.

We calculate the heat current and rectification in different coupling regimes and considering a periodic driving applied to the qubit. The rectification displays the signatures of multi-photon processes that occur when the qubit-resonator coupling enters the nonperturbative regime.

[1] A. Ronzani *et al.*, Nat. Phys. 14, 991 (2018)
[2] J. Senior, A. Gubaydullin, B. Karimi, J. T. Peltonen, J. Ankerhold, and J. P. Pekola, Commun. Phys. 3, 40 (2020)
[3] B. Bhandari, P. Andrea Erdman, R. Fazio, E. Paladino, and F. Taddei, Phys. Rev. B 103, 155434 (2021)
[4] L. Tesser, B. Bhandari, P. A. Erdman, R. Fazio, E. Paladino, and F. Taddei, New J. Phys. 24, 035001 (2022)

TT 54.7 Thu 16:45 HSZ 304

Qubit reset using frequency modulation by AC Stark effect — •Jami Rönkkö, Vasilii Sevriuk, Antti Vepsäläinen, and Fabian Marxer — IQM Quantum Computers, Espoo, Finland

We present a theory for an unconditional reset scheme utilizing qubit's frequency modulation by AC Stark effect and a coupled lossy resonator. In AC Stark effect, off-resonant microwave drive shifts the frequency of a qubit without causing strong Rabi oscillations. Modulating the frequency of this drive creates sidebands around the qubit frequency. By setting the modulation frequency equal to the difference between the qubit and resonator frequencies, one of the sidebands becomes resonant with the resonator frequency. This leads to the transfer of the qubit excitation to the lossy resonator, resulting in a qubit reset. With typical parameters, the reset is achieved in only tens of nanoseconds

TT 54.8 Thu 17:00 HSZ 304

Fabrication of a superconducting transmission line in a planar design on a spin-doped crystalline membrane — •Georg Mair[1,2], Ana Strinic[1,2,3], Niklas Bruckmoser[1,2], Michael Stanger[1], Andreas Erb[1,2], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85747 Garching, Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Scaling up the density of superconducting qubits on a chip is reaching its limits, and a supplementing microwave quantum memory is a promising way to enhance the computing power [1]. Rare-earth doped crystals are potential candidates to realize such microwave quantum memories, due to the long coherence times of their spin states [2]. For efficient operation, one needs to have precise control over the distribution of strength and orientation of the oscillating magnetic field inside the sample. Here, we introduce a novel, planar superconducting transmission line design based on a thin crystalline $CaWO_4$ membrane. The transmission line is designed to exhibit high transmission in the range of $1 - 8\,\mathrm{GHz}$, i.e. the frequency range of the hyperfine transitions of the rare-earth ions in near-zero external magnetic field. Fabrication techniques are explained and transmission spectra recorded at cryogenic temperatures are discussed.

[1] É. Gouzien and N. Sangouard, Phys. Rev. Lett. **127**, 140503 (2021)
[2] N. Kukharchyk et al. New J. Phys. **20**, 023044 (2018)

TT 54.9 Thu 17:15 HSZ 304

Quantum state storage in spin ensembles — •Patricia Oehrl[1,2], Julian Franz[1,2], Manuel Müller[1,2], Nadezhda Kukharchyk[1,2,3], Kirill G. Fedorov[1,2], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Garching, Germany — [3]Munich Center for Quantum Science and Technologies (MCQST), Munich, Germany

The storage of quantum states is considered as a key element for successful realization of a multimode quantum network, enabling various applications, such as secure communication and distributed quantum computing [1]. In order to allow for connection of multiple quantum nodes without frequency conversion, several requirements have to be met, such as frequency compatibility and connectability between chosen quantum systems. As superconducting quantum circuits operate in the microwave regime, solid-state spin ensembles with their exceptional coherence times are promising candidates [2]. Here, we present a hybrid system consisting of a superconducting lumped-element microwave resonator coupled to a phosphorus donor electron spin ensemble hosted in isotopically engineered silicon. We show experimental results toward the storage of quantum states and their retrieval based on Hahn-echo type pulse sequences.

We acknowledge financial support from the Federal Ministry of Education and Research of Germany (project number 16KISQ036).

[1] M. Pompili et al., Science 372, 6539 (2021)
[2] M. Steger et al., Science 336, 1280 (2012)

TT 54.10 Thu 17:30 HSZ 304

Broadband electron spin resonance spectroscopy of rare earth spin ensembles at mK temperatures — •Ana Strinic[1,2,3], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[2,1,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Garching, Germany — [2]Walther-Meißner-Institut, Bavarian Academy of Sciences, Garching, Germany — [3]Munich Center for Quantum Science and Technologies, Munich, Germany

Rare earth spin ensembles exhibit spin coherence times in the millisecond range and possess transitions at microwave frequencies [1,2]. These properties make them attractive candidates for realizing microwave quantum memories, which can be directly interfaced with superconducting quantum processors. In principle, there are two options for the implementation of spin-based quantum memories: (i) coupling them to resonators, or (ii) interfacing them with an open transmission line. In particular, the latter is considered for multi-modal concepts or the storage of information based on atomic frequency comb protocols. In this work we characterize the electron spin resonance Hamiltonian of an ^{167}Er spin ensemble in a $^{7}LiYF_4$ host crystal at mK temperatures using a broadband microwave spectroscopy approach. We find good agreement with published g and hyperfine tensors, which is key for the implementation of microwave quantum memory schemes at low magnetic fields.

[1] P.-Y. Li et al., Phys. Rev. Appl. 13, 024080 (2020)
[2] A. Ortu et al., Nat. Mater. 17, 671 (2018)

TT 55: Dynamics and Chaos in Many-Body Systems I (joint session DY/TT)

Time: Thursday 15:00–17:30 Location: MOL 213

TT 55.1 Thu 15:00 MOL 213

Imperfect Many-Body Localization in Exchange-Disordered Isotropic Spin Chains — •Julian Siegl and John Schliemann — University of Regensburg

We study many-body localization in isotropic Heisenberg spin chains with the local exchange parameters being subject to quenched disorder. The Hamiltonian is invariant under global SU(2)- rotations and incorporates therefore a nonabelian symmetry. Systems of common spin length 1/2 and 1 are studied numerically using random matrix techniques. In both cases we find a transition from an ergodic phase at small disorder strength to an incompletely localized phase at stronger disorder. The transition is signaled by a maximum of the sample-to-sample variance of the averaged consecutive-gap ratio. The incompletely localized phase found here is distinguished from a fully localized system by the scaling behavior of the sample-to-sample variance.

TT 55.2 Thu 15:15 MOL 213

Magnetic Dipole Clusters - Resurrection of Catastrophe Machines — •Ingo Rehberg and Simeon Völkel — Experimental Physics, University of Bayreuth

Hysteretic transitions between stable configurations of a hexagonal magnetic dipole cluster [1] are set in a broader context by revealing the nature of the corresponding instabilities [2]. Following the animation of this bifurcation scenario [3], we present an experimental setup where the height of the centre dipole serves as the bifurcation parameter. This catastrophe machine demonstrates the two instabilities forming the hysteresis loop, and it might provide a hint to the unresolved puzzle of the slowing down of one of the eigenmodes [4].

[1] Andrew D.P. Smith et al., JMMM 549, 168991 (2022).
[2] Simeon Völkel et al., JMMM 559, 169520 (2022).
[3] https://doi.org/10.5281/zenodo.6380539 (18.5.2022).
[4] Peter T. Haugen et al., Chaos 32, 063108 (2022).

TT 55.3 Thu 15:30 MOL 213

Signatures of the interplay between chaos and local criticality on the dynamics of scrambling in many-body systems — Felix Meier[1], •Mathias Steinhuber[2], Juan Diego Urbina[2], Daniel Waltner[1], and Thomas Guhr[1] — [1]University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — [2]University of Regensburg, Universitätsstr. 31, 93040 Regensburg, Germany

Fast scrambling, quantified by the exponential initial growth of Out-of-Time-Ordered-Correlators (OTOCs), is the ability to efficiently spread quantum correlations among the degrees of freedom of interacting systems, and constitutes a characteristic signature of local unstable dynamics. As such, it may equally manifest both in systems displaying chaos or even in integrable systems around criticality. We discuss the results from our recent publication [1], where we go beyond these two well-studied regimes with an exhaustive study of the interplay between local criticality and chaos. We address many-body systems with a well-defined classical (mean-field) limit, as coupled large spins and Bose-Hubbard chains, thus allowing for semiclassical analysis. Our aim is to investigate the dependence of the exponential growth of the OTOCs, defining the quantum Lyapunov exponent $\lambda_{\rm q}$ on quantities derived from the classical system with mixed phase space, specifically the local stability exponent of a fixed point $\lambda_{\rm loc}$ as well as the maximal Lyapunov exponent $\lambda_{\rm L}$ of the chaotic region around it.

[1] Meier, F., Steinhuber, M., Urbina, J. D., Waltner, D. & Guhr, T. arxiv:2211.12147

TT 55.4 Thu 15:45 MOL 213

Characterizing quantum chaoticity of kicked spin chains — •Tabea Herrmann, Maximilian F. I. Kieler, and Arnd Bäcker — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Quantum many body systems are commonly considered as quantum chaotic if their spectral statistics, such as the level spacing distribution, agree with those of random matrix theory. Using the example of the kicked Ising chain we demonstrate that even if both level spacing distribution and eigenvector statistics agree well with random matrix predictions, the entanglement entropy deviates from the expected Page curve. We propose a new measure of the effective spin interactions and obtain the corresponding random matrix result. By this the deviations of the entanglement entropy can be understood.

TT 55.5 Thu 16:00 MOL 213

Entanglement Characterization of Measurement-Induced Phase Transition in Fermionic Chains — •Jiangtian Yao[1,2], Sebastian Diehl[1], and Michael Buchhold[1] — [1]Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

We report characterization of measurement-induced phase transition in Gaussian fermionic chains. We use various entanglement measures to characterize the two phases as well as the nature of the transition. Through a numerical study on the entanglement spectra, we observe closure of the entanglement gap in the critical phase and relate the scaling of the closure to the effective central charge of the system. In addition, we numerically extract the effective Luttinger liquid parameter of the system and use it to characterize the critical phase. Lastly, we use the scaling behavior of the effective Luttinger liquid parameter as well as the Schmidt gap to estimate the critical point for the phase transition.

15 min. break

TT 55.6 Thu 16:30 MOL 213

Dynamical characterization of the chaotic phase in the Bose-Hubbard model — David Peña Murillo and •Alberto Rodríguez — Departamento de Física Fundamental, Universidad de Salamanca, E-37008 Salamanca, Spain

We study the dynamical manifestation of the Bose-Hubbard model's chaotic phase [1] by analysing the temporal behaviour of connected two-point density correlations on experimentally accessible time scales up to a few hundred tunneling times. The time evolution of initial Mott states with unit density in systems including up to 17 bosons (Hilbert space dimension $\approx 10^9$) reveals that the chaotic phase can be unambiguously identified from the early time fluctuations of the considered observable around its equilibrium value [2]. The emergence of the chaotic phase is also seen to leave an imprint in the initial growth of the time signals. The possibility to discern specific features of this many-body chaotic phase, on top of the universal prediction of random-matrix theory, from these experimentally accessible measures is explored.

[1] L. Pausch *et al.*, Phys. Rev. Lett. 126, 150601 (2021)
[2] D. Peña Murillo, MSc Thesis, Universidad de Salamanca (2022)

TT 55.7 Thu 16:45 MOL 213

Universal Eigenvalue Distribution for Locally Interacting Quantum Systems — •Tobias Helbig, Tobias Hofmann, Ronny Thomale, and Martin Greiter — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Wigner has shown [1] that the eigenvalue distribution of a Gaussian orthogonal or unitary ensemble of random matrices approaches a semicircle in the thermodynamic limit. Here, we show that the joint eigenvalue distribution of locally interacting quantum systems, that is, ensembles of finite dimensional subsystems with local interactions between them, approaches a Gaussian distribution as the number of subsystems is taken to infinity [2]. In the talk, we present our analytical results supported by numerical data and discuss possible implications of a Gaussian density of states for physical problems.

[1] E. P. Wigner. On the statistical distribution of the widths and spacings of nuclear resonance levels. Mathematical Proceedings of the Cambridge Philosophical Society, 47(4): 790-798 (1951).
[2] T. Hofmann, T. Helbig, R. Thomale, and M. Greiter. In preparation.

TT 55.8 Thu 17:00 MOL 213

Power-law decay of correlations after a global quench in the massive XXZ chain — •Flávia Braga Ramos[1], Andrew Urichuk[2,3], Imke Schneider[1], and Jesko Sirker[3] — [1]Fachbereich Physik und Research Center OPTIMAS, Technische Universität Kaiserslautern, Kaiserslautern, Germany — [2]University of Manitoba, Winnipeg, Canada — [3]Bergische Universität Wuppertal, Wuppertal, Germany

While there have been great advances in understanding the final equilibration of integrable systems after a quantum quench, relatively little is known about their precise relaxation towards the steady state. In this context, the XXZ chain provides a playground for the investigation of interaction effects in out-of-equilibrium properties of quantum many-body systems. We investigate the relaxation dynamics of equal-time correlations in the antiferromagnetic phase of the XXZ spin-1/2 chain following a global quantum quench of the anisotropy parameter. In particular, we focus on the relaxation dynamics starting from an initial Néel state. Using the exact solution of an effective free-fermion model, state-of-art density matrix renormalization group simulations, and the quench-action approach, we show that the late-time relaxation is characterized by a power-law decay $\sim t^{-3/2}$ independent of anisotropy. Overall, we find remarkable agreement in the results obtained from the distinct approaches.

TT 55.9 Thu 17:15 MOL 213

Universal correlations in chaotic many-body quantum states: lifting Berry's Random Wave Model into Fock space — Rémy Dubertrand[1], Juan-Diego Urbina[2], Klaus Richter[2], and •Florian Schöppl[2] — [1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, NE1 8ST Newcastle upon Tyne, United Kingdom — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Using a semiclassical analysis based on Berry's ansatz [1] we investigate the universal statistical features of eigenstate correlations in chaotic mesoscopic many-body quantum systems, focusing on Bose-Hubbard lattices, where the existence of a classical (mean-field) limit allows for the use of many-body semiclassical methods [2]

For this, we first have to lift Berry's ansatz into the many-body space by expanding the microscopic correlations and the conjectured multi-variant Gaussian distribution of expansion coefficients into the Fock space of quantum fields. Together with numerical evidence, which supports the extension to multi-point correlations of the known Gaussian distribution for a single expansion coefficient, the universality of eigenstate correlations can be extended well beyond random matrix theory, where these correlations are absent. Our results bring the correlation backbone of eigenfunctions into a precise signature of quantum chaos in many-body mesoscopic systems.

[1] M. V. Berry, Journal of Physics A: Mathematical and General **10**, 2083 (1977) [2] K.Richter, J.D. Urbina, and S. Tomsovic. "Semiclassical roots of universality in many-body quantum chaos," (2022)

TT 56: Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management I (joint session O/TT)

Data have been identified as major resource of the 21st century, unlocking great potential if refined and processed in the right way. In scientific research, particularly modern data science concepts like machine learning or neural networks enable novel types of data analysis with often strong predictive power. This Focus Session aims at providing a framwork for presenting and discussing novel concepts, tools and platforms for managing experimental research data related to surface science and solid-state physics. In particular, in light of the German NFDI initiative, where several consortia are actively working on tackling the imminent challenges of research data management in experimental solid-state physics, this Focus Session will offer an ideal environment for exchange among researchers, and bringing these novel developments into the labs. The intended topics include the description of experimental data and meta data generation workflows, meta data schemas and file formats, electronic lab notebooks, novel tools for handling and analyzing scientific research data, as well as sharing and searching platforms according to F.A.I.R. principles.

Organizers: Martin Aeschlimann (TU Kaiserslautern), Laurenz Rettig (FHI Berlin) and Heiko Weber (U Erlangen)

Time: Thursday 15:00–18:30 Location: WIL A317

Topical Talk TT 56.1 Thu 15:00 WIL A317

Introducing a FAIR research data management infrastructure for experimental condensed matter physics data — •Christoph Koch — Humboldt-Universität zu Berlin, Department of Physics & IRIS Adlershof, Berlin, Germany

Digitization and an increase in complexity and price of experimental materials characterization techniques, an increase in accuracy and system size of computational solid state physics (or computational materials science), and the maturation of machine learning tools to extract patterns from large amounts of very diverse (annotated) data promise an acceleration of materials development by synergistically combining research data from many sources. While some labs start to upload their (raw) research data to data repositories, this is only a first but not sufficient step in leveraging the above-mentioned potential, since such repositories are typically either specific to a very particular technique or agnostic to the content of the data being uploaded. In both cases the research data cannot easily, and definitely not without significant human effort, be compared to and integrated with experimental data from other sources, or numerical predictions. In this talk I will report on recent progress of the FAIRmat NFDI consortium in extending the novel materials discovery laboratory (NOMAD), the world's largest data base for ab-initio computational materials data, to ingest experimental research data on the synthesis and characterization of materials in a machine-accessible manner, i.e. annotated with well-defined and interoperable metadata, achieved by establishing links between related (experimental and computational) quantities.

TT 56.2 Thu 15:30 WIL A317

Introducing an electronic laboratory notebook in a collaborative research center — •Sebastian T. Weber[1], Aneta Daxinger[1], Philipp Pirro[1], Marek Smaga[1], Christiane Ziegler[1], Mathias Kläui[2], Georg von Freymann[1], Baerbel Rethfeld[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau — [2]Institute of Physics, Johannes Gutenberg University Mainz

The basis of a FAIR data management is a well-described and detailed documentation of every single step of the experiment and data analysis. In recent decades, however, the focus has shifted from analog measuring instruments and analytical calculations to computer-based experiments and simulations. This has lead to a large increase in the numbers of measurements and observed quantities and therefore in the amount of data generated. Consequently, traditional paper lab notebooks have reached their limits. Electronic lab notebooks (ELNs) are better suited for storing, indexing, searching and retrieving a large amount of entries. In particular, the automated filling-in of meta data can lead to a reduction in the workload of the scientists in the long term.

We present the lessons learned on challenges and advantages with the introduction of a joint electronic lab notebook within our collaborative research center CRC/TRR173 *Spin+X*. We report on our experiences in the daily work of the scientists and in education in student labs.

TT 56.3 Thu 15:45 WIL A317

An efficient workflow for processing single event dataframes. — •Steinn Ýmir Ágústsson[1], M. Zain Sohail[2,3], David Doblas Jiménez[4], Dmytro Kutnyakhov[3], and Laurenz Rettig[5] —

[1]Aarhus University, DK — [2]RWTH, Aachen — [3]DESY, Hamburg — [4]Eu-XFEL, Schenefeld — [5]FHI, Berlin

Single event resolved data streams measured by delay-line-detectors allow to correlate each measured photoelectron with the state of the experimental apparatus. This allows corrections and calibrations to be applied on a shot-to-shot basis and a flexible investigation of correlations between various measurement parameters.

We are developing an open-source python package[1], where highly optimized dataframe management and binning methods enable leveraging the full potential of event-resolved data structures. The flexible design of the pipeline allows processing any event-resolved data stream.

With momentum microscopy as the primary target application, we developed axis calibration and artifact correction methods designed to be agnostic to the experimental apparatus. These methods are tested on data generated by microscopes at FELs (HEXTOF@FLASH) as well as at HHG sources (FHI), but are easily exended to other end-stations using similar detection techniques.

Our aim is to provide tools for the community which will reduce the development time for each end station, as well as an open and accessible data processing pipeline, built around the FAIR data principles.

[1] github.com/openCOMPES/sed

TT 56.4 Thu 16:00 WIL A317

FAIR Data Infrastructure for Computation: Advanced many-body methods. — •José M. Pizarro[1], Nathan Daelman[1], Joseph F. Rudzinski[1,2], Luca M. Ghiringhelli[1], Roser Valentí[3], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Institut für Theoretische Physik, Goethe University Frankfurt am Main — [4]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena

Big-data analyses and machine-learning approaches have recently emerged as a new paradigm to study and predict properties of materials. In order to perform these analyses, materials data have to be structured in a FAIR (findable, accessible, interoperable, and reusable) format [1]. While most of the current databases deal with density-functional-theory (DFT) calculations, there is a clear need for developing FAIR-data schema for methodologies going beyond DFT. Methods such as the *GW* approximation, dynamical mean-field theory, and time-dependent DFT allow to calculate excited- and many-body-states properties beyond DFT, thus having a direct quantitative comparison with experiments. In this talk, we will introduce the achievements and challenges undertaken within the FAIRmat consortium towards fully structuring the (meta)data of all these techniques. We demonstrate how users can analyze the data and compare with angle-resolved photoemission spectroscopy.

[1] M. Scheffler et al., Nature **604**, 635 (2022).

TT 56.5 Thu 16:15 WIL A317

Electronic Laboratory Notebooks for FAIR Data Management; Evaluation and Recommendations for Solutions at Research Infrastructures — •Philipp Jordt[1], Wiebke Lohstroh[2], and Bridget Murphy[1] — [1]IEAP, Kiel University, Germany — [2]MLZ, Technische Universität München, Germany

Electronic Laboratory Notebooks (ELN) are the digital counterpart to the classical handwritten paper notebook and play a vital role in the implementation of FAIR data standards. Modern ELN solutions range from simple note taking applications to integrated tools, combining documentation, inventory management, progress tracking and more. Nowadays, ELNs are becoming more prominent in research laboratories around the world, replacing paper notebooks. This evaluation of basic needs was carried out in the context of the DAPHNE4NFDI consortia. Of special interest is the view on ELNs for combined use at large scale facilities and in the home laboratory. Thus, the requirements regarding implementation, deployment, authentication, etc., may differ from those for single or laboratory use at universities. An overview of different concepts and existing solutions is given. Multiple ELNs have been evaluated during test runs at large scale facilities and a survey on existing solutions was held. From these results, a list of ELN specifications is presented, ranging from useful to necessary. These insights may serve as a guideline for evaluating or implementing ELNs in the future.

TT 56.6 Thu 16:30 WIL A317

Ontology for Experimental Data — •Sandor Brockhauser — Center for Materials Science Data, Humboldt-Universität zu Berlin, Germany

Ontology is the scientific field of formal knowledge representation. This field contributes to Data Science and helps Experimentalist to properly annotate their data and metadata on a FAIR way. During the last decades several different ways have been developed in the field of Ontology for describing knowledge as a set of information and their relationships. These include Information mapping, Concept maps, Topic maps, Mind maps, Knowledge graphs, BORO (Business Objects Reference Ontology), RDF (Resource Description Framework), OWL (Web Ontology Language), ORO (Object-Role Modeling), UML (Unified Modeling Language), ISO 15926 (standard for data sharing), OLOG (mathematical framework for knowledge representation), GELLISH (ontology language for data storage and communication), etc. For describing experimental facts, we suggest using an ontology in OWL which is derived from the NeXus community standard. It represents all the concepts developed for explaining experiments and experimental data, just like the relationships between them. Such representation allows connecting the concepts defined in NeXus also to other ontologies. Additionally, any data management systems, like NOMAD which accepts experiment data provided in the NeXus standard, can immediately link the data and metadata to the ontology and make them interoperable.

15 min. break

Topical Talk TT 56.7 Thu 17:00 WIL A317

Open Research Data for Photons and Neutrons: Applications in surface scattering and machine learning — •Linus Pithan — Universität Tübingen, Institut für Angewandte Physik - DAPHNE4NFDI

Open (F.A.I.R.) research data is becoming a key ingredient for data driven machine learning (ML) applications that requires access to existing data of preceding experiments - which goes well beyond data collected in the context of one's own experiments which one might keep in a secret drawer. We will discuss current possibilities as well as future opportunities and challenges with special emphasis on surface scattering. Embedded in the DAPHNE4NFDI (DAta from PHoton and Neutron Experiments) consortium we present efforts on how data catalogs may serve as backbone for F.A.I.R. datasets provided by synchrotron and neutron sources or through community efforts. Besides suitable metadata collection also the harmonization of data- and metadata formats are issues still to be tackled especially for systematic access to fully analyzed, experimental datasets (e.g. by adopting NeXus community conventions). After a broader overview and shining light on the SciCat meta-data catalog system,[1] we discuss as application examples efforts in the field of reflectometry (XRR, NR) [2,3] and X-Ray scattering and diffraction (WAXS, GIWAXS and XPCS).[1,4]

[1] V. Starostin, L. Pithan et al. 2022, SRN, Vol. 35, No. 4
[2] A. Greco et al. 2022, J. Appl. Cryst. 55 362
[3] L. Pithan et al., Refl. dataset, 10.5281/zenodo.6497438
[4] V. Starostin et al. 2022, npj Comp. Mat. 8, 101

TT 56.8 Thu 17:30 WIL A317

NOMAD OASIS as a Tool for Electron and Atom Probe Microscopists — •Markus Kühbach — Department of Physics, Humboldt-Universität zu Berlin, Germany

Embracing the FAIR principles for sharing data and knowing how to work with different tools in research data management systems is becoming an invaluable skill in a scientist's daily life. Embracing such systems of tools, one of which is offered with NOMAD OASIS, allows you to start organizing your research data locally. Learning such tools will train you to understand what schemes and electronic lab notebooks are and how the data and metadata are processed by these tools. Example implementations of specific workflows can give you ideas where to start from and how to customize these tools for the needs of your own research and colleagues. Thereby, you can provide feedback which supports the evolution and improvement of the research data management system.

NOMAD OASIS offers you many examples which show now also how data and metadata of specific experiments can be parsed into a standardized representation. These examples teach users through detailing how data can be entered, viewed, and organized with customizable schemes in NOMAD. Furthermore, the examples suggest strategies for how the information in NOMAD can be accessed for generic or domain-specific data analytics tools.

In my talk, I will go through one or two of these examples specific to electron microscopy (orientation imaging microscopy or spectroscopy).

TT 56.9 Thu 17:45 WIL A317

FAIR Data Infrastructure for Computation: Introducing the parsers for Quantum Monte Carlo and ALF — •Jonas Schwab[1], José M. Pizarro[2], Jefferson Stafusa E. Portela[1], Luca M. Ghiringhelli[2], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin

DFT calculations lead to low-energy effective models. A modern example would be Kitaev types spin Hamiltonains for $RuCl_3$. Once the model is specified, many different many-body calculations can be carried out. Here, we will concentrate on the ALF [1] implementation of the auxiliary field quantum Monte Carlo algorithm that can deal with general models that includes the ones produced by DFT calculations. Being a Monte Carlo method, the ALF library produces stochastic time series. We will discuss how to implement this workflow in the NOMAD Repository & Archive (https://nomad-lab.eu) and concentrate on a FAIR meta-data scheme. The first challenges are to define the models in a searchable way as well as standards for the Monte Carlo time series. In this talk we will discuss the present state of this project for the special case of the ALF-library and how users can exploit the benefits of the NOMAD repository to find, compare and resuse our QMC data.
[1] F. F. Assaad et al., SciPost Phys. Codebases **1** (2022).

TT 56.10 Thu 18:00 WIL A317

CAMELS - A Configurable Instrument Control Software for FAIR Data — •Alexander Fuchs[1,3], Johannes Lehmeyer[1,3], Michael Krieger[1,3], Heiko B. Weber[1,3], Patrick Oppermann[2,3], and Heinz Junkes[2,3] — [1]Lehrstuhl für Angewandte Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft (FHI), Berlin — [3]FAIRmat, Humboldt-Universität zu Berlin, Berlin, Germany

We are developing a configurable measurement software (CAMELS), targeted towards the requirements of experimental solid-state physics. Here many experiments utilize a multitude of measurement devices used in dynamically changing setups. CAMELS [1] will allow to define instrument control and measurement protocols using a graphical user interface (GUI). This provides a low entry threshold enabling the creation of new measurement protocols without programming knowledge or a deeper understanding of device communication. The GUI generates python code that interfaces with instruments and allows users to modify the code for specific applications and implementations of arbitrary devices if necessary. Even large-scale, distributed systems can be implemented. CAMELS is well suited to generate FAIR-compliant output data. Nexus standards, immediate NOMAD integration and hence a FAIRmat compliant data pipeline can be readily implemented.
[1] https://github.com/FAU-LAP/CAMELS

TT 56.11 Thu 18:15 WIL A317

OpenSemanticLab: Usecase Device Repository — •Matthias A. Popp and Simon Stier — Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg, Germany

Fully automated experiments provide benefits regarding precision, repeatability, as well as data quality and therefore gain more and more popularity. However, setting them up can be time consuming, especially when computer interface information has to be manually transferred from device manuals to software.

In order to implement FAIR principles precise descriptions of measurement setups and instrumentation are necessary. Currently, this results in extra workload for experimental scientists.

With our framework OpenSemanticLab, we address this shortcoming by providing a central metadata repository for scientific instruments. The ontology-based repository meets both human (GUI) and machine requirements (APIs). A device ontology helps finding and classifying devices. In an associated Python package, abstract device drivers and concrete device metadata can be combined into executable workflows. Overall, this approach not only strengthens the transparency of research according to FAIR principles, but also significantly reduces the implementation effort for complex setups.

TT 57: Poster: Superconductivity I

Time: Thursday 15:00–18:00 Location: P2/OG2

TT 57.1 Thu 15:00 P2/OG2

Influence of reduced dimensionality on the superconducting properties of ultrathin aluminum films — Werner M.J. van Weerdenburg[1], •Anand Kamlapure[1], Eirik Holm Fyhn[2], Xiaochun Huang[1], Niels P.E. van Mullekom[1], Manuel Steinbrecher[1], Peter Krogstrup[3], Jacob Linder[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University, 6525 AJ Nijmegen, the Netherlands — [2]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [3]NNF Quantum Computing Programme, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen, Denmark

Study of superconductivity (SC) in lower dimensional systems is vital to devices involving multilayers and heterostructures for future quantum information applications. In this work, using scanning tunneling microscopy/spectroscopy, we study SC in ultrathin epitaxial Al films on Si(111) as we approach the 2D limit. With reducing thickness, we observe enhancement of SC where critical temperature and gap size shows threefold enhancement. In addition, we characterize the vortex structure in presence of strong Zeeman fields and find evidence for extended vortices showing paramagnetic Meissner effect originating from triplet pairing contributions. These results illustrate two striking influences of reduced dimensionality and present a new platform to study SC in presence of large magnetic fields. Reference: arXiv:2210.10645(2022).

TT 57.2 Thu 15:00 P2/OG2

Demonstration of 300 mm CMOS-compatible superconducting HfN and ZrN thin films — •Roman Potjan[1,3], Raik Hoffmann[1], Marcus Wislicenus[1], Benjamin Lilienthal-Uhlig[1], and J. Wosnitza[2,3] — [1]Fraunhofer Institute for Photonic Microsystems (IPMS), Center Nanoelectronic Technologies (CNT), Dresden, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

The increasing interest in quantum computing is pushing the development of new superconducting materials for semiconductor fab process technology. However, these are often facing CMOS process incompatibility. In contrast to common CMOS materials such as TiN and TaN, reports on the superconductivity of other suitable transition-metal nitrides are scarce, despite potential superiority. Hence, we demonstrate fully CMOS-compatible fabrication of HfN and ZrN thin films on state-of-the-art 300 mm semiconductor process technology, employing reactive DC magnetron sputtering on silicon wafers. Mechanical stress, thickness, and roughness measurements of the thin films imply process compatibility. Material phase and stoichiometry in bulk and interfaces are investigated by structural analysis. HfN and ZrN exhibit transitions into the superconducting state with critical temperature up to 5.1 and 6.1 K, respectively. A decrease in critical temperature with decreasing film thickness indicates geometric limitations and proximity effects of the interfaces. The results prepare a scalable application of HfN and ZrN in quantum computing and related applications.

TT 57.3 Thu 15:00 P2/OG2

Unraveling Charge Transfer to Understand Superconductivity in MgB_2 — •Simon Marotzke[1,2], Jan Oliver Schunck[1,3], Amina Alic[4], Octave Duros[4], Moritz Hoesch[1], Alessandro Nicolaou[5], Gheorghe Sorin Chiuzbaian[4], and Martin Beye[1] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [3]Universität Hamburg, Hamburg, Germany — [4]Sorbonne Université, Paris, France — [5]Synchrotron SOLEIL, Saint-Aubin, France

Magnesium diboride (MgB_2) holds the world-record for the highest transition temperature ($T_C = 39$ K) in a conventional Bardeen-Cooper-

Schrieffer (BCS)-type, i.e., phonon-mediated, superconductor. The undoped electron configuration of MgB_2 is still disputed as contradicting results on the appearance of charge transfer upon crossing T_C have been reported. To settle this question, we conducted high-resolution resonant X-ray emission spectroscopy (XES) as well as X-ray absorption spectroscopy (XAS) measurements around the boron K-edge at the SEXTANTS beamline at the synchrotron SOLEIL. In order to investigate the charge transfer between in-plane and out-of-plane states, we varied the polarization of the incoming photons as well as the incidence and emission angle. We report on differences in the spectral intensity for both the absorption and emission spectra upon crossing T_C to be first indications of changes in the density of the boron $2p$ states. Complementary density of states calculations showing good agreement with the experimental data were performed.

TT 57.4 Thu 15:00 P2/OG2

Strain device for *in-situ* uniaxial strain measurements of strongly correlated electron materials in scanning tunneling microscopy — •Carolina A. Marques[1], Danyang Liu[1], Alexander Steppke[1,2], and Fabian D. Natterer[1] — [1]University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland — [2]Paul Scherrer Institut Forschungsstrasse 111 5232 Villigen PSI Switzerland

Uniaxial strain is an effective way to tune the properties of strongly correlated electron systems without introducing disorder. One seminal example is the doubling of the critical temperature of Sr_2RuO_4.

Strain devices for the *in-situ* application of strain have been used in several different measurement techniques: transport, specific heat, angle-resolved photoemission spectroscopy, muon spin relaxation, and neutron scattering measurements. Here, we describe the design and construction of a strain device compatible with a scanning tunneling microscope. Our piezo-element based strain-cell is temperature compensated and enables the continuous tuning of strain, allowing to monitor local strain response. It opens up the possibility to locally track changes to the low-energy electronic states as a function of strain, giving insight into the underlying physical mechanisms.

TT 57.5 Thu 15:00 P2/OG2

Magnon dispersion of $SrRuO_3$ studied by inelastic neutron scattering experiments — Kevin Jenni[1], •Akshay Tewari[1], Stefan Kunkemöller[1], Agustinus Agung Nugroho[2], Russell Ewings[3], Yvan Sidis[4], Astrid Schneidewind[5], Paul Steffens[6], and Markus Braden[1] — [1]*II*. Phys. Institut, Universität zu Köln — [2]Institut Teknologi Bandung, Bandung 40132, Indonesia — [3]ISIS Pulsed Neutron and Muon Source, United Kingdom — [4]Laboratoire Léon Brillouin, Gif-sur-Yvette CEDEX, France — [5]Jülich Centre for Neutron Science (JCNS), Garching, Germany — [6]Institut Laue Langevin, Grenoble, France

Weyl points in the ferromagnetic state in $SrRuO_3$ not only determine anomalous magnetotransport properties but also modify the spin dynamics leading to a peculiar temperature dependence of both the spin gap and of the stiffness in the ferromagnetic state [1]. In contrast the magnon chirality in $SrRuO_3$ remains normal, i.e. right handed [2]. To extend the analysis of the magnon dispersion we performed inelastic neutron scattering experiments with the time-of-flight technique as well as with polarization analysis. The magnon dispersion can be followed to about 30 meV and there is no indication for a crossover into a Stoner continuum. There is evidence for additional coupling beyond just the nearest neighbors. In addition magnon excitations exhibit pronounced broadening that further increases upon heating possibly related to the strong coupling between ferromagnetism and conductivity in $SrRuO_3$.

[1] K. Jenni et al. Phys. Rev. Lett. **123**, 17202 (2019). [2] K. Jenni et al. Phys. Rev. B. **105**, L180408 (2022).

TT 57.6 Thu 15:00 P2/OG2

Screening in a two-band model for infinite-layer nickelate — •Tharathep Plienbumrung[1,2], Maria Daghofer[1,2], Michael Schmid[3], and Andrzej M. Oles[4,5] — [1]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Stuttgart, Germany — [2]Center for Integrated Quantum Science and Technology, University of Stuttgart, Stuttgart, Germany — [3]Waseda Research Institute for Science and Engineering, Waseda University, Tokyo, Japan — [4]Max Planck Institute for Solid State Research, Stuttgart, Germany — [5]Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland

Considering two-band model for infinite-layered nickelates, containing d- and s-like orbitals, on two-dimensional lattice. The extended nature of the s-like orbital leads to less electronic correlation. We thus parameterize the electronic correlations of the s-like orbital by introducing *screening parameter*. With exact diagonalization, we calculate the pairing symmetries and other electronic properties of the two-band model on two-dimensional lattice. We find that the screening strength of the s-like band plays an important role in the electronic properties of the two-band model. Interestingly, depending on the screening strength of s-like band, we find both d- and s-wave pairing symmetries within the two-band model. In strong screening, the d-wave pairing is found while the s-wave pairing is formed in the weak screening regime. The phase diagram of the two-band model for different ratio of J/U is also presented.

TT 57.7 Thu 15:00 P2/OG2

Magnetic and thermoelectric properties of Bi-substituted $La_{0.95-x}Bi_xSr_{0.05}CoO_3$ — •Divya Prakash Dubey and Ratnamala Chatterjee — IIT Delhi Hauz Khas New Delhi 110016 India

We present the results of a comprehensive investigation of electric and thermal transport properties of polycrystalline Bi substituted $La_{0.95-x}Bi_xSr_{0.05}CoO_3$ for x=0,0.1 and 0.2 (LBSCO-0, 1 & 2). The electrical resistivity reflects the semiconducting nature with interesting n-type to p-type transition   52K for LBSCO-1 and LBSCO-2 samples. The substitution of higher atomic weight elements Bi at La site drastically affects overall thermal conductivity by reducing the lattice contribution (κ 0.12W/m-K at T= 50K) and also enhance the Seebeck coefficient (S   354 μV/K). The increase in the resistivity and Seebeck coefficient for Bi-substituted system is related to the decrease in the available charge carrier concentration (5.12 10^{20} cm^3). The phonon mediated charge transport via phonon drag effect below 50K and a large increment in ZT   0.17 at RT for LBSCO-2 composition has been observed that is 1-order larger to pristine undoped LBSCO-0 and even higher to the other existing cobaltite*s-based thermoelectric choice.

TT 57.8 Thu 15:00 P2/OG2

High pressure T-P phase diagram of $2H$-$TaSe_2$ — •Yuliia Tymoshenko[1], Xingchen Shen[1], Amir-Abbas Haghighirad[1], Tom Lacmann[1], Gaston Garbarino[2], and Frank Weber[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, 71 avenue des Martyrs, CS 40220, Grenoble 38043, France

Many layered materials featuring charge-density waves (CDW), a modulation of the electronic density of states, acquire a superconducting ground state often associated with a quantum critical point (QCP) of the CDW order. Although $2H$ polymorph of tantalum diselenide ($2H$-$TaSe_2$) with a layered hexagonal crystal structure is one of the most studied CDW systems, to the best of our knowlege, previous studies of the phase diagram have not been carried out at pressures sufficient to suppress the CDW order at low temperatures. We investigated the CDW phase diagram in its most crucial but still unexplored area and determined the CDW quantum critical point in $2H$-$TaSe_2$ under pressure via high-resolution synchrotron x-ray diffraction (XRD). Its position together with previously published resistivity measurements and our recent ambient-pressure study of the soft phonon mode at the CDW transition enable us to argue that this compound likely has a CDW quantum critical point closely connected to the emergent superconducting phase. This can serve as a textbook example where both phases are mediated by the same mechanism, electron-phonon coupling of the CDW soft phonon mode.

TT 57.9 Thu 15:00 P2/OG2

Clarifying the origin of CDW and finding the routes to superconductivity in 1T-$TiSe_2$ — •Andrii Kuibarov[1], Alexander Fedorov[1,2], Rui Lou[1,2], Yuliia Shemerliuk[1], Oleksandr Suvorov[1], Saicharan Aswartham[1], Bastian Rubrecht[1], Dmitry Efremov[1], Helmuth Berger[3], Bernd Büchner[1], and Sergey Borisenko[1] — [1]Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II — [3]Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne

The relationship between charge density waves (CDW) and superconductivity was always one of the important questions of solid-state physics. Even though they are often observed on the phase diagram next to each other, it is still unknown whether CDW competes or cooperates with superconductivity. Utilizing the photon energy-dependent ARPES we investigate the 3D electronic structure of well-known CDW-bearing material $TiSe_2$, superconductor Cu_xTiSe_2, and TiSeS. Our results suggest that neither Mott nor the excitonic insulator model is applicable to the electronic structure of $TiSe_2$. In contrast to the generally accepted model, we find a crucial agreement with the conventional band structure calculations, which predict the absence of the energy gap in this material.

Additionally, we perform temperature-dependent ARPES studies and show that the CDW phase remains in doped superconducting samples Cu_xTiSe_2. On the basis of the obtained results, we propose a mechanism for both CDW and superconductivity $TiSe_2$ family.

TT 57.10 Thu 15:00 P2/OG2

Nematic susceptibility in heavily hole-doped iron based superconductors — •Franz Eckelt[1], Xiaochen Hong[1], Vilmos Kocsis[2], Vadim Grinenko[2], Chul-Ho Lee[3], Bernd Büchner[2], and Christian Hess[1] — [1]Bergische Universität Wuppertal, 42097 Wuppertal, Germany — [2]Leibniz-Institute for Solide State and Materials Research (IFW-Dresden), 01069 Dresden, Germany — [3]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan

We investigate the elastoresistivity of the heavily hole doped iron-based superconductor $Ba_{1-x}K_xFe_2As_2$ in the range x= 0.68 - 0.98 using a piezoelectric measurement technique. We observe a divergent increase in elastoresistance along the [100] direction during cooling for all samples studied so far. We discuss our findings in terms of nematic fluctuations and Fermi surface effects in the vicinity of a Lifshitz transition.

TT 57.11 Thu 15:00 P2/OG2

Towards topological superconductivity on the surface of LiFeAs — •Luise Merkwitz[1], Andrii Kuibarov[1], Rui Lou[1,2], Alexander Fedorov[1,2], Sabine Wurmehl[1], Saicharan Aswartham[1], Igor Morozov[1], Bernd Büchner[1], and Sergey Borisenko[1] — [1]Leibniz-Institute for Solid State Research, IFW-Dresden, D-01171 Dresden, Germany — [2]Helmholtz-Zentrum Berlin, BESSY, D-12489 Berlin, Germany

Realisation of topological superconductivity is theoretically possible in iron-based superconductors, where the s-wave pairing in the bulk can induce superconductivity of the topological surface states. The detection of the latter by angle-resolved photoemission spectroscopy (ARPES) in LiFeAs and FeSeTe systems is questionable since the bulk-originated dispersions can mimic the Dirac crossing and inverted gap is expected to be very small (of the order of 5 meV). The only feasible possibility to detect topological surface states in such a small gap is to bring it to the Fermi level where the scattering is minimal. We have synthesized differently doped $LiFe_{1-x}Y_xAs$ (Y=Co, V) crystals and performed synchrotron-based ARPES studies to map k_z-dispersion in detail. Our results demonstrate the principal possibility of tuning the binding energy of the inverted gap in these systems and point to the optimal composition where this binding energy is close to zero. In addition, our results reveal considerable renormalization anisotropy of the Fe d-states never detected earlier.

TT 57.12 Thu 15:00 P2/OG2

The superconducting symmetries of $CeRh_2As_2$ — •Fabian Jakubczyk[1,2], Julia M. Link[1,2], and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Multiphase unconventional superconductivity is a rare phenomenon, which has recently been discovered in the tetragonal but locally noncentrosymmetric heavy-fermion compound $CeRh_2As_2$. Here, the transition between two distinct superconducting phases occurs as a function of magnetic field applied along the c axis and the formation of superconductivity takes place around $T_{SCI} = 0.26\,\mathrm{K}$. At $\mu_0 H^* \approx 4\,\mathrm{T}$ the superconductor changes from a low-field to a high-field state with a large critical field of $\mu_0 H_{c2} = 14\,\mathrm{T}$. However, for in-plane fields only the low-field phase appears, with $\mu_0 H_{c2} = 2\,\mathrm{T}$. Recent As-NQR experiments further increased the variety of intriguing phenomena in this material, for they detected the onset of antiferromagnetism within the superconducting low-field phase, i.e. at $T_N < T_{SCI}$. In order to study the coexistence and interplay of the potential superconducting and magnetic phases, as well as the effect of an external magnetic field, we conduct a symmetry analysis followed by the construction of a Landau-type energy functional. Thereby we can give a statement about the probable symmetries of the superconducting states.

TT 57.13 Thu 15:00 P2/OG2

Flat bands of surface states in chiral symmetric superconductors — •Clara Johanna Lapp[1,2], Julia M. Link[1,2], and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, Technische Universität Dresden, 01069 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Nodal noncentrosymmetric superconductors can support flat bands of zero-energy surface states in part of their surface Brillouin zone if they obey time-reversal symmetry. These bands are protected by a winding number that relies on chiral symmetry, which in these systems is realized as the product of time-reversal and particle-hole symmetry. We examine which symmetry conditions a model must obey such that a winding number is well defined and can be nonzero. In particular, time-reversal symmetric Bogoliubov-de Gennes Hamiltonians which conserve one spin component can be interpreted as chiral symmetric in each of the spin-blocks and exhibit a nonzero winding number that protects zero energy surface modes. Moreover, we classify which types of sublattice symmetry lead to nonzero winding numbers.

TT 57.14 Thu 15:00 P2/OG2

Eliashberg theory calculations for magnetically mediated superconductivity — •Ran Tao and Malte Grosche — Department of Physics, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom

Computational modelling for realistic material parameters can speed up the search for new unconventional superconductors.
We have implemented calculations of the superconducting transition temperature in Eliashberg theory for spin fluctuation mediated superconductivity and validated them by reproducing previously published results in simple systems (e.g. [1]). Next, our code has been extended to a minimal model for iron-based superconductors, namely a 2D compensated metal with varying Fermi surface volume and interaction strength. Developing this approach further in the spirit of the UppSC code (e.g. [2]), numerical calculations are used to investigate the effects of applied field and to assist the discovery of new unconventional superconductors by surveying large numbers of candidate materials.

[1] P. Monthoux and G. G. Lonzarich, Phys. Rev. B 59, 14598 (1999)
[2] A. Aperis, P. Maldonado, and P. M. Oppeneer, Phys. Rev. B 92, 054516 (2015)

TT 57.15 Thu 15:00 P2/OG2

Yu-Shiba-Rusinov states in unconventional superconductors — •Michael Hein[1], Wolfgang Belzig[1], and Juan Carlos Cuevas[2] — [1]Universität Konstanz, Konstanz, Germany — [2]Universidad Autónoma de Madrid, Madrid, Spain

Recently there has been a huge effort to investigate individual magnetic impurities on superconducting surfaces in the context of scanning tunneling microscopy (STM) [1]. These STM-based experiments have enabled to elucidate the properties of the in-gap superconducting bound states known as Yu-Shiba-Rusinov states. These bound states are a key signature of the interplay between magnetism and superconductivity at the atomic scale and, in turn, they lead to a strong local modification of the superconducting state. In this regard, we present here our theoretical efforts to understand the physics of YSR states in the context of unconventional superconductivity, with special attention to the so-called Ising superconductors. We show that the study of YSR states can provide a very valuable way to reveal the underlying properties of unconventional superconductors.

[1] B. W. Heinrich, J. I. Pascual, and K. J. Franke, Prog. Surf. Sci. 93, 1 (2018)

TT 57.16 Thu 15:00 P2/OG2

RKKY interaction in non-centrosymmetric superconductors — •Finja Tietjen and Jacob Linder — Department of Physics, Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491, Trondheim, Norway

Recent advances in experimental studies have raised interest in how spin interactions are manifested in unconventional superconductors, which can potentially be used for spintronic devices. In particular, superconducting triplet states featuring spin-polarized Cooper pairs are expected to qualitatively alter spin interaction compared to non-superconducting materials.

We consider the RKKY-interaction between two impurity spins in a non-centrosymmetric superconductor. Such superconductors feature antisymmetric spin-orbit coupling and, generally, coexisting singlet and triplet Cooper pairs. The RKKY-interaction is treated perturbatively with a Schrieffer-Wolff transformation within the Bogoliubov-de Gennes framework. Exact numerical studies complement the analytical approach and show local decreases in the total superconducting gap as well as a change in local density of states at impurity sites. The RKKY interaction is affected by the superconductor and the corresponding change in the ground-state spin configuration is also clearly visible. We expect that the spin configuration can thus be externally controlled by entering or leaving the superconducting state.

Ongoing studies on the exact dependencies as well as advances in the analytical approach promise further insights closer to the conference date.

TT 57.17 Thu 15:00 P2/OG2

Analytical parquet renormalization group for multipocket systems — •Nora Taufertshöfer, Matteo Dürrnagel, and Ronny Thomale — Theoretische Physik I, Universität Würzburg

Materials with multi-pocket fermiology may exhibit unconventional superconductivity which arises from inter-pocket scattering. Studying this problem in the weak coupling regime by renormalization group (RG) methods requires a perturbative expansion in each flow step.

As electronically driven instabilities are predominantly governed by states close to the Fermi surface, the RG analysis can be restricted to a few distinct momentum channels between the Fermi pockets. The parquet RG [1] embeds the truncation of the flow equations into a rigorous analytical scheme to investigate superconductivity and its interplay with various competing phases. Within this framework we discuss the relevance of nematic fluctuations in a 2D model for GaAs/AlAs heterostructures, which may host the possibility for gate-tunable unconventional superconductivity [2].

[1] S. Maiti and A. V. Chubukov, Phys. Rev. B **82**, 214515 (2010)
[2] A. V. Chubukov and S. A. Kivelson, Phys. Rev. B **96**, 174514 (2017)

TT 57.18 Thu 15:00 P2/OG2

Higgs mode in superconductors with Rashba spin-orbit coupling — •Tobias Kuhn and Björn Sothmann — Fakultät für Physi, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

When a superconductor is periodically driven by electromagnetic radiation, the superconducting order parameter shows radial oscillation with twice the driving frequency. This so called Higgs mode can be excited resonantly when the driving frequency equals the absolute value of the order parameter. Here, we study Higgs modes for superconductors with Rashba spin-orbit coupling using two methods. We discuss the resonance condition by analyzing the dynamics of Anderson pseudospins. In addition, we use Floquet Green's functions to generalize the pseudospin approach and discuss the impact of spin-orbit coupling on the order parameter dynamics.

TT 57.19 Thu 15:00 P2/OG2

Order-parameter evolution in the FFLO phase — •H. Kühne[1], S. Molatta[1], T. Kotte[1], D. Opherden[1], G. Koutroulakis[2], J.A. Schlueter[3,4], G. Zwicknagl[5], S.E. Brown[6], and J. Wosnitza[1,7] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]UC Santa Barbara, USA — [3]ANL, Argonne, USA — [4]NSF, Alexandria, USA — [5]IMP, TU Braunschweig — [6]UC Los Angeles, USA — [7]IFMP, TU Dresden

The Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state represents a general concept of pairing in multi-component Fermi liquids with strong population imbalance. In the superconducting FFLO state, the spin polarization varies as the modulus of the spatially modulated superconducting gap amplitude, and, thus, its modulation amplitude represents the order parameter. Indeed, NMR experiments of the organic superconductors β''-$(ET)_2SF_5CH_2CF_2SO_3$ and κ-$(ET)_2Cu(NCS)_2$ showed the emergence of inhomogeneous line broadening, stemming from the spatially modulated spin polarization. We report on our studies of the temperature-dependent order parameter of the superconducting FFLO state. For that, we utilize ^{13}C NMR spectroscopy of β''-$(ET)_2SF_5CH_2CF_2SO_3$. From a comparison of the NMR spectra to a comprehensive modeling, we determine the evolution of the local spin-polarization modulation amplitude upon condensation of the FFLO state. Further, the modeling allows to quantify the decrease of the average spin polarization, stemming from the spin-singlet coupling of the superconducting electron pairs.

TT 57.20 Thu 15:00 P2/OG2

Comparison of window-type and cross-type Nb/Al-AlO$_x$/Nb Josephson tunnel junctions — •Fabienne Bauer[1], Martin Neidig[1], Christian Enss[2], and Sebastian Kempf[1] — [1]Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology — [2]Kirchhoff Institute of Physics, Heidelberg University

Josephson tunnel junctions (JJs) are the heart of numerous superconducting electronic devices such as SQUIDs, qubits or parametric amplifiers. Out of the multitude of junction variants, Nb/Al-AlO$_x$/Nb junctions have somehow become the state of the art as they are resilient to thermal cycling and additionally show a very high junction quality and reproducibility of characteristic junction properties. Against this background, we present two anodization-free fabrication processes for Nb/Al-AlO$_x$/Nb Josephson junctions. One is a variant of the selective niobium etching process (SNEP) for fabricating window-type junctions. The second is a process for producing self-aligning, low-capacitance cross-type Josephson junctions. For comparing both processes, we comprehensively characterized fabricated junctions by studying resonance phenomena in unshunted dc-SQUIDs to determine the intrinsic junction capacitance and determined characteristic junction figures of merit. We show that both of our processes yield very high quality JJs. However, our cross-type Josephson junctions turn out not only to greatly simplify the fabrication process and to provide much lower junction capacitance, but also to show a greatly improved homogeneity of critical current density distribution as determined by analysing the magnetic field dependence of the critical current.

TT 57.21 Thu 15:00 P2/OG2

Process optimisation for the fabrication of cross-type Nb/Al-AlO$_x$/Nb Josephson junctions — •A. Stoll, F. Bauer, L. Münch, D. Hengstler, A. Ferring-Siebert, F. Krämer, N. Kahne, D. Mazibrada, A. Fleischmann, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany.

Josephson tunnel junctions (JJs) are the basic element of many superconducting electronic devices such as qubits or superconducting quantum interference devices (SQUIDs). Since many applications demand a large number of Josephson junctions, a reliable wafer-scale fabrication process yielding JJs with a reproducible and uniform high quality is required. Very often window-type JJs are used, in which the JJ area is defined by openings in an insulating layer. The size of the JJ is thus limited by the alignment accuracy, therfore causing the need for low critical current densities j_c and in turn long oxidation times. The transition to cross-type JJs is motivated by reducing the junction area as well as parasitic capacities, and in turn suppressing or completely removing parasitic effects, e.g. *LC*-resonances, with the additional benefit of simplistic and time efficient fabrication steps. We present how we optimised and retained the quality of our cross-type Nb/Al-AlO$_x$/Nb junctions, for which quality checks of our in-house sputter-deposited niobium films and oxidized aluminium layers were carried out, including the measurement of the critical temperature T_c, stress of the niobium film and junction specific quality features. The parameters for the magnetron sputtering, like the Ar-pressure and power of the sputtering source, were optimised accordingly.

TT 57.22 Thu 15:00 P2/OG2

Realization of He-FIB induced Josephson junction THz detectors in YBCO thin films — •Kenny Fohmann, Christoph Schmid, Eric Dorsch, Edward Goldobin, Dieter Koelle, and Reinhold Kleiner — Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany

We designed and fabricated ultrawideband thin-film antennas from the high-temperature superconductor $YBa_2Cu_3O_{7-\delta}$ (YBCO) partially covered with Au. By using a focused He ion beam (He-FIB) we "draw" a Josephson Junction (JJ) [1] into the microbridge footpoint of the spiral antenna. Under microwave irradiation the JJ exhibits Shapiro steps in the $I-V$ characteristic.

We report on design optimization. This includes improved matching of the impedances of the antenna and the JJ in an ultrawide frequency band by using a logarithmic periodic antenna. Moreover, we performed simulations using CST Studio-Suite to improve the coupling of a plane-wave signal to the antenna.

To characterize the antennas, we compare the excitation of the JJ embedded in a simple linear YBCO bridge (~ 1 mm) with the one embedded in the footpoint of the antenna, for frequencies up to 40 GHz. The ultimate goal of such an antenna with a YBCO JJ is to detect the radiation from a BSCCO-mesa (placed on another chip nearby) in the frequency range $\gtrsim 0.5$ THz. The latest measurements will be presented.

[1] B. Müller et al., Phys. Rev. Appl. **11**, 044082 (2019)

TT 57.23 Thu 15:00 P2/OG2

Investigation and optimization of $YBa_2Cu_3O_{7-\delta}$ Josephson junctions written with a focused He ion beam — •Christoph Schmid[1], Max Karrer[1], Katja Wurster[1], Moritz Meichsner[1], Isabelle Vandermoeten[1], Noor Hasan[1], Ramón Manzorro[2,3], Javier Pablo-Navarro[2,3], Cesar Magen[2,3], Dieter Koelle[1], Reinhold Kleiner[1], and Edward Goldobin[1] — [1]Physikalisches Institut, Center for Quantum Science and LISA$^+$, Universität Tübingen, Germany — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, Spain — [3]Laboratorio de Microscopías Avanzadas (LMA), Universidad de Zaragoza, Spain

We use a focused He Ion Beam (He-FIB) to "write" Josephson barriers across $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin-film bridges. Such Josephson junctions (JJs) exhibit RCSJ-like I–V characteristics, and the dependence of critical current vs. magnetic field resembles a Fraunhofer pattern [1]. Scanning transmission electron microscopy (STEM) shows that He-FIB irradiation modifies locally ($\sim$ 10 nm) the YBCO crystal structure that can partially heal with time. Electric transport measurements provide the evolution of the JJ parameters with time or thermal annealing. Those reveal barrier recovery processes and show how to stabilize the JJ parameters on short time scales. Furthermore, we investigated the interaction of two and more JJs placed close to each other and biased in series. Using a multi-terminal arrangement we found some unexpected behavior that will be discussed. Several approaches to synchronize arrays of He-FIB written JJs are investigated.
[1] B. Müller et al., Phys. Rev. Applied **11**, 044082 (2019)

TT 57.24 Thu 15:00 P2/OG2

On-chip driving of a phase-slip junction for dual Shapiro steps — •David Scheer and Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

A single Josephson junction in the phase-slip regime exhibits Bloch oscillations that relate current to frequency if supplied with a DC voltage-bias. If additionally an AC-drive is applied to the junction, the Bloch oscillations can synchronize with the driving frequency. This leads to the emergence of dual Shapiro steps with constant current in the IV-curve of the junction with the current determined by the driving frequency. An AC-drive in the required frequency regime of > 10GHz is challenging to implement experimentally without detrimental effects due to stray capacitances. We investigate the use of a Josephson junction with a DC-bias as an on-chip AC-voltage source. We discuss the relevant coupling parameters between the oscillations caused by the DC-Josephson effect and the Bloch oscillations as well as the back action of the Bloch oscillations on the Josephson oscillations. We identify the regime in which the back action is minimized in order to obtain a steady voltage source to create dual Shapiro steps.

TT 57.25 Thu 15:00 P2/OG2

MOCCA: A 4k-pixel molecule camera for the position and energy resolved detection of neutral molecule fragments — •Daniel Kreuzberger[1], Christian Enss[1], Andreas Fleischmann[1], Lisa Gamer[2], Loredana Gastaldo[1], Christopher Jakob[2], Ansgar Lowack[1], Oldřich Novotny[2], Andreas Reifenberger[1], Dennis Schulz[1], and Andreas Wolf[2] — [1]Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg

The MOCCA detector is a 4k-pixel high-resolution molecule camera based on metallic magnetic calorimeters and read out with SQUIDs that is able to detect neutral molecule fragments with keV kinetic energies. 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 measures the energy and position of incident particles on the detector, even with multiple particles hitting the detector simultaneously.

We present a new read-out scheme which uses only 32 SQUID channels for the 4096 pixels of the detector as well as some new fabrication details including copper-filled through-wafer vias to heat-sink the detector to the wafer backside. In addition we present the results of first characterization measurements.

TT 57.26 Thu 15:00 P2/OG2

Towards large-area 256-pixel MMC arrays for high resolution X-ray spectroscopy — •Andreas Abeln, Steffen Allgeier, Axel Brunold, Lars Eisenmann, Daniel Hengstler, Lukas Münch, Alexander Orlow, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

Metallic Magnetic Calorimeters (MMCs) are energy-dispersive cryogenic particle detectors. Operated temperatures below 50 mK, they provide very good energy resolution, high quantum efficiency as well as linearity over a large energy range. In many precision experiments on X-ray spectroscopy the photon flux is small, thus a large active detection area is desirable. Therefore, we develop arrays with increasing number of pixels. For a cost-effective read-out of a growing number of detector channels we investigate different multiplexing techniques.
In this contribution we present the design of a novel 16×16 pixel MMC array. The pixels provide a total active area of 4 mm × 4 mm and are equipped with 5 μm thick absorbers made of gold. This ensures a stopping power of at least 50 % for photon energies up to 20 keV. The expected energy resolution is ΔE = 1.4 eV (FWHM) at an operating temperature of 20 mK. We give an overview about the microfabrication process and focus on the challenging task of producing through wafer vias to heat sink the MMC pixels to the wafer backside. These vias are realized by holes etched through the silicon substrate and subsequently lined with gold to achieve high thermal coupling between detector pixels and the cryostat.

TT 57.27 Thu 15:00 P2/OG2

A dedicated 2-dimensional array of metallic magnetic microcalorimeters to resolve the 29.18 keV doublet of ^{229}Th — •A. Brunold, A. Abeln, S. Allgeier, J. Geist, D. Hengstler, A. Orlow, L. Gastaldo, A. Fleischmann, and C. Enss — Heidelberg University

The isotope ^{229}Th has the nuclear isomer state with the lowest presently known excitation energy, which possibly allows to connect the fields of nuclear and atomic physics with the potential application as a nuclear clock. In order to excite this very narrow transition with a laser a precise knowledge of the transition energy is needed. Recently the isomer energy (8.338±0.024) eV [Kraemer et al., arXiv:2209.10276, 2022] could be precisely determined. To get additional valuable insights, we will improve our recent high-resolution measurement [Sikorsky et al., PRL 125, 2020] of the γ-spectrum following the α-decay of ^{233}U. This decay results in excited ^{229}Th with a nuclear state at 29.18 keV. Resolving the doublet, that results from subsequent deexcitation to the ground and isomer state, respectively, would allow an independent measurement of the isomer energy and the branching ratio of these transitions. To resolve this doublet, we develop a 2D detector array consisting of 8×8 metallic magnetic calorimeters (MMCs). MMCs are operated at millikelvin temperatures and convert the energy of a single incident γ-ray photon into a temperature pulse which is measured by a paramagnetic temperature sensor. The detector array features an active detection area of 4 mm^2, a stopping power of 63.2% for 30 keV photons and an energy resolution below 3 eV (FWHM).

TT 57.28 Thu 15:00 P2/OG2

X-ray spectroscopy of U^{90+} ions with a 64-pixel metallic magnetic calorimeter array — •A. Orlow[1], S. Allgeier[1], A. Abeln[1], A. Brunold[1], M. Friedrich[1], A. Gumberidze[2], D. Hengstler[1], F. M. Kröger[2,3,4], P. Kuntz[1], A. Fleischmann[1], M. Lestinsky[2], E. B. Menz[2,3,4], Ph. Pfäfflein[2,3,4], U. Spillmann[2], B. Zhu[4], G. Weber[2,3,4], Th. Stöhlker[2,3,4], and C. Enss[1] — [1]KIP, Heidelberg University — [2]GSI/FAIR, Darmstadt — [3]IOQ, Jena University — [4]HI Jena

Metallic magnetic calorimeters (MMCs) are energy-dispersive X-ray detectors which provide an excellent energy resolution over a large dynamic range combined with a very good linearity. MMCs convert the energy of each incident photon into a temperature pulse which is measured by a paramagnetic temperature sensor. The resulting change of magnetisation is read out by a SQUID magnetometer.

To investigate electron transitions in U^{90+} at CRYRING@FAIR within the framework of the SPARC collaboration, we developed the 2-dimensional maXs-100 detector array. It features 8x8 pixels with a detection area of 1 cm^2 and a stopping power of 40 % at 100 keV. Four on-chip thermometers allow to correct for temperature drifts and to achieve an energy resolution of 40 eV at 60 keV. We show preliminary X-ray spectra of the recent U^{90+} beamtime. Due to the small rate of emitted X-rays, a good supression of background radiation is mandatory, which was ensured by a coincidence measurement with a particle detector. To increase the stopping power to above 60 % at 100 keV we develop a new maXs-100 detector with 100 μm thick absorbers.

TT 58: Poster: Superconductivity II

Time: Thursday 15:00–18:00 Location: P2/OG3

TT 58.1 Thu 15:00 P2/OG3

Low temperature MMC-based muon veto for IAXO — •Daniel Unger, Christian Enss, Andreas Fleischmann, Daniel Hengstler, Ashish Jadhav, and Loredana Gastaldo — Kirchhoff Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

An array of Metallic Magnetic Calorimeter (MMC) operated at a few mK in a dilution refrigerator is considered as a possible focal plane detector for the IAXO helioscope. For such an experiment, the background rate must be smaller than $10^{-6}\,\mathrm{keV^{-1}cm^{-2}s^{-1}}$. However, we expect the rate of events related to cosmic muons to be two orders of magnitude larger. A traditional muon veto composed by scintillating panels would have to cover the full cryostat, a volume of about $3\,\mathrm{m}^3$. A cryogenic muon veto surrounding the $150\,\mathrm{cm}^3$ volume of the detector module could veto muon related events more efficiently. We present the development of a large-area MMC-based muon veto. Muons will be detected through their energy deposition while traversing a silicon wafer with thickness of 0.4 mm and an area of $30\,\mathrm{cm}^2$. We discuss the design and the fabrication challenges of the muon veto in addition to the prototype setup for testing purposes. We aim to characterize the performance of the large silicon detector and at the same time study the spectrum of muon related events detected by the MMC array as well as of the residual background due to natural radioactivity. Finally, we evaluate the suitability of MMC arrays for low background measurements.

TT 58.2 Thu 15:00 P2/OG3

Dc-SQUID readout with high dynamic range and intrinsic frequency-domain multiplexing capability — •L. Münch, A. Abeln, N. Kahne, F. Krämer, D. Hengstler, L. Hoibl, D. Mazibrada, D. Richter, A. Stoll, A. Fleischmann, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Dc superconducting quantum interference devices (dc-SQUIDs) are periodic flux-to-voltage converters whose linear flux range is rather small. For this reason, a flux locked loop (FLL) circuit is typically used to linearize the output signal and increase the dynamic range. However, the measurement of large signals while maintaining the excellent noise performance of SQUIDs sets high demands on the digitizer sampling the SQUID signal in terms of voltage resolution. Furthermore, FLL operation often sets a practical limit for the realization of massive multi-channel SQUID systems since feedback wires have to be routed to every SQUID.
In this contribution, we discuss a SQUID readout approach which relaxes the hardware requirements of a SQUID system while maintaining a linearized output signal and a large dynamic range. At the same time, it allows for reducing the number of wires within multi-channel SQUID systems due to its intrinsic frequency-domain multiplexing (FDM) capability. We introduce the basic concept of our readout approach and demonstrate its intrinsic FDM-capability using a custom-made four channel multiplexer device. We also present a new chip design optimized for the read-out of a novel 16 x 16 pixel MMC array.

TT 58.3 Thu 15:00 P2/OG3

Integrated two-stage SQUID-chip with 6 nH input impedance — •David Mazibrada, Fabian Krämer, Alexander Stoll, Nicolas Kahne, Lukas Münch, Daniel Hengstler, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

SQUIDs are sensitive superconducting magnetic flux to voltage converters, whose operation is based on the Josephson effects. To increase the signal-to-noise ratio of a SQUID-based readout system one can amplify the signal with an N-SQUID series array. We present our first integrated two-stage chip design which combines a single current sensing dc-SQUID as front-end and a 18-dcSQUID series array as amplifier stage, in one compact, well thermalized chip. This not only eliminates the need for two separate chips, but also achieves low signal propagation delay and larger bandwidth. Compared to our most recent single-stage current sensing SQUIDs, the first stage SQUID features a 2-turn input coil with increased inductance of 6 nH increasing the input current sensitivity by a factor of about 2. To counteract the resistive heating of the two-stage setup, large thermalization pads made of gold are implemented to thermalize the resistive elements and in addition the chip can be thermally anchored to the sample holder by means of gold bonds. In future designs lossy striplines will be used in order to provide delocalized broad-band damping and suppress effects of parasitic resonances without introducing new noticeable sources of noise.

TT 58.4 Thu 15:00 P2/OG3

Identification of noise sources in superconducting microstructures — •R. Yang, A. Fleischmann, D. Hengstler, M. Herbst, D. Mazibrada, L. Münch, A. Reifenberger, C. Ständer, and C. Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

Improving the performance of a superconducting device often means identifying and eliminating noise. Many potential noise sources are independent of the specific experimental set-up and transferable across many device categories such as qubits, SQUIDs, and superconducting detectors. We have constructed a stand-alone device able to representably probe specific noise sources. The set-up consists of a Wheatstone-like bridge of microfabricated superconducting inductors and a pair of two-stage dc-SQUID read-out chains. Cross-correlation removes noise contributions from the read-out electronics giving us the sum total of all noise in the superconducting circuit. If, in comparison, the Wheatstone bridge is AC-driven, we can measure a sample material's magnetic noise via the material's complex AC susceptibility using the fluctuation-dissipation theorem. The experiment is performed at temperatures between $T = 10\,\mathrm{mK}$ and 1000 mK in the frequency range from $f = 100\,\mathrm{mHz}$ to 100 kHz on an experimental holder with excellent thermal coupling and shielding. We present first results of measurements on SiO_2 and Ag:Er thin films and compare these results with previous measurements on Au:Er. In addition, we demonstrate our device's ability to probe the dynamics of magnetic moments in a sample material.

TT 58.5 Thu 15:00 P2/OG3

Recent insights into low frequency excess flux noise in superconducting quantum devices — •Anna Ferring-Siebert, Fabian Kaap, David Mazibrada, Lukas Münch, Matthew Herbst, Andreas Fleischmann, Christian Enss, and Sebastian Kempf — Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

In many applications low frequency excess flux noise (EFN), with a frequency dependence of $1/f^\alpha$, limits the performance of superconducting quantum devices such as SQUIDs and Qubits. Although it was long believed that its magnitude expressed in units of magnetic flux $S_\Phi(1\,\mathrm{Hz})$ and exponent α are fairly independent of the device material and inductance, there meanwhile exist hints for the contrary. It is also known that EFN can depend on the equipment used for device fabrication, the reason for that however remained unknown up to now.
In this contribution, we discuss origins of fabrication induced EFN as well as means to minimize it. In particular, we show that material layers deposited with commercial deposition equipment can contain magnetic impurities causing EFN. In this context, we present how we have modified commercial sputtering sources to reduce EFN and provide evidence for a relationship between EFN amplitude and the DC magnetization of the deposited material layers. Finally, recent measurements investigating the dependence of EFN on device inductance are discussed, suggesting that energy sensitivity $\varepsilon(1\,\mathrm{Hz}) = S_\Phi(1\,\mathrm{Hz})/(2L)$, rather than magnetic flux noise, is the more appropriate metric to describe EFN.

TT 58.6 Thu 15:00 P2/OG3

Impedance engineering of flux-pumped Josephson traveling wave parametric amplifier — •Daniil E. Bazulin[1,2], Kedar E. Honasoge[1,2], Leon Koch[1,2], Niklas Bruckmoser[1,2], Yuki Nojiri[1,2], Thomas Luschmann[1,2], Achim Marx[1], Stefan Filipp[1,2,3], and Kirill G. Fedorov[1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Scalable quantum computing with superconducting qubits relies on ef-

ficient and fast readout of multiple qubits. This goal can be achieved by exploiting broadband Josephson Traveling Wave Parametric Amplifiers (JTWPAs). Here, we investigate fabrication and characterization of a specific type of the JTWPA based on aluminium Superconducting Nonlinear Asymmetric Inductive eLements (SNAILs) exploiting the 3-wave mixing down-conversion process. This approach allows for separating signal and pump paths, which is expected to enhance the overall JTWPA performance by mitigating back action amplification processes and avoiding the pump depletion. Additionally, we implement a single-layer 50 Ω impedance matching approach by exploiting fish-bone capacitors fabricated simultaneously with the Josephson junctions. This technique avoids using extra dielectric layers, which are typical sources of losses and noise in JTWPAs.

TT 58.7 Thu 15:00 P2/OG3

Large-scale fabrication of Josephson parametric devices — •Maria-Teresa Handschuh[1,2], Kedar E. Honasoge[1,2], Yuki Nojiri[1,2], Niklas Bruckmoser[1,2], Leon Koch[1,2], Daniil Bazulin[1,2], Florian Fesquet[1,2], Fabian Kronowetter[1,2,4], Michael Renger[1,2], Wun K. Yam[1,2], Achim Marx[1], Rudolf Gross[1,2,3], and Kirill G. Fedorov[1,2] — [1]Walther-Meißner-Institut, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 Munich, Germany — [4]Rohde & Schwarz GmbH & Co. KG, 81671 Munich, Germany

The rapid progress in the field of quantum information processing with superconducting circuits requires the development of large-scale fabrication to increase fabrication efficiency, reproducibility as well as to reduce costs. Moreover, many advanced quantum applications and experiments rely on using multiple nominally identical chips, such as flux-driven Josephson parametric amplifiers (JPAs) [1]. To this end, the goal is to establish good control over various fabrication parameters, such as critical current density and microwave losses, in JPAs with Nb/Al-AlOx/Nb Josephson junctions on 4-inch high-resistivity silicon wafers. We provide a detailed analysis of the related parameter distribution across the wafer and make proposals for future improvements.

[1] K. G. Fedorov et al., Sci. Adv. 7, eabk0891 (2021)

TT 58.8 Thu 15:00 P2/OG3

Microwave quantum memory based on rare earth doped crystal — •Jianpeng Chen[3,1,2], Ana Strinic[3,1,2], Achim Marx[1,3], Kirill G. Fedorov[1,3], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[3,1,2] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology, 80799 Munich, Germany — [3]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany

Quantum memory is an essential element in the development of future quantum technologies, such as quantum computing circuits and quantum communication links. Specifically, crystals doped with rare earth ions are promising competitive candidates due to their long coherence times [1] and potential multiplexing capability [2]. Here, we aim to couple coherent microwave signals to rare earth ion dopants in yttrium orthosilicate crystals (Y2SiO5) at 10 mK. We will discuss the impact of the transmission line design on the efficiency of quantum information storage and its multimodality potential.

We acknowledge financial support from the Federal Ministry of Education and Research of Germany (project number 16KISQ036).

[1] M. Zhong, Nature 517, 177 (2015)
[2] A. Ortu et al., Quantum Sci. Technol. 7, 035024 (2022)

TT 58.9 Thu 15:00 P2/OG3

Non-Markovian effects in Er:YSO — •Owen Thomas Huisman[1,2,4], Ana Strinic[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[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]Delft University of Technology, Delft, Netherlands

Erbium doped Y_2SiO_5 (Er:YSO) has proven to be a suitable platform to realise quantum memory protocols based on microwave ESR techniques [1]. The successful storage and retrieval of a microwave quantum state depends on the coherence and relaxation of spectral holes burned in inhomogeneously broadened spin transitions. Recent work has shown that relaxation and decoherence processes in Er:YSO at sub-Kelvin temperature may be affected by the phonon bottleneck process [2]. Several attempts have been made to develop a microscopic theory of the phonon bottleneck [3,4]. In this work, we attempt to connect the phonon bottleneck to more recent investigations of non-Markovian open quantum systems [5]. We propose an experiment to confirm the presence of non-Markovian effects in Er:YSO and justify the connection with a phonon bottleneck.

[1] S. Probst et al., Phys. Rev. B 92, 014421 (2015)
[2] R. P. Budoyoet al., Appl. Phys. Express 11, 043002 (2018)
[3] D. A. Garanin, Phys. Rev. B 75, 094409 (2007)
[4] D. A. Garanin, Phys. Rev. B 77, 024429 (2008)
[5] C.-F. Li et al., EPL 127, 50001 (2019)

TT 58.10 Thu 15:00 P2/OG3

Microwave single-shot quantum key distribution — •Florian Fesquet[1,2], Fabian Kronowetter[1,2,4], Michael Renger[1,2], Nadezhda Kukharchyk[1,2], Hans Huebl[1,2,3], Achim Marx[1], Rudolf Gross[1,2,3], and Kirill. G. Fedorov[1,2] — [1]Walther-Meißner-Institut, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [4]Rohde & Schwarz GmbH, 81671 Munich, Germany

Security of modern classical data encryption often relies on computationally hard-to-solve problems. A potential remedy for this challenge is quantum communication (QC) which takes advantage of the laws of quantum physics to provide secure exchange of information. Here, quantum key distribution (QKD) represents a powerful tool, allowing unconditionally secure QC between remote parties. A demand for QC at microwave frequencies has emerged due to the tremendous progress in quantum information processing with superconducting circuits. To this end, we present a realization of a continuous-variable QKD protocol based on displaced squeezed microwave states. We use a Josephson parametric amplifier (JPA) to generate squeezed microwave states at cryogenic temperatures. By implementing a single-shot quadrature readout with a second JPA in the phase-sensitive regime with quantum efficiency of 38 %, we demonstrate the unconditional security of this microwave QKD protocol. We analyze these results in terms of losses and noise in order to map them on possible real-world scenarios.

TT 58.11 Thu 15:00 P2/OG3

3D-Integration of superconducting qubits using flip-chip bump bonding technology — •Franziska Wilfinger[1,2], Ivan Tsitsilin[1,3], and Stefan Filipp[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 (MCQST), Munich, Germany

Superconducting quantum circuits are typically realized in a planar architecture. This approach is, however limited to dozens of qubits due to the complexity of routing signal lines when scaling beyond. 3D-integration can overcome these limitations by separating circuit components on different layers and on different chips. One promising 3D-integration strategy is to assemble two chips, patterned on one side, through flip-chip bonding using indium bumps. Quantum components such as qubits and couplers containing Josephson junctions can then be separated from the control- and readout-lines on different faces. Here, we discuss design concepts and test-structures in a flip-chip architecture and their simulated performances with respect to quality factors, decay rates and gate times. Finite-element simulation is applied to extract design parameters such as the qubit coupling to readout- and control lines and to other qubits. These parameters are optimized in order to achieve a performance comparable with planar structures. Moreover, the influence of inaccuracies in fabrication is investigated by simulating varying distance parameters and analyzing their impact on relevant quantities.

TT 58.12 Thu 15:00 P2/OG3

Probing the density of states of defects in superconducting flux qubits — •Benedikt Berlitz, Alexander Konstantin Händel, Alexey V. Ustinov, and Jürgen Lisenfeld — Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Material defects forming two-level systems (TLS) present a source of decoherence and unwanted degrees of freedom in superconducting quantum circuits. Current theoretical models make different assumptions about the frequency dependence of the TLS' density of states (DOS). To measure the TLS' DOS in a wide frequency range, spanning from about 0.1 to 20 GHz, we fabricated flux qubits as TLS detectors. Measuring the DOS will enhance our understanding of the underlying physics of TLS in amorphous materials.

TT 58.13 Thu 15:00 P2/OG3

Fast quantum state tomography with superconducting qubits — •Andras Di Giovanni[1], Adrian Aasen[3], Moritz Reh[3], Martin Gärttner[3], Markus Griedel[2], Hannes Rotzinger[1,2], and Alexey Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe — [2]Institut für Quantenmaterialien und Technologien, Karlsruher Institut für Technologie, Karlsruhe — [3]Kirchhoff-Institut für Physik, Heidelberg

Quantum simulators promise insights into quantum many-body problems in regimes where classical simulation methods hit a complexity wall. One challenge towards this goal is to develop well characterized building blocks that allow to scale system sizes up while conserving reliability in terms of errors. A promising platform for building such quantum simulators are superconducting quantum circuits. We characterize small-scale quantum processors in the time domain with single-shot accuracy and minimal hardware and post-processing overhead. For this purpose we use reactive basis rotations based on greedy algorithms and adaptive Bayesian tomography. We present experimental results measured on a transmon qubit and compare the data with theoretical predictions.

TT 58.14 Thu 15:00 P2/OG3

Infrared filters for superconducting qubit applications — •Markus Griedel[1,2], Sebastian Koch[2], Alex Stehli[2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Institut for Quantum Materials and Technologies (IQMT), Karlsruhe Institut for Technology (KIT) — [2]Physikalisches Institut (PHI), Karlsruhe Institut for Technology (KIT)

Superconducting qubits are manipulated and read out using microwave signals which are generated at room temperature and guided through coaxial cables to the milikelvin temperature stage. One common problem of coax cables is their high transparency to infrared radiation originating from a rather high photon flux sources at elevated temperatures of cryostat stages. Filtering out the infrared radiation requires a low-pass filter with a sharp cutoff in the micro- or low mm-wave frequency range. We present simulations as well as experimental data on a new generation of powder based filters. The samples are investigated over the full band of infrared radiation using conventional detectors as well as superconducting qubits directly.

TT 58.15 Thu 15:00 P2/OG3

Superconducting flux qubits with stacked Josephson junctions — •Alex Kreuzer[1], Hossam Tohamy[1], Thilo Krumrey[1], Markus Griedel[1,2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie (KIT) — [2]Institut für Quantenmaterialien und -technologien (IQMT), Karlsruher Institut für Technologie (KIT)

Josephson junctions are often employed as nonlinear inductive elements in superconducting qubits as they allow to tailor specific circuit properties. The promising flux qubit types as fluxonium or quarton qubits require compact inductances which are often implemented as arrays of Josephson junctions. Here, the stray capacitance originating, for instance, from the capacitive coupling of an array island to ground, introduces the major limitation of this approach, since it introduces parasitic resonances at GHz frequencies which may degrade the overall qubit performance. We explore the possibility of implementing the qubit inductances by stacking Josephson junctions vertically and thus reducing the capacitance to ground. We present transport as well as microwave measurement data of stacked Josephson junctions and flux qubits made from them. Furthermore, we present a comparison of our experimental data with a detailed numerical simulation.

TT 58.16 Thu 15:00 P2/OG3

Flux escape mitigation in gradiometric fluxonium qubits — •Denis Bénâtre[1], Mathieu Féchant[1], Martin Spiecker[1,2], and Ioan Pop[1,2] — [1]IQMT, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]PHI, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Superconducting fluxonium qubits have grown in the past decade as an interesting alternative to the now standard transmons. In 2022, Gusenkova et al. proposed a new design, the gradiometric fluxonium qubit, whose two loops have shown to suppress sensitivity to homogeneous magnetic field and open the door for its use in hybrid quantum systems. However, these devices undergo flux escape triggered by radioactive and cosmic impacts, and thus require shielding from ionizing radiation, e.g. in deep-underground facilities [Gusenkova et al., 2022]. We present new designs of gradiometric fluxoniums aimed at intrinsically mitigating the rate of trapped flux escape.

TT 58.17 Thu 15:00 P2/OG3

Towards millimeter-wave superconducting qubits — •Philipp Lenhard, Jürgen Lisenfeld, and Alexey V. Ustinov — Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Superconducting circuits are a promising platform to realize a solid-state quantum computer. However, scaling up to larger multi-qubit circuits is severely hindered by decoherence of various origins. While contemporary qubits are typically operated between 3 and 6 GHz resonance frequencies, here we investigate qubit designs for millimeter-wave operation frequencies between 80 and 110 GHz. We present first spectroscopic measurements of resonant energy level transitions in a current-biased Josephson junction in the millimeter-wave regime. In addition, we show simulations of designs for integrating qubits and readout resonators in 3D-waveguides.

TT 58.18 Thu 15:00 P2/OG3

Towards dissipatively coupled photon-pressure circuits — •Janis Peter, Mohamad Adnan el Kazouini, Emily Guo, Kevin Uhl, and Daniel Bothner — Physikalisches Institut, Center for Quantum Science (CQ) and LISA$^+$, Universität Tübingen, Germany

Photon-pressure circuits are a superconducting all-circuit equivalent of cavity optomechanics. They recently gained a lot of attention since they are providing a new toolbox for sensing and controlling radiofrequency (rf) photons by high-frequency (hf) circuits. In contrast to optomechanical systems, this platform only consists of LC circuits without any mechanical resonators. As a result they offer a larger flexibility regarding device parameters and a simplified fabrication process. Until now, photon-pressure circuits have been realized using the so-called dispersive interaction: the rf-resonator modulates the resonance frequency ω_0 of the hf-circuit. To reach the quantum regime by ground state cooling, dispersively coupled devices need to be in the so-called sideband-resolved regime, that is, the resonance frequency Ω_0 of the rf-resonator is much larger than the decay rate of the hf-circuit κ (typically several 100 kHz). Extending the quantum regime to even lower frequency photons ($\lesssim$ 1 MHz) requires a different interaction: dissipative photon-pressure coupling, where κ is modulated instead of ω_0. We present our progress on implementing a dissipative photonpressure interaction between two superconducting circuits and discuss in this context simulation, fabrication, device design and intermediate experimental milestones.

TT 58.19 Thu 15:00 P2/OG3

Towards non-classical state preparation in photon-pressure circuits — •Mohamad Adnan El Kazouini, Janis Peter, Emily Guo, Kevin Uhl, and Daniel Bothner — Physikalisches Institut, Center for Quantum Sciences (CQ) and LISA$^+$, Universität Tübingen, Germany

Photon-Pressure is a non-linear interaction between two electromagnetic modes in LC circuits, which gained considerable attention in the past years due to its unique possibilities to sense and control radio-frequency photons. To date, several milestone experiments have been performed such as interferometric radio-frequency thermometry, the observation of parametric strong-coupling, and the realization of resolved-sideband cooling of a low-frequency LC circuit ($\sim$ 100 MHz) into its quantum ground state. Although photon-pressure is in principle providing the possibilities, non-classical states like quantum squeezed and entangled states of MHz photonic modes have not been realized yet in these systems. Those states, however, have the potential to enhance quantum-limited sensing of bosonic modes in the radio-frequency regime, an application of photon-pressure systems that have been discussed for instance in the context of the search for dark-matter axions. In our poster, we will present our progress in developing photon-pressure devices that are being engineered toward the preparation of non-classical radio-frequency photon states and we will discuss the next steps and our future plans.

TT 58.20 Thu 15:00 P2/OG3

Towards room temperature microwave quantum teleportation — •Wun Kwan Yam[1,2], Michael Renger[1,2], Simon

Gandorfer[1,2], Florian Fesquet[1,2], Kedar Honasoge[1,2], Fabian Kronowetter[1,2,3], Yuki Nojiri[1,2], Achim Marx[1], Rudolf Gross[1,2,4], and Kirill G. Fedorov[1,2] — [1]Walther-Meißner-Institut, BAdW, 85748 Garching, Germany — [2]Physik-Department, TUM, 85748 Garching, Germany — [3]Rohde & Schwarz GmbH & Co. KG, 81671 Munich, Germany — [4]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Microwave quantum communication enables efficient and unconditionally secure exchange of quantum states. This paves the way towards distributed quantum computing and open-air quantum key distribution. One of the relevant quantum communication protocols is quantum teleportation. In the microwave regime, quantum teleportation has been successfully demonstrated by using superconducting Josephson circuits in a cryogenic setup. To investigate the limits of microwave quantum teleportation under more realistic application scenarios, we study the influence of thermal noise and losses in microwave communication channels. We show that the teleportation protocol is robust against noise in the feedforward channel and analyze experimental limits of distributing entanglement via thermal channels. Furthermore, we describe the experimental implementation of microwave quantum teleportation with the room temperature feedforward and consider microwave quantum teleportation in the open air.

TT 58.21 Thu 15:00 P2/OG3

Experimental investigations and flow simulation of regenerator configurations of a single stage GM-type pulse tube cooler — •Elias Eisenschmidt[1,3], Jack-Andre Schmidt[2,3], Bernd Schmidt[2,3], Jens Falter[3], and Andre Schirmeisen[2,3] — [1]Technische Hochschule Mittelhessen, Friedberg, Germany — [2]Justus-Liebig-university, Giessen, Germany — [3]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany

Pulse tube coolers are increasingly used in industry and research due to their low vibrations and long service intervalls. The regenerator and especially the filling of the regenerator has a great influence on the cooling capacity as well as the achievable, minimum temperatures. The temperature-dependent heat storage capacity of the materials used in the regenerator is usually the main focus of attention when selecting regenerator fillings. [1, 2]

This poster deals with the pressure drop of two regenerator fillings of stainless steel spheres and sieves. Steady-state and transient measurements of the two regenerator fillings will be discussed. In comparison of the two fillings used, the meshes show lower pressure drops, resulting in a higher cooling efficiency as regenerator filling, while spheres are more cost efficient in time and acquisition.

[1] N. Almtireen et. al., J. Low Temp. Phys. 199, 1179 (2020)
[2] P. P. Steijaert, Thermodynamical aspects of pulse-tube refrigerators, Technische Universiteit Eindhoven (1999)

TT 58.22 Thu 15:00 P2/OG3

Characterization of the cooling power on a two stage 4 K pulse tube cooler operated with solenoid valves — •Xaver Herrmann[1], Jack-André Schmidt[1,2], Bernd Schmidt[1,2], Jens Falter[2], and André Schirmeisen[1,2] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany — [2]TansMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany

Closed-cycle cryocoolers have become an important tool for low temperature scientific research[1]. Here we focus on Gifford-McMahon (GM) type pulse tube coolers (PTC), which offer low maintenance and long measurement periods. In order to create a temperature difference between the cold and hot end of the cooler, Helium is periodically compressed an expanded within the cooler. In order to do so a valve - commonly a rotary valve - allows high pressure Helium to enter the cooler or to relieve the pressure within. The high and low pressure levels are supplied by a Helium compressor[2]. In order to reduce complexity and improve flexibility of the system[3], this poster will look into the operation of a two stage 4 K PTC with solenoid valves. This removes the rotary valve from the system and therefore allows for easy access and change of parameters like high- and low-pressure duration, quiet times after high- and low-pressure pulse or frequency.

[1] R. Güsten et al., Nature 568, 357 (2019)
[2] R. Radebaugh, J. Phys.: Condens. Matter 21, 164219 (2009)
[3] S. Wild, Fortschr.-Ber. VDI Reihe 19 Nr. 105, Düsseldorf 1997

TT 58.23 Thu 15:00 P2/OG3

Development of a miniaturized, modular, nuclear demagnetization stage — •Leo Maximov[1], Nico Huber[1], Andreas Bauer[1], Keiya Shirahama[2], and Christian Pfleiderer[1] — [1]Physik-Department, Technical University of Munich, D-85748 Garching, Germany — [2]Keiyo University, Hiyoshi 3-14-1, Kohoku-ku, Yokohama, Japan

Experimental studies of condensed matter systems at sub-milli Kelvin temperatures are effectively only possible by virtue of nuclear adiabatic demagnetization refrigeration (NADR). While copper is the most commonly used refrigerant for NADR, both the development and operation of copper based NADR-stages are technically demanding and limited due to the very low starting temperatures needed for demagnetization. To overcome these limitations, hyperfine-enhanced refrigerants may be used. Here, we present the design and implementation of a compact, miniaturized, modular nuclear demagnetization stage for optional use with a conventional dilution refrigerator. Comprising a superconducting aluminum heat switch, a demagnetization stage using $PrNi_5$ with a bespoke superconducting coil, and a CMN thermometer, the setup is conceived for exploratory studies in the milli-Kelvin regime and below.

TT 58.24 Thu 15:00 P2/OG3

Study of the magnetocalotic effect in $[Ni(C_4H_3O_4)_2(H_2O)_4]$ - A Potential Realization of a Spin-1 Spatially Anisotropic Square Lattice with Ferromagnetic Interactions — •Petro Danylchenko, Róbert Tarasenko, Erik Čižmár, Vladimír Tkáč, Alžbeta Orendáčová, and Martin Orendáč — Institute of Physics, Faculty of Science, Pavol Jozef Šafárik University, Park Angelinum 9, 04154 Košice, Slovakia

The magnetocaloric effect in $[Ni(C_4H_3O_4)_2(H_2O)_4]$ was investigated using specific heat and magnetization measurements in the temperature range from 0.4 K to 50 K in magnetic fields up to 7 T. A magnetic entropy change -11.2 $JK^{-1}kg^{-1}$ at a temperature of about 3.5 K is achieved for magnetic field of 7 T. The temperature dependence of the magnetic specific heat in a zero magnetic field was compared with an $S = 1$ model with single-ion anisotropy parameters D and E (axial and rhombic). The best agreement was found for the parameters $D/k_B = 7.82$ K and $E/k_B = 2.15$ K. The divergence which appears between experimental and theoretical data at non-zero magnetic fields indicates the presence of additional factors in the system such as exchange interaction between magnetic ions. Broken-symmetry DFT calculations provided the values of ferromagnetic exchange interactions, $J_1/k_B = 1.50$ K and $J_2/k_B = 1.44$ K. The presence of such ferromagnetic correlations may explain the enhanced magnetocaloric effect. *Supported by project No. APVV-18-0197.*

TT 58.25 Thu 15:00 P2/OG3

Noise thermometers for mK- and μK-temperatures in high magnetic fields — •Pascal Willer, Christian Ständer, Nathalie Probst, Andreas Reiser, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany.

To measure the temperature in the presence of high magnetic fields is one of the big challenges in solid state physics labs. We developed a prototype of a cross-correlated, current sensing noise thermometer for mK-temperatures for application in high magnetic fields. The basic concept relies on the thermal motion of charge carriers in a bulk metal resistor. Two DC-SQUIDs detect the corresponding noise signal which is then recorded via two identical but independent amplifier chains. The method of cross correlation is used to eliminate uncorrelated noise contributions from the amplifier chains. As resistor materials we use the alloys $Ag_{60}Cu_{40}$ as well as $Pt_{92}W_8$, the latter being characterized by an extremely small temperature dependence of the electrical resistivity as well as the smallest magneto-resistance known to date. We show that this approach towards a relative primary thermometer for high magnetic fields is able to cover the complete temperature range below 4 K. We discuss the design and the necessary considerations of both thermometers and present first experimental results at mK temperatures.

TT 58.26 Thu 15:00 P2/OG3

Variable temperature probe stick with 2D coil system — •Claudia Köhn[1], Sylke Bechstein[2], and Doreen Wernicke[3] — [1]Entropy GmbH, Abbestr. 2-12, 10587 Berlin — [2]PTB, Abbestr. 2-12, 10587 Berlin — [3]Entropy GmbH, Gmunder Str. 37a, 81379 München

Within a technology transfer cooperation with PTB, Entropy made a probe stick for characterization of superconducting devices commercially available. It is an easy to use dip stick that can be cooled down directly in the liquid helium transport vessel while providing the possibility to vary temperature and apply magnetic fields.

The stick has two temperature stages. A 4.2 K stage and one with variable temperature (vT) stage, that can be heated up to 10 K with a temperature stability of 1 mK.

The device under test at the vT stage is placed inside a 2D coil system providing up to 500 mT parallel and 100 mT perpendicular to the chip. Homogeneity is 5% within a 1.5 mm radius around the center in the chip plane. At the moment we are optimizing the fabrication process of the coil bodies to provide better homogeneity of the magnetic field perpendicular to the chip.

TT 58.27 Thu 15:00 P2/OG3

Cryogenic scanning tunneling microscope — •Julia Besproswanny[1], Sebastian Schimmel[1], Ronny Schlegel[2], Danny Baumann[2], Bernd Büchner[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Christian Hess[1] — [1]University of Wuppertal, 42119 Wuppertal, Germany — [2]IFW Dresden, 01069 Dresden, Germany

We report the construction of a compact cryogenic scanning tunneling microscope. The design will allow to study local electronic structures at temperatures down to 2.5 K and magnetic fields of up to 15 T with atomic resolution in real space and a high energy resolution of 2 meV at 6 K. The microscope has a scanning range of 1μm x 1μm and a built-in cleaving mechanism that renders it possible to cleave the samples at a cryogenic temperature. Samples can be exchanged within a day while the measurement time can reach up to 6 weeks. These qualities combined with its compact and portable design make this STM a comfortable tool to study low temperature phenomena, e.g. superconductivity.

TT 58.28 Thu 15:00 P2/OG3

Cyclotron resonance on germanium probed by coplanar microwave resonators — •Anastasia Bauernfeind, Frederik Bolle, Martin Dressel, and Marc Scheffler — 1. Physikalisches Institut, University of Stuttgart, Stuttgart, Germany

Cyclotron resonance is a powerful way to investigate the Fermi surface of various materials. In our research we performed cyclotron resonance experiments on the semiconductor germanium by using metallic coplanar waveguides (CPW). In comparison to conventional three-dimensional cavity resonators, CPW resonators have the advantage of multiple well-accessible resonances. Furthermore, CPWs open the possibility of implementation in a dilution refrigerator, which makes the performance down to the mK regime possible, which is also interesting for Kondo insulators. By using a superconducting magnet (up to 8T) and the access to a broad frequency range in the microwave regime (up to 25 GHz), we were able to investigate the cyclotron resonance in germanium in detail. Here we analysed the frequency-, temperature- (2-40K) and power dependence of the cyclotron resonance signal. Beside the investigation of the electronic bands, we present interesting phenomena like the generation of charge carriers by the power of the microwave electric field and the process of impact ionization in p-doped germanium.

TT 58.29 Thu 15:00 P2/OG3

Sample environment communication protocol (SECoP) — •Klaus Kiefer[1], Georg Brandl[2], Niklas Ekström[3], Enrico Faulhaber[4], Thomas Herrmannsdörfer[5], Bastian Klemke[1], Thorsten Kracht[6], Anders Pettersson[3], Lutz Rossa[1], and Markus Zolliker[7] — [1]HZB, Berlin — [2]FZJ, Garching — [3]ESS, Lund — [4]TUM, Garching — [5]HZDR, Dresden — [6]DESY, Hamburg — [7]PSI, Villigen

We would like to present the Sample Environment Communication Protocol (SECoP), a software and initiative that addresses the standardization of communication between instrument-control software, sample-environment equipment (SE), and acquisition of metadata. The International Society for Sample Environment (ISSE) has developed SECoP in order to support a wide research community by tackling the challenges of data acquisition in daily laboratory routine, ([1] and references therein). Using SECoP as a common standard for controlling SE equipment will save resources and intrinsically give the opportunity to supply standardized and FAIR-data compliant SE metadata. It will also supply a well-defined interface for user-provided SE equipment, e.g. shared by different research facilities and of industry. In this poster presentation we will give an overview of the present status of SECoP and the developments within the SECoP@HMC project supported by the Helmholtz Metadata Collaboration. We would also like to advertize the SECoP booth at the exhibition of this conference, a possibility to get a first practical experience with SECoP.

[1] K. Kiefer et al., J. Neutron Res. 21, 181 (2020)

TT 58.30 Thu 15:00 P2/OG3

Lab::Measurement – measurement control with Perl 5 — Mia Schambeck, Erik Fabrizzi, Simon Reinhardt, and •Andreas K. Hüttel — Institute for Experimental and Applied Physics, Universität Regensburg, Regensburg, Germany

`Lab::Measurement` is a collection of object-oriented Perl 5 modules for control of test and measurement devices. It allows for quickly setting up complex tasks with diverse hardware. Instruments can be connected via GPIB (IEEE 488.2), USB, or VXI-11 / raw network sockets on Ethernet. Internally, third-party backends as, e.g., Linux-GPIB, the NI-VISA library, or Zurich Instruments' LabOne API are used, in addition to lightweight drivers for USB and TCP/IP-based protocols. This enables cross-platform portability of measurement scripts between Linux and Windows machines. Based on roles within `Moose` that provide communication standards such as SCPI, dedicated instrument driver classes take care of internal details. A high-level sweep layer allows for fast and flexible creation of nested measurement loops, where, e.g., several input variables are varied and data is logged into a customizable folder structure. Sweeps can also be retrieved directly from an instrument as, e.g., a spectrum or network analyzer. Further features include live plotting and obtaining attested timestamps for measurement data. Recent enhancements focus on support for the Nanonis Tramea quantum measurement system and for fast measurements using arbitrary waveform generators as voltage sources. `Lab::Measurement` is free software and available at `https://www.labmeasurement.de/`

[1] S. Reinhardt *et al.*, Comp. Phys. Comm. **234**, 216 (2019)

TT 58.31 Thu 15:00 P2/OG3

Modeling a vibrating carbon nanotube Josephson junction — •Andreas K. Hüttel[1,2], Keijo Korhonen[2], and Pertti Hakonen[2] — [1]Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Low Temperature Laboratory, Department of Applied Physics, Aalto University, P.O. Box 15100, 00076 Aalto, Finland

A carbon nanotube suspended between superconducting electrodes acts simultaneously as nanomechanical resonator and as a Josephson junction. Its energy-dependent density of states and with that position-dependent critical current further adds to the complexity of the system, as does both mechanical and electronic nonlinearity.

Using parallelized Julia code[1], we numerically solve the coupled differential equation system of the driven (via an ac gate voltage and/or ac current or voltage bias) system for realistic device parameters and characterize the evolving steady state. Specific attention is given to the impact of the Josephson junction behaviour on the mechanical resonance frequency and the vibration amplitude, and on the impact of the carbon nanotube motion on the phase evolution of the junction.

[1] https://julialang.org/

TT 59: Poster Session: Topology

Time: Thursday 15:00–18:00 Location: P2/OG4

TT 59.1 Thu 15:00 P2/OG4

Density-dependence of surface transport in tellurium-enriched nanograined bulk Bi_2Te_3 — •Sepideh Izadi[1], Ahana Bhattacharya[2], Sarah Salloum[3], Stephan Schulz[3], Martin Mittendorff[2], and Gabi Schierning[1] — [1]Bielefeld University, Department of Physics, 33615 Bielefeld, Germany — [2]University of Duisburg-Essen, Department of Physics, 47057 Duisburg, Germany — [3]University of Duisburg-Essen, Department of Chemistry, 45141 Essen, Germany

Three-dimensional topological insulators (3D TI) demonstrate conventional parabolic bulk bands together with protected Dirac surface states. Bi_2Te_3 material is considered as a well-known 3D TI model, however, due to its complicated defect chemistry, high number of charge carriers in the bulk dominate transport signal, even as nanograined structures. Herein we introduce Te-enriched Bi_2Te_3 nanoparticles synthesis as a method to control the bulk charge carrier density. Therewith, defects-free and stoichiometric Bi_2Te_3 nanoparticles with sizes between 4 and 40 nm are synthesized using ionic-liquid based approach. Grain boundaries along Bi_2Te_3 facets are investigated using high resolution transmission electron microscopy (HRTEM). The resulting nanoparticles were compacted into nanograined pellets of varying porosity, thereby emphasizing the surface transport contribution. The nanograined pellets were characterized by a combination of electrical transport together with THz time-domain reflectivity measurements. Using the Hikami-Larkin-Nagaoka (HLN) model, a characteristic coherence length of 200 nm that is considerably larger than nanograins diameter is reported.

TT 59.2 Thu 15:00 P2/OG4

Topological phases in $TaRhTe_4$: from monolayer to bulk — •Xiao Zhang — Leibniz Institute for Solid State and Material Research, Dresden, Germany

Topological phases are studied in different dimensional $TaRhTe_4$ using the method of density functional theory (DFT). We find that bulk $TaRhTe_4$ is a Weyl semimetal, whereas both monolayer and bilayer $TaRhTe_4$ display features of quantum spin Hall (QSH) insulator. A complete phase diagram linking monolayer, bilayer, and bulk $TaRhTe_4$ is obtained by varying intra- and inter-bilayer distance of the three-dimensional structure. It contains phases of Weyl semimetal, weak topological insulator, and normal insulator.

TT 59.3 Thu 15:00 P2/OG4

Quantum transport through resonant Dirac states in topological insulator nanowire constrictions — •Michael Barth[1], Maximilian Fürst[1], Cosimo Gorini[2], and Klaus Richter[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

Quantum transport in topological insulator (TI) nanowires is expected to be mediated by surface states which wrap phase coherently around the circumference [1]. The spectrum corresponds to a quantized and gapped Dirac cone, where the gap is present because of a Berry phase of π which arises due to spin-momentum locking. In this work, we numerically study transport in TI constrictions which are subjected to an axial magnetic field. More specifically, we consider a realistic junction of a narrow TI wire which is smoothly connected at its two ends to broad TI leads and calculate the transmission through the setup with respect to the Fermi energy and the magnetic field. The latter is tuned to close the Berry gap [2]. It turns out, that perpendicular field components in the constriction lead to the formation of magnetic barriers which result in resonant Dirac states. The proposed system can be used to spectroscopically study the Dirac spectrum with respect to its gate and flux dependence. Moreover, different transport regimes are identified, which depend on the length of the central wire segment.

[1] J. H. Bardarson, P. W. Brouwer, and J. E. Moore Phys. Rev. Lett. **105**, 156803 (2010)
[2] J. Ziegler et al., Phys. Rev. B **97**, 035157 (2018)

TT 59.4 Thu 15:00 P2/OG4

Topological insulator as barrier in Josephson junction — •Anton Montag, Alexander Ziesen, and Fabian Hassler — RWTH Aachen University, Aachen, Germany

We numerically study the behavior of a long Josephson junction in a superconductor-topological insulator-superconductor setup. An s-wave superconductor is deposited on the disordered surface of a three-dimensional topological insulator proximitizing the surface states on both sides of the junction. The normal region is probed by a local tunnelling contact. We simulate the tunnel spectrum at energies below the bulk gap of the topological insulator as a function of the phase difference of the superconducting order parameter across the junction. The low-energy spectrum can be divided into trivial Andreev bound states usually appearing at higher energies and chiral edge modes which become gapless at a phase difference of π. Since the latter are topologically protected, they are essentially not affected by symmetry preserving onsite potential disorder on the topological insulator surface. We show the simulated tunnel spectra for various disorder configurations and compare it to analytical calculations.

TT 59.5 Thu 15:00 P2/OG4

Towards the quantum anomalous Hall effect in magnetic topological insulator structures — •Justus Teller[1,2], Erik Zimmermann[1,2], Micheal Schleenvoigt[1,2], Gerrit Behner[1,2], Kristof Moors[1,2], Peter Schüffelgen[1,2], Gregor Mussler[1,2], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany

Three-dimensional topological insulators (TIs) are a material class which may enable robust topological quantum computing by using so-called Majorana zero modes. Published theoretical work predicts the Majorana state to exist in hybrid structures of superconductors and magnetic topological insulators which exhibit the quantum anomalous Hall effect (QAHE). We present magnetotransport measurements of Cr-doped magnetic $(Bi_{0.27}Sb_{0.73})_2Te_3$ layers. At 1.2 K, the uniformly Cr-doped samples exhibit a magnetic signature whose behaviour is probed under gate influence. Based on these measurements, an existing QAHE is ruled out. The results are compared to a magnetic TI heterostructure which is comprised of a plain TI layer embedded into two layers of magnetic TI. This structure reveals the QAHE. The temperature dependence of the effect is measured. In addition, the magnetic energy gap is probed by a gate dependent measurement. The QAHE is improved by current adjustment.

TT 59.6 Thu 15:00 P2/OG4

Axial topological insulator based DC SQUID in external SQUID layout — •Jan Karthein[1,3], Erik Zimmermann[1,3], Max Vassen Carl[1,3], Gerrit Behner[1,3], Abdur Rehman Jalil[1,3], Gregor Mussler[1,3], Peter Schüffelgen[1,3], Hans Lüth[1,3], Detlev Grützmacher[1,2,3], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Peter Grünberg Institut (PGI-10), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany

A three-dimensional topological insulator (TI) nanowire proximitized with a superconductor is predicted to be host to Majorana bound states that provide a platform for fault-tolerant quantum computation. Recently, axial TI-nanowire based DC SQUIDs showed coherent oscillations originating from the interference of topological surface states. We fabricate an axial TI-nanowire based DC SQUID with a neighboring Josephson junction completely in-situ, using selective-area growth and shadow mask fabrication techniques. An out-of-plane magnetic field is able to tune the flux inside the so formed external SQUID loop, while being decoupled from the in-plane magnetic field that tunes the flux inside the TI-nanowire. Coherent SQUID oscillations are visible when sweeping both the out-of-plane and in-plane magnetic field, proving that the axial TI-nanowire based DC SQUID and the external DC SQUID are experiencing phase-coherent transport.

TT 59.7 Thu 15:00 P2/OG4

Controlling the real-time dynamics of a spin coupled to the helical edge states of the Kane-Mele model — •Robin Quade[1] and Michael Potthoff[1,2] — [1]I. Institute of Theoretical Physics, De-

partment of Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

The time-dependent state of a classical spin locally exchange coupled to an edge site of a Kane-Mele model in the topologically non-trivial phase is studied numerically by solving the full set of coupled microscopic equations of motion for the spin and the electron system. Dynamics in the long-time limit is accessible thanks to dissipative boundary conditions, applied to all but the zigzag edge of interest. We study means to control the state of the spin via transport of a spin-polarization cloud through the helical edge states. The cloud is formed at a distant edge site using a local magnetic field to inject an electron spin density and released by suddenly switching off the injection field. This basic process, consisting of spin injection, propagation of the spin-polarization cloud, and scattering of the cloud from the classical spin, can be used to steer the spin state in a controlled way. We find that the effect of a single basic process can be reverted to a high degree with a subsequent process. Furthermore, we show that by concatenating several basic injection-propagation-scattering processes, the spin state can be switched completely and that a full reversal can be achieved.

TT 59.8 Thu 15:00 P2/OG4

Fermi-surface investigation of CaCdGe and CaCdSn — •B.V. Schwarze[1,2], F. Husstedt[1,2], M. Uhlarz[1], D. Kaczorowski[3], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence-ct.qmat, HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Poland

CaCdSn and CaCdGe are nodal-line semimetal candidate materials. These materials have one-dimensional lines or loops of topologically protected band-touching nodes. They sparked interest, due to their unique response to high magnetic or electric fields, including giant linear magnetoresistance and high charge-carrier mobility. These properties make them candidates for future technological applications. Band-structure calculations [1, 2] show for both systems non-topological and topological valence bands with the nodal band crossings above the Fermi level. Previous measurements of the magnetoresistance provide some support for the topological nature of the materials. Here, we present our investigation of the Fermi surfaces of CaCdSn and CaCdGe by use of de Haas-van Alphen measurements and band-structure calculations. Our measurements reveal many quantum-oscillation frequencies, which are not predicted by calculations. This discrepancy calls the calculated band structures [1, 2] and, thus, the precise nature of the topology of these systems into question.

[1] A. Laha et al., Phys. Rev. B 102, 035164 (2020).
[2] E. Emmanouilidou et al., Phys. Rev. B 95, 245113 (2017).

TT 59.9 Thu 15:00 P2/OG4

Ultrasound propagation in candidate material for electron hydrodynamics, Weyl semimetal WTe_2 — •Rafal Wawrzynczak[1], Stanislaw Galeski[1,2], and Johannes Gooth[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Physikalisches Institut, Universität Bonn, Nussallee 12, D-53115 Bonn, Germany

Interactions between electrons might lead to the appearance of a regime where the dominating time-scale is defined by momentum-conserving processes. This is manifested by electron liquid exhibiting features characteristic for classical liquids, like Poiseuille flow, resulting in non-Ohmic, sample-width-dependent resistivity. This was recently observed in a two-dimensional metal $PdCoO_2$ and two Weyl semimetals. Neither of the observations was accounted for with complete microscopic description. For WTe_2 there was proposed a mechanism based on the electron-electron scattering process involving a virtual phonon.

Here we report results of ultrasound propagation study performed on WTe_2 Weyl semimetal. We have analyzed temperature and field dependence of propagation of longitudinal and two transverse modes of different polarization propagating along the a crystallographic directions. The data shows anomalous decrease in speed of the longitudinal mode below 10 K and non-monotonous T-dependence of its attenuation. Moreover, quantum oscillations observed in all six measured quantities reveal the details of coupling between measured phonon modes and different parts of systems Fermi surface.

TT 59.10 Thu 15:00 P2/OG4

Photo-thermal imaging of $ZrTe_5$ in the quasi-quantized Hall regime — •Erica Warth Pérez Arias[1], Rafal Wawrzyńczak[1], Stansilaw Galeski[1], Johannes Gooth[2], Claudia Felser[1], and Fabian Menges[1] — [1]Max Planck Institute for Chemical Physics of Solids, Germany — [2]University of Bonn, Germany

$ZrTe_5$ has recently gained attention due to various intriguing experimental observations including the chiral magnetic effect [1] and the quasi-quantized 3D quantum Hall effect [2]. However, it remains challenging to probe the characteristic features of gapless surface and edge states experimentally. Addressing this challenge, we devised an optoelectronic detection scheme based on cryogenic magneto-optical laser scanning microscopy. The technique relies on a global electrical read-out of locally-induced currents, and contrasts previous all-optical studies of photogalvanic effects. We characterized $ZrTe_5$ single crystals with this approach and visualized rich spatial patterns of photo-induced transport as function of temperature and magnetic field. Remarkably, current maps obtained in the quasi-quantized Hall regime display long-range photoresponse over mm-distances and oscillations in magnetic field, hinting towards charge movement of ambient carriers in the system [3] driven by the photo-thermal effect [4] and the external magnetic field.

[1] Q. Li et.al., Nat. Phys. 12, 550-554 (2016)
[2] S. Galeski et.al., Nat. Commun. 12, 3197 (2021)
[3] J. C. W. Song et.al., Phys. Rev. B 90, 075415 (2014)
[4] Y. Wang et.al., arXiv:2203.17176 [cond-mat.mtrl-sci] (2022)

TT 59.11 Thu 15:00 P2/OG4

Anomalous transverse transport and phase transitions in Weyl semimetals RAlSi (R = La, Ce) — •erjian cheng — Leibniz Institute for Solid State and Materials Research (IFW-Dresden), 01069 Dresden, Germany

The noncentrosymmetric RAlPn (R = rare earth elements, Pn = Si or Ge) with the space-inversion (SI) symmetry breaking and/or the time-reversal (TR) symmetry breaking host multiple types of Weyl fermions, providing a fertile platform for the exploration of novel topological matter states. In particular, when magnetic configuration couples with the electronic wavefunctions, exotic anomalous transverse transport phenomena emerge. Here, by resorting to electrical and thermoelectrical transport, we systematically studied the ferromagnetic CeAlSi and its nonmagnetic analog LaAlSi, revealing the anomalous Hall effect (AHE) and/or anomalous Nernst effect (ANE). In addition, for LaAlSi, quantum oscillations reveal five frequencies. Moreover, a temperature-induced Lifshitz transition is unveiled in LaAlSi. For CeAlSi, magnetism enhances the anomalous transverse transport, implying that magnetism tunes the positions of Weyl nodes. Besides, high-pressure electrical transport and X-ray diffraction (XRD) measurements were also implemented, demonstrating multiple phase transitions. These results indicate that LaAlSi and CeAlSi provide unique and tunable systems to explore exotic topological physics, and a potential paradise for an array of promising applications for spintronics.

TT 59.12 Thu 15:00 P2/OG4

Electronic structure of topological superconductor candidate Li_2Pd_3B — •Gabriele Domaine[1], Jonas A. Krieger[1], Wei Yao[1], Changjiang Yi[2], Claudia Felser[2], Stuart S. P. Parkin[1], and Niels B. M. Schröter[1] — [1]Max Planck Institute for Microstructure Physics, Halle, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Chiral crystals are known to host a number of exotic quasiparticles which carry large Chern numbers and, as they are unconstrained from the celebrated spin statistics connection, can exhibit a range of unconventional (effective) spins [1]. These include, for instance, spin 3/2 Rarita-Schwinger, Kramers-Weyl, spin-1 and multifold fermions, which can be considered a generalization of conventional Weyl-fermions [2]. Here we present our preliminary results for the first Angle-Resolved Photoemission Spectroscopy (ARPES) measurements of the chiral crystal Li_2Pd_3B which is expected to host an as-yet unobserved multifold topological superconducting phase of class DIII, which is time reversal invariant), even without odd parity paring [3]. The superconducting gap is expected to arise from the intraband coupling at time-reversal invariant momentum points leading to an unconventional multiband gap function and nodal rings [4].

[1] N. B. M. Schröter et al. Nat. Phys. 15, 759 (2019)
[2] B. Bradlyn et al., Science 353, 6299 (2016)
[3] Z. S. Gao et al., Quantum Front 1, 3 (2022)
[4] C. Lee et al., Phys. Rev. B 104, L241115 (2021)

TT 59.13 Thu 15:00 P2/OG4

Implementing superconductor/skyrmion-host heterostructures using exfoliated Fe_3GeTe_2 on NbN — •Maximilian Daschner[1,2], Thomas Reindl[2], Marion Hagel[2], Jürgen Weis[2], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Max-Planck Institute for Solid State Research, Stuttgart, Germany

Experimental coupling of chiral magnetism and superconductivity through the proximity effect is a challenging and unexplored field that can lead to novel physics. Chiral magnets host topological excitations known as skyrmions that, when coupled to the vortices in a superconductor, are predicted to form Majorana fermions at its boundaries and vortex cores. The van-der-Waals material Fe_3GeTe_2 is known to host a skyrmion state over temperature and field ranges that depend on the sample thickness. We have exfoliated flakes of Fe_3GeTe_2 from a high quality crystal grown by vapour transport, deposited them on a NbN film and patterned electrical contacts using standard e-beam lithography techniques. The resulting Hall bar shaped nanodevices provide a convenient system for investigating skyrmion/superconductor interactions: Hall measurements above the superconducting transition temperature T_c3 in combination with magnetic force measurements survey the skyrmion state as a function of applied field, and measurements of the critical current density below T_c3 probe skyrmion-assisted vortex nucleation and pinning.

TT 59.14 Thu 15:00 P2/OG4

Pressure-dependent structural instabilities and transport phenomena in candidate topological semimetal $LaSb_2$ — •Theodore Weinberger, Christian de Podesta, Jiasheng Chen, Stephen Hodgson, and Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, United Kingdom

At low temperatures, and in the presence of large magnetic fields, $LaSb_2$ exhibits large, linear, non-saturating magnetoresistance, defying Fermi liquid behaviour. This phenomenon is thought to be caused by the onset of charge density wave order (CDW) below a sharp, hysteretic anomaly seen in resistivity data at ~ 355 K. This anomaly is rapidly pushed to lower temperatures under applied hydrostatic pressure, where above 6 kbar, it is fully suppressed. Surprisingly, the anomalous magnetoresistance persists to pressures beyond 20 kbar even after the suppression of the resistive anomaly. Hence, we suggest that the magnetoresistance is not driven by the onset of CDW order. Instead, we propose that the high temperature anomaly corresponds to a structural transition, similar to that seen in $CeSb_2$, which is supported by *ab initio* density functional theory calculations. Further, these calculations indicate that the Fermi surface of LaSb2 contains small pockets in both its high and low pressure structures. Small Fermi surface pockets suggest that $LaSb_2$'s band structure might feature topological, Dirac-like, cones which may explain the observed large, linear magnetoresistance.

TT 59.15 Thu 15:00 P2/OG4

2π domain walls for tunable Majorana devices — •Daniel Hauck[1], Stefan Rex[2,3], and Markus Garst[1] — [1]Karlsruhe Institute of Technology, Institute for Theoretical Solid State Physics, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [3]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe

Superconductor-magnet hybrid structures provide a platform for investigating topological phases with localized Majorana states. Such states have previously been predicted for elongated Skyrmions in the magnetic layer. Here we consider 2π domain walls that can be easily controlled experimentally. Depending on the boundary conditions, we demonstrate that localized Majorana states can be found at both ends of such walls. This establishes 2π domain walls as tunable elements for the realization of Majorana devices.

TT 59.16 Thu 15:00 P2/OG4

DMRG simulations of the one-dimensional anyon Hubbard model — •Yannick Werner, Maximilian Kiefer-Emmanouilidis, Pascal Jung, and Sebastian Eggert — Department of Physics, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany

The recent detection of anyons in setups of ultra-cold gases has further encouraged the in-depth studies of anyonic systems. Although the existence of conventional anyons is limited to two dimensions, a realization of fractional exchange statistics in a 1D system is possible which leads to a continuous interpolation between bosons and (pseudo-)fermions. In this poster we present the effects of perturbations i.e. local impurities, in a one-dimensional anyonic Hubbard model with onsite and nearest neighbor interactions on local densities, correlation functions and density transport. Here anyonic statistics are fulfilled by mapping bosonic operators via Jordan-Wigner-transformation, leading to a density dependent Peierl's phase in the hopping term. Additionally, in the case of small filling rates, we compute and analyze numerically the Luttinger parameter via Density Matrix Renormalization Group methods and compare it with analytical results.

TT 59.17 Thu 15:00 P2/OG4

Dynamical structure factor of an anyonic Luttinger liquid — •Pascal Jung, Martin Bonkhoff, Yannick Werner, and Sebastian Eggert — Department of Physics and Research Center Optimas, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany

Luttinger liquids are a powerful tool to describe the low-energy excitations of bosonic and fermionic systems in one spatial dimension. Anyonic systems, which allow a continuous transition between those two fundamental types of statistics, can be included in this framework by an additional coupling of the current and density excitations. This results into different velocities for the left and right movers, breaking the spatio-temporal symmetries.

To study the effects of this symmetry breaking on experimentally verifiable quantities, characteristic correlation functions are calculated. Using these, the dynamical structure factor for a finite system is determined. The broken symmetry leads here to a characteristic imbalance between left and right movers with typical power laws. Furthermore, the impact of local impurities is investigated using the perturbative renormalization group. These results are compared to numerical simulations obtained by the DMRG algorithm.

TT 59.18 Thu 15:00 P2/OG4

Quantum spin dynamics in the spin-chain compound Cu_2OH_3Br — •Anneke Reinold[1], Kirill Amelin[2], Zhiying Zhao[3], Changqing Zhu[1], Patrick Pilch[1], Hans Engelkamp[4], Toomas Rõõm[2], Urmas Nagel[2], and Zhe Wang[1] — [1]TU Dortmund University, Germany — [2]National Institute of Chemical Physics and Biophysics, Tallinn, Estonia — [3]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, China — [4]Radboud University, Nijmegen, The Netherlands

In low-dimensional quantum magnets, exotic spin phenomena can emerge due to strong spin fluctuations. Here we investigate spin dynamics of the quantum spin-chain compound Cu_2OH_3Br by high-resolution terahertz spectroscopy as a function of temperature and in high magnetic fields. Below the Néel temperature T_N=9.3 K, this compound exhibits a unique magnetic structure consisting of alternating ferromagnetic and antiferromagnetic spin-1/2-chains of Cu^{2+}-ions [1,2]. In this ordered phase we observed magnetic excitations, which are characteristic for this unique spin structure and consistent with results of inelastic neutron scattering [2]. Moreover, we are able to track these spin excitations in applied magnetic fields crossing field-induced phase transitions [1].

[1] Z. Y. Zhao *et al.*, J. Phys.: Condens. Matter **31**, 275801 (2019)
[2] H. Zhang *et al.*, Phys. Rev. Lett. **125**, 037204 (2020)

TT 60: Quantum Dots, Quantum Wires, Point Contacts

Time: Thursday 17:15–19:00 Location: HSZ 03

TT 60.1 Thu 17:15 HSZ 03

Spin-texture topology in curved circuits driven by spin-orbit interactions — Alberto Hijano[1,2], Eusebio J. Rodríguez[3], •Dario Bercioux[4,5], and Diego Frustaglia[3] — [1]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain — [2]Department of Condensed Matter Physics, University of the Basque Country UPV/EHU, 48080 Bilbao, Spain — [3]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain — [4]Donostia International Physics Center (DIPC), 20018 Donostia–San Sebastián, Spain — [5]IKERBASQUE, Basque Foundation for Science, Plaza Euskadi 548009 Bilbao, Spain

We study the response of spin carriers to the effective field textures developed in curved one-dimensional circuits subject to the joint action of Rashba and Dresselhaus spin-orbit interactions. By using a quantum network technique, we establish that the interplay between these two non-Abelian fields and the circuit's geometry modify the geometrical characteristics of the spinors, particularly on square circuits, leading to the localisation of the electronic wave function and the suppression of the quantum conductance. We propose a topological interpretation by classifying the corresponding spin textures in terms of winding numbers.

[1] A. Hijano *el al.*, arXiv:2209.11653 [cond-mat.mes-hall]

TT 60.2 Thu 17:30 HSZ 03

Stochastic resonance of electron tunneling in a quantum dot in spite of a periodically blind eye — •Eric Kleinherbers, Hendrik Mannel, Johann Zöllner, Marcel Zöllner, Martin Geller, Axel Lorke, and Jürgen König — Faculty of Physics and CENIDE, University Duisburg-Essen, 47057 Duisburg, Germany

The key idea of stochastic resonance is to amplify a signal by adding noise. For electron tunneling in a quantum dot, this can be used to facilitate a periodic electron transfer, where during each period a single electron enters and leaves the quantum dot. In stochastic resonance, the noise (tunneling) rate must be well adjusted to the frequency of the periodic drive that is applied to the quantum dot. The Fano factor is a possible indicator of this effect [1]. Here, we study the full counting statistics and, in particular, factorial cumulants as higher-order indicators of stochastic resonance. We discuss experimental data of electron tunneling into and out of a self-assembled InAs quantum dot, where the full counting statistics is measured using a resonance fluorescence readout scheme. We find that even if the detector is blind during half of each period, a stochastic resonance is visible in the full counting statistics.

[1] T. Wagner *et al.*, Nat. Phys. 15, 330 (2019)

TT 60.3 Thu 17:45 HSZ 03

Modifications of the local dissipation profile imposed by quantum point contacts — •Nico Leumer — Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Recent experimental progress provides access to local temperature changes on the nanoscale, three orders of magnitude lower than the sample temperature itself [1]. Since electric current is accompanied by an energy loss of the charge carriers, this advance implies that the dissipated power became in fact a local observable. The key role is adopted by electron-phonon interactions transferring the electronic energy loss to the bulk material and thus; stimulating the sample temperature profile.

Quantum point contacts (QPC) have been reported to modify the dissipation and, especially, the energy loss of charge carriers may be distributed asymmetrically around the QPC. Inspired by this feature, we develop a theory to determine why, where and how much dissipation occurs in experimental relevant geometries.

[1] D. Halbertal et al., Nature 539, 407 (2016)
[2] C. Blaas-Anselmi et al., SciPost Phys. 12, 105 (2022)

TT 60.4 Thu 18:00 HSZ 03

Resonant tunneling energy harvesters: Improving performance via quantum interference. — •José Balduque[1] and Rafael Sánchez[1,2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain. — [2]Condensed Matter Physics Center (IFIMAC), and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain.

The spectral filtering of quantum dots can be used for heat to power conversion in electronic conductors. A proposal based on resonant-tunneling three-terminal devices [1] has been recently verified experimentally [2]. Two quantum dots connect the two terminals of a conductor to a hot electronic cavity where carriers exchange heat via thermalization. We propose the heat source to be separated from the conductor via a beam-splitter (e.g., the tip of a scanning microscope) that mediates the system-bath coupling. The resulting ballistic electron propagation gives rise to interferences [3] able to improve the engine performance, both in the extracted power and efficiency [4].

[1] A.N. Jordan *et al.*, Phys. Rev. B **87**, 075312 (2013)
[2] G. Jaliel *et al.*, Phys. Rev. Lett. **123**, 117701 (2019)
[3] R. Sánchez *et al.*, Phys. Rev. B **104**, 115430 (2021)
[4] J. Balduque and R. Sánchez, in preparation.

TT 60.5 Thu 18:15 HSZ 03

Vibrational instabilities arising from non-conservative current-induced forces in nanosystems: A comparison of quantum and semi-classical approaches — •Samuel Rudge, Christoph Kaspar, and Michael Thoss — Institute of Physics, University of Freiburg, Germany

Understanding the vibrational dynamics of molecular junctions is of paramount importance to creating junctions that are mechanically stable. In systems with more than one vibrational degree of freedom, instabilities can arise due to non-conservative current-induced forces, an effect that can occur at lower voltages than the well-understood mechanism of current-induced heating [1].

In recent years, such non-conservative forces have been largely explored with semi-classical Langevin-type equations for the vibrational degrees of freedom, where the electronic friction tensor and average electronic force can be analyzed directly [1]. In this work, however, we employ both a semi-classical Langevin equation as well as a quantum master equation approach to explore instabilities in a model system with two electronic levels and two vibrational modes. Both approaches derive from the numerically exact hierarchical equations of motion (HEOM) method [2], and the resulting analysis is able to show in which regimes such semi-classical treatments can be used.

[1] J. T. Lü *et al.*, Phys. Rev. B **85**, 245444 (2012)
[2] S.L. Rudge, Y. Ke, and M. Thoss, arXiv:2211.14215 (2022)

TT 60.6 Thu 18:30 HSZ 03

Asymmetric couplings of quantum dot systems to environments — •Lukas Litzba, Nikodem Szpak, Eric Kleinherbers, and Jürgen König — Fakultät für Physik, Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany

We study systems with a few quantum dots, represented by the Fermi-Hubbard model, coupled to several Markovian baths with different coupling strengths. On the one hand, we compare different approximations (such as Redfield equation, coherent Lindblad approximation [1]) for a Master equation in first order of the quantum dot–bath coupling for strongly interacting electrons. On the other hand, we find exact solutions for non-interacting electrons. We compare the results for different coupling strength regimes and discuss the qualitative changes in the system behavior. Thereby we observe significant effects of the coupling asymmetry on energy coherences, which is linked to local versus global coupling. We look closer at systems from two to ten dots and study the non-equilibrium dynamics based on dressed excitation energies of the system as well as the associated damping rates. In this context we find transitions from global to local coupling behavior with increasing coupling strength asymmetry.

[1] E. Kleinherbers, N. Szpak, J. König, R. Schützhold, PRB 101, 125131 (2020)

TT 60.7 Thu 18:45 HSZ 03

Relaxation dynamics in Fermi-Hubbard systems coupled to environment — •Nikodem Szpak[1], Gernot Schaller[2], Ralf Schützhold[2,3], and Jürgen König[1] — [1]Theoretische Physik und CENIDE, Universität Duisburg-Essen, Lotharstr. 21, 47048 Duisburg — [2]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden — [3]Institut für Theoretis- che Physik, Technische Universität Dresden, 01062 Dresden

We study a chain of quantum dots coupled to enviroment and describe it with the Fermi-Hubbard model coupled to fermionic baths. For different coupling regimes (interdot vs bath-dot) we derive separate Lindblad master equations and compare their properties. It is shown that for strong repulsive onsite (Coulomb) interactions and low bath temperatures the system quickly reaches a low-energy sector described effectively by the Heisenberg model. Within this sector the further dynamics depends strongly on the relative coupling strengths. For weak bath-dot coupling, the system relaxes globally to the unique anti-ferromagnetic ground state with zero total spin. For strong bath-dot coupling, the system increases its total spin to the maximal possible value and ends up in (degenerate) states exhibiting ferromagnetic order. We provide rigorous derivations as well as numerical examples.

[1] E. Kleinherbers, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 101, 125131 (2020)
[2] G. Schaller, F. Queisser, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 105, 115139 (2022)

TT 61: Focus Session: Correlations in Moiré Quantum Matter II

Time: Thursday 17:45–19:00 Location: HSZ 201

TT 61.1 Thu 17:45 HSZ 201

Magnetism and metallicity in Moiré transition metal dichalcogenides — •Patrick Tscheppe[1], Jiawei Zang[2], Marcel Klett[1], Seher Karakuzu[3], Thomas Maier[4], Michel Ferrero[5,6], Andrew Millis[2,3], and Thomas Schäfer[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Department of Physics, Columbia University, 538 West 120th Street, New York, New York 10027, USA — [3]Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, New York 10010, USA — [4]Computational Sciences and Engineering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6164, USA — [5]CPHT, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91128 Palaiseau, France — [6]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The Moiré transition metal dichalcogenide homobilayer WSe_2 has recently been observed both to undergo continuous Mott transitions and to display quantum critical behavior, while also allowing for high tunability of its electronic parameters. At the same time, the effective low-energy physics of WSe_2 is believed to be adequately described by a simple one-band Hubbard model. We study the rich interplay between perfect nesting and dynamical as well as non-local correlations in this model using the cellular dynamical mean-field theory (CDMFT) in conjunction with the dynamical cluster approximation (DCA). In this way we elucidate the nature of both interaction and magnetic field-driven metal-insulator crossovers, previously observed in experiments.

TT 61.2 Thu 18:00 HSZ 201

Switching between Mott-Hubbard and Hund physics in Moiré quantum simulators — •Siheon Ryee and Tim Wehling — I. Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany

Mott-Hubbard and Hund electron correlations have been realized thus far in separate classes of materials. In this talk, we show that a single Moiré homobilayer encompasses both kinds of physics in a controllable manner. We develop a microscopic multiband model which we solve by dynamical mean-field theory to nonperturbatively address the local many-body correlations. We demonstrate how tuning with twist angle, dielectric screening, and hole density allows to switch between Mott-Hubbard and Hund correlated states in twisted WSe_2 bilayer. The underlying mechanism bases on controlling Coulomb-interaction-driven orbital polarization and energetics of concomitant local singlet and triplet spin configurations. From comparison to recent experimental transport data, we find signatures of a filling-controlled transition from a triplet charge-transfer insulator to a Hund-Mott metal. Our finding establishes twisted transition metal dichalcogenides as a tunable platform for exotic phases of quantum matter emerging from large local spin moments.

TT 61.3 Thu 18:15 HSZ 201

Tunable topological order of pseudo spins in semiconductor heterostructures — Clemens Kuhlenkamp[1,2,3], •Wilhelm Kadow[1,2], Atac Imamoglu[3], and Michael Knap[1,2] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, D-80799 München, Germany — [3]Institute for Quantum Electronics, ETH Zürich, CH-8093 Zürich, Switzerland

We propose a novel platform to realize highly-tunable, frustrated Hubbard physics with topological order in multi-layer Moiré structures. Identifying a layer degree of freedom as a pseudo spin, allows us to retain SU(2) symmetry, while controlling ring exchange processes and concurrently quenching the kinetic energy by large external magnetic fields. This way, a broad class of interacting Hofstadter states and their transitions can be studied. Remarkably, in the limit of strong interactions the system becomes Mott insulating and we find exceptionally stable spin liquid phases which are induced by the magnetic field. As the magnetic flux can be easily tuned in Moiré systems, our approach provides a promising route towards the experimental realization and control of topologically ordered phases of matter. We also discuss how layer pseudo-spin can be probed in near-term experiments.

TT 61.4 Thu 18:30 HSZ 201

Nontrivial quantum geometry of multiband systems and implications for flat bands — •Johannes Mitscherling — Department of Physics, University of California, Berkeley, California 94720, USA

Studying the geometry of wave function manifolds helps us to identify and understand phenomena whose descriptions are not captured by the sole knowledge of the energy dispersion. A prominent example of recent interest is the distance between wave functions captured by the quantum metric. Flat-band systems are promising candidates for novel fascinating quantum metric effects since well-known contributions to observables that depend on the slope or curvature of the dispersion vanish. For instance, the dominant contribution to the superfluid stiffness and the dc electrical conductivity is proportional to the integrated quantum metric for flat bands. In this talk, I will address the role of band degeneracy in these quantum metric effects. I will use the developed framework for dc electrical conductivity [PRB 105, 085154 (2022), PRB 106, 165133 (2022)] to contrast nondegenerate and degenerate band manifolds. We will explore the common mathematical description in terms of Grassmannian manifolds and its concrete implications, such as lower bounds and the nonadditivity of the quantum metric. I close by illustrating how these concepts can be directly extended to other observables.

J.M. acknowledges support by the German National Academy of Sciences Leopoldina through grant LPDS 2022-06.

TT 61.5 Thu 18:45 HSZ 201

Magnetism in twisted bilayer graphene with heterostrain — Ahmed Missaoui[1], Florie Mesple[2], Javad Vahedi[3], Andreas Honecker[1], Vincent Renard[2], and •Guy Trambly de Laissardière[1] — [1]Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, Cergy-Pontoise, France — [2]Université Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, Grenoble, France — [3]Jacobs University, School of Engineering and Science, Bremen, Germany

The discovery of correlated insulators and superconductivity due to flat bands in twisted bilayer graphene (TBG) at so-called “magic angles” has stimulated the study of their magnetic properties [1]. Furthermore, it is now well established that heterostrain, which is generally present in the samples, is a key parameter in understanding the actual shape of the flat bands [2]. Here, we present a theoretical study of magnetism in magic-angle TBG combining a Hubbard model and the mean-filed approach including non-collinear magnetic terms. We show how heterostrain strongly modifies the magnetization and the local order of magnetic state for realistic Coulomb interaction values.

[1] J. Vahedi *et al.*, SciPost Phys. **11**, 083 (2021) and references therein
[2] L. Huder *et al.*, Phys. Rev. Lett. **120**, 156405 (2018);
F. Mesple *et al.*, Phys. Rev. Lett. **127**, 126405 (2021)

TT 62: Ultrafast Dynamics of Light-Driven Systems

Time: Friday 9:30–11:45 Location: HSZ 03

TT 62.1 Fri 9:30 HSZ 03

Ultrafast dynamics of spin-density wave order in $BaFe_2As_2$ under high pressures — Ivan Fotev[1,2], Stephan Winnerl[1], Saicharan Aswartham[3], Sabine Wurmehl[3,4], Bernd Büchner[3,4], Harald Schneider[1], Manfred Helm[1,2], and •Alexej Pashkin[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]IFW Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany

We utilize pump-probe spectroscopy to measure the quasiparticle relaxation dynamics of $BaFe_2As_2$ in a diamond anvil cell at pressures up to 4.4 GPa and temperatures down to 8 K. Tracing the amplitude of the relaxation process results in an electronic phase diagram that illustrates the variation of the spin-density wave (SDW) order across the whole range of the applied pressures and temperatures. We observe a slowing down of the SDW relaxation dynamics in the vicinity of the phase transition boundary. However, its character depends on the trajectory in the phase diagram: the slowing down occurs gradually for the pressure-induced transition at low temperatures and abruptly for the thermally-driven transition. Our results suggest that the pressure-induced quantum phase transition in $BaFe_2As_2$ is related to the gradual worsening of the Fermi-surface nesting conditions.

TT 62.2 Fri 9:45 HSZ 03

Probing the superconducting transition in a cuprate superconductor by multi-dimensional terahertz spectroscopy — •Albert Liu[1], Danica Pavicevic[1], Michael Fechner[1], Pedro Lozano[2], Genda Gu[2], and Andrea Cavalleri[1,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Brookhaven National Laboratory, New York, USA — [3]Oxford University, Oxford, UK

We develop two-dimensional terahertz spectroscopy in both a noncollinear and reflection geometry. We demonstrate the technique by distilling the terahertz optical response of a superconducting plasma into its constituent nonlinearities, up to fifth-order. Subsequent measurements at temperatures approaching and crossing the phase transition reveal a phase-disordering transition in lieu of a BCS transition. An outlook for probing light-induced superconducting states will be provided.

TT 62.3 Fri 10:00 HSZ 03

Tracing the dynamics of the superconducting order via transient THG — •Minjae Kim[1,2,3], Gennady Logvenov[2], Bernhard Keimer[2], Dirk Manske[2], Lara Benfatto[4], and Stefan Kaiser[1,2,3] — [1]Institute of Solid State and Materials Physics, Technical University Dresden, 01062 Dresden, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [3]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [4]Department of Physics and ISC-CNR, Sapienza University of Rome, 00185 Rome, Italy

Nonlinear THz third harmonic generation (THG) was shown to directly probe internal degrees of freedoms of the superconducting condensate and its exposure to external collective modes in the framework of driven Higgs modes [1-3]. Here we extend this idea to light-driven nonequilibrium states in superconducting La2-xSrxCuO4 establishing a transient Higgs spectroscopy. We perform an optical pump-THz-THG drive experiment and using 2D-spectroscopy we disentangle the driven TH response into the excited quasiparticles and condensates response. As such the light induced changes of the THG signals probe the ultrafast pair breaking dynamics and transient pairing amplitude of the condensate.

[1] Nat. Comm. 11, 1 (2020)
[2] Nat. Comm. 11, 287 (2020)
[3] arXiv:2109.09971

TT 62.4 Fri 10:15 HSZ 03

Influence of impurities on the Higgs mode in noncentrosymmetric superconductors — •Simon Klein and Dirk Manske — Max-Planck Institut für Festkörperforschung, Stuttgart, Deutschland

Recent interest for collective amplitude (Higgs) excitations focused on third harmonic generation (THG) experiments in single- and multiband superconductors, both for singlet *s*- and *d*-wave gap structure. A resonance in the THG intensity appears, when matching the driving frequency to the energy of the corresponding investigated mode, leading to a phase jump at the resonance frequency. We extend these studies to superconductors without an inversion symmetry, which can be effectively described by a two-band model with an order parameter, consisting of spin singlet (even parity) and spin triplet (odd parity) components. We calculate the THG response, showing that it contains contributions from three distinguishable sources, namely the Higgs mode, the Leggett mode and quasiparticles. In the clean limit the quasiparticle contributions dominate the collective modes for all singlet-triplet ratios of the gap structure. By including already a small amount of impurities in the system, we find a significant enhancement of the Higgs mode contributions to the THG signal. Furthermore, we notice a significant change in the phase jump, which helps to differentiate between clean and dirty superconductors.

15 min. break

TT 62.5 Fri 10:45 HSZ 03

Non-equilibrium phenomena in a two-band superconductor MgB_2 driven by narrow-band THz pulses — •Sergei Sobolev[1], Amon Lanz[1], Tao Dong[2], Alexej Pashkin[3], Amrit Pokharel[1], Zi Zhao Gan[2], Li Yu Shi[2], Nan Lin Wang[2], Stephan Winnerl[3], Manfred Helm[3], and Jure Demsar[1] — [1]Uni-Mainz, Mainz — [2]Peking Uni., Beijing — [3]HZDR, Dresden

Excitation of a superconductor (SC) with a low energy electromagnetic pulse leads to a non-equilibrium state, which may profoundly differ from a quasi-thermal one, driven by optical excitation. Such a non-equilibrium may be especially pronounced in a multi-band SC. Here, we report on systematic time-resolved studies of the dynamics of the SC order following resonant excitation with intense narrow-band THz pulses in thin films of MgB_2, the prototype two-band SC with two distinct superconducting gaps. We demonstrate that the temperature and excitation density dependent dynamics qualitatively follows the behavior predicted by the phenomenological Rothwarf-Taylor model for dynamics in a single gap BCS superconductor implying strong coupling between the two condensates on the ps timescale. Tracking the dependence of the amplitude of the THz driven gap suppression, however, displays a pronounced minimum near $0.6T_c$, that cannot be accounted by the phenomenological model. Comparison of the results to those obtained by excitation with NIR pulses suggests that resonant THz excitation results in long-lived (100 ps timescale) non-thermal quasiparticle distribution, which gives rise to Eliashberg-type enhancement of superconductivity, competing with pair-breaking.

TT 62.6 Fri 11:00 HSZ 03

Semi-classical analysis of high harmonic spectra in Dirac materials — •Wolfgang Hogger[1], Vanessa Junk[1], Alexander Riedel[1], Cosimo Gorini[2], Juan-Diego Urbina[1], and Klaus Richter[1] — [1]Institute for theoretical physics, University of Regensburg, Germany — [2]Université Paris-Saclay, CEA, CNRS, SPEC, 91191, Gif-sur-Yvette, France

The study of high-order harmonic generation (HHG) in solids by virtue of intense laser pulses provides a fascinating platform to study ultrafast electron dynamics as well as material properties. We theoretically investigate HHG on the basis of massive Dirac Fermions, serving as a prototypical model for topologically non-trivial matter. The high harmonic spectra resulting from a numerical solution of the equations of motion for the density-matrix are supplemented and compared to a semiclassical saddle-point analysis known as the Lewenstein or simpleman model[1,2]. We demonstrate that HHG can be interpreted as a result of interfering classical trajectories generated at different half-cycles of the laser pulse. A transparent and compact analytical formula for the high harmonic spectrum in the limit of long pulses is provided and discussed regarding the range of its validity as well as corrections arising from short waveforms.

[1] M. Lewenstein, P. Balcou, M. Y. Ivanov, A. L'Huillier, and P. B. Corkum, Phys. Rev. A 49, 2117 (1994)
[2] G. Vampa, C. R. Mcdonald, G. Orlando, D. D. Klug, P. B. Corkum, and T. Brabec, Phys. Rev. Lett. 113, 073901 (2014)

TT 62.7 Fri 11:15 HSZ 03

Driven lattice fluctuations in quantum paraelectric $SrTiO_3$ — •Michael Fechner[1], Michael Först[1], Ankit Disa[1], Michele Buzzi[1], Alex von Hoegen[1], Gal Orenstein[2], Viktor Krapivin[2], Quỳnh Le Nguyen[2], Roman Mankowsky[3], Mathias Sander[3], Henrik Lemke[3], Yunpei Deng[3], Mariano Trigo[2], and Andrea Cavalleri[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Stanford Linear Accelerator Center, Menlo Park, United States of America — [3]Paul Scherrer Institute, Villigen, Switzerland

Enhanced fluctuations are the precursors of quantum phase transition. In the case of ferro- and antiferrodistortive structural transitions, these fluctuations arise at specific points in reciprocal space. Here we use time-resolved x-ray diffuse scattering to show how a resonantly driven zone center optical phonon in cubic $SrTiO_3$ selectively modulates lattice fluctuations at the Brillouin zone boundary. On short time scales, enhanced and oscillating lattice fluctuations are found at the R-point, which reduce to below the equilibrium value on the picosecond time scale. We attribute the fast dynamics to a finite-momentum fourth-order phonon-phonon interaction between the driven infrared-active Ti-O stretch mode and the antiferrodistortive zone-boundary soft mode. The long-term reduction indicates nonlinear coupling of the antiferrodistortive distortions to strain. We discuss the implications of these findings for the recently observed light-induced ferroelectric state of $SrTiO_3$[1].
[1] T.F. Nova et al., Science 364, 1075 (2019)

TT 62.8 Fri 11:30 HSZ 03

Decay of photoinduced orbital excitations in the spin-Peierls system TiOCl: a study from first principle — •Paul Fadler[1], Philipp Hansmann[1], Kai Phillip Schmidt[1], Angela Montanaro[2], Daniele Fausti[1,2], and Martin Eckstein[3] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]University of Trieste — [3]Universität Hamburg

In spin-Peierls materials, the magnetic interactions caused by the electronic correlations drive a phase transition in which the unit cell is distorted. TiOCl is a quasi one-dimensional transition metal oxide with well-defined orbital (d-d) excitations that transitions to a spin-Peierls state below 67K, by doubling the unit cell along the 1-D chain. Recently, optical transmissivity measurements after a double pump excitation into the orbital excitations revealed a dependence of the decay time on the excitation sequence, which may indicate different lifetimes of various orbital excitations. To unveil the microscopic origins of this observation, we study a material-realistic multi-orbital Hubbard Hamiltonian derived from ab initio density-functional theory. The localized strong-coupling native of TiOCl then allows for perturbative elimination of charge-excitations, leading to a spin-orbital model of Kugel-Khomskii type. We compute its spin dispersion in the absence of orbital excitations. Based on this, and the computed intra and inter-orbital matrix elements, we then estimate the decay time of orbital excitations via (multi) spinon emission, and compare to the experimental findings.

TT 63: Superconductivity: Theory

Time: Friday 9:30–13:15 Location: HSZ 103

TT 63.1 Fri 9:30 HSZ 103

Sharp Kohn-like phonon anomalies due to charge order can strongly enhance the superconducting T_c — •Alessio Zaccone — Department of Physics, University of Milan, 20133 Milano, Italy

Phonon softening is a ubiquitous phenomenon in condensed matter systems which is usually associated with charge density wave (CDW) instabilities and anharmonicity. The interplay between phonon softening, CDW and superconductivity is a topic of intense debate. In this work, the effects of anomalous soft phonon instabilities on superconductivity are studied based on a recently developed theoretical framework that accounts for phonon damping and softening within the Migdal-Eliashberg theory [1]. Model calculations [2] show that the phonon softening in the form of a dip in the phonon dispersion relation, either acoustic or optical (including the case of Kohn-type anomalies typically associated with CDW), can cause a manifold increase of the electron-phonon coupling constant λ. This, under certain conditions, which are consistent with the concept of optimal frequency introduced by Bergmann and Rainer, can produce a large increase of the superconducting transition temperature T_c. These results suggest the possibility of reaching high-temperature superconductivity by exploiting soft phonon anomalies restricted in momentum space.
[1] M. Baggioli, C. Setty, A. Zaccone, Phys. Rev. B 101, 214502 (2020)
[2] arXiv:2211.12015v2

TT 63.2 Fri 9:45 HSZ 103

Universal suppression of superfluid weight by non-magnetic disorder in s -wave superconductors independent of quantum geometry and band dispersion — •Alexander Lau[1], Sebastiano Peotta[2], Dmitry I. Pikulin[3], Enrico Rossi[4], and Timo Hyart[1,2] — [1]MagTop, IF PAN, Warsaw, Poland — [2]Aalto University, Finland — [3]Microsoft Quantum, Redmond, USA — [4]William & Mary, Williamsburg, USA

Motivated by the experimental progress in controlling the properties of the energy bands in superconductors, significant theoretical efforts have been devoted to study the effect of the quantum geometry and the flatness of the dispersion on the superfluid weight. In conventional superconductors, where the energy bands are wide and the Fermi energy is large, the contribution due to the quantum geometry is negligible, but in the opposite limit of flat-band superconductors the superfluid weight originates purely from the quan- tum geometry of Bloch wave functions. Here, we study how the energy band dispersion and the quantum geometry affect the disorder-induced suppression of the superfluid weight [1]. In particular, we consider non-magnetic disorder and s -wave superconductivity. Surprisingly, we find that the disorder-dependence of the superfluid weight is universal across a variety of models, and independent of the quantum geometry and the flatness of the dispersion. Our results suggest that a flat-band superconductor is as resilient to disorder as a conventional superconductor.
[1] SciPost Phys. 13, 086 (2022)

TT 63.3 Fri 10:00 HSZ 103

Correction to Morel-Anderson-Tolmachev pseudopotential from nonlocal Coulomb interaction in 2D superconductors — •Manuel Simonato, Malte Rösner, and Mikhail I. Katsnelson — Radboud University, Nijmegen, NL

The repulsive Coulomb interaction between electrons is detrimental to conventional superconductivity. The widely accepted model to account for this is to describe this repulsion with a purely local interaction of strength μ_C. Morel, Anderson, and Tolmachev then showed that the superconducting quantities are effectively described by a renormalized parameter μ_C^*, as a direct consequence of the energy scale separation between phonons and electrons. In 2D the screening properties are less efficient and modeling the Coulomb repulsion with a strictly local interaction can result in inaccurate description. We therefore study how superconducting properties are affected by nonlocal Coulomb repulsions. We find that the superconducting state can still be accurately described when a revised Coulomb pseudopotential $\tilde{\mu}_C^*$ is used. We show that the revised parameter, which accounts for nonlocal interactions, is always larger that the convetional μ_C^*. The non-local Coulomb interaction thus suppresses superconductivity and the critical temperature even further. Analyzing the Bethe-Salpeter equation describing the screening of Coulomb interaction in 2D, we obtain an analytical expression for $\tilde{\mu}_C^*$, and show that the structure of the nonlocal Coulomb interaction weakens the screening effects from high-energy pair fluctuations and therefore yields larger values of the pseudopotential.

TT 63.4 Fri 10:15 HSZ 103

Coherence and pairing fluctuations in strongly correlated superconductors — •Niklas Witt[1,2], Sergey Brener[1], Yusuke Nomura[3], Ryotaro Arita[4,5], Alexander Lichtenstein[1,2], and Tim Wehling[1,2] — [1]University of Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Germany — [3]Keio University Japan — [4]University of Tokyo, Japan — [5]RIKEN CEMS, Japan

The fundamental properties of superfluids and superconductors are determined by the spatial coherence of the macroscopic condensate. Central to this characterization is the knowledge of the coherence length ξ, as it specifies the relevant length scales for fluctuations pertinent to, e.g., the formation of vortex latices or magneto-thermal transport. While the description of ξ is well established in weak-coupling BCS theory and Eliashberg-theory, it is a generally unknown quantity in strongly correlated superconductors, where spatiotemporal fluctuations influence the critical temperature [1] and might underlie light-induced enhancement of superconductivity [2].

In this work, we establish a link to directly calculate the coherence length for superconductors with strong electron correlations from microscopic theories and first principles. We illustrate with the example of Alkali-doped fullerides (A_3C_{60}) how proximity of superconducting and Mott-localized states impact superconducting coherence, pairing fluctuations, and critical temperature. Our analysis shows Eliashberg-type behavior of strongly correlated superconductors.

[1] Emery & Kivelson, Nature **374** (1995)
[2] Fausti et al., Science **331** (2011)
Mitrano et al., Nature **530** (2016)

TT 63.5 Fri 10:30 HSZ 103

Superconductivity from repulsive interactions due to strong-coupling to a Mott-insulating layer — •Clara S. Weber[1,2], Dante M. Kennes[1], and Martin Claassen[2] — [1]RWTH Aachen, Aachen, Germany — [2]University of Pennsylvania, Philadelphia, USA

While superconductors in their conventional form are established by effective attractive interactions, mechanisms for emergent electronic pairing from strong repulsive electron-electron interactions remain under considerable debate. Here, we establish a strong-coupling mechanism that realizes intertwined superconductivity and magnetic order in a Kondo-like bilayer system with purely repulsive interactions, composed of a two-dimensional Mott insulator with strong Hubbard interactions coupled to a layer of weakly-interacting itinerant electrons. Remarkably, this model allows for a rigorous strong-coupling analysis, where we find that itinerant electrons in the nearly-metallic layer are subject to an effective attractive electron-electron interaction as a function of magnetic ordering in the Mott-insulating layer. We carefully study this behavior numerically using large scale DMRG calculations and find that the superconducting behavior persists in a wide parameter range beyond the strong-coupling regime. Additionally, we classify the rich magnetic phase diagram and find a 2-site antiferromagnetic and a 4-site antiferromagnetic phase, along with a phase separation regime. Finally, we discuss possible applications and realizations of the proposed mechanism.

TT 63.6 Fri 10:45 HSZ 103

Simulating superconducting properties of overdoped cuprates: The role of inhomogeneity — Mainak Pal[2], •Andreas Kreisel[1], William A. Atkinson[3], and Peter J. Hirschfeld[2] — [1]Niels Bohr Institute, University of Copenhagen, Denmark — [2]Department of Physics, University of Florida, USA — [3]Department of Physics and Astronomy, Trent University, Canada

Theoretical studies of disordered d-wave superconductors have focused, with a few exceptions, on optimally doped models with strong scatterers. Addressing recent controversies about the nature of the overdoped cuprates, however, requires studies of the weaker scattering associated with dopant atoms. Here we study simple models of such systems in the self-consistent Bogoliubov-de Gennes (BdG) framework, and compare to disorder-averaged results using the self-consistent-T-matrix-approximation (SCTMA). Despite surprisingly linear in energy behavior of the low-energy density of states even for quite disordered systems, the superfluid density in such cases retains a quadratic low-temperature variation of the penetration depth, unlike other BdG results reported recently. We trace the discrepancy to smaller effective system size employed in that work. Overall, the SCTMA performs remarkably well, with the exception of highly disordered systems with strongly suppressed superfluid density. We explore this interesting region where gap inhomogeneity dominates measured superconducting properties, and compare with overdoped cuprates.

[1] M. Pal, A. Kreisel, W.A. Atkinson, P.J. Hirschfeld arXiv:2211.13338 (2022)

TT 63.7 Fri 11:00 HSZ 103

Finite energy Cooper pairing in multiband superconductors — •Masoud Bahari[1], Song-Bo Zhang[2], Chang-An Li[1], Sang-Jun Choi[1], Carsten Timm[3], and Björn Trauzettel[1] — [1]University of Würzburg, Würzburg, Germany — [2]University of Zürich, Zürich, Switzerland — [3]Technische Universität Dresden, Dresden, Germany

Extensive efforts have been carried out to understand the superconducting pairing symmetry since the birth of Bardeen-Cooper-Schrieffer theory. In weakly interacting systems, the essential ingredient is a weak effective electron-electron interaction at the Fermi energy resulting in particular bulk properties including superconducting gaps possibly with nodes.

We demonstrate and discuss the bulk and surface spectral properties of a novel pairing mechanism that occurs at finite excitation energies in multiband superconductors. In the bulk, it is manifested by the appearance of superconducting coherence peaks in the density of states at finite energies. Interestingly, on the surface, we predict the emergence of a pair of helical topological Dirac surface cones when the finite energy pairing is odd-parity.

Finally, we propose aluminum in proximity with (111) surface of gold to realize the bulk properties of finite energy pairing. We discuss the pairing symmetry of the system by employing the density-functional theory, and an analytical model based on the Bogoliubov-de Gennes formalism. The signature of such a pairing gives important information about the correct pairing symmetry of a superconductor.

15 min. break

TT 63.8 Fri 11:30 HSZ 103

Fragmented Cooper pair condensation in striped superconductors — •Alexander Wietek — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, Dresden 01187, Germany

Condensation of bosons in Bose-Einstein condensates or Cooper pairs in superconductors refers to a macroscopic occupation of a few single- or two-particle states. A condensate is called *fragmented* if not a single, but multiple states are macroscopically occupied. While fragmentation is known to occur in particular Bose-Einstein condensates, we propose that fragmentation naturally takes place in striped superconductors. To this end, we investigate the nature of the superconducting ground state realized in the two-dimensional t*t**J model. In the presence of charge density modulations, the condensate is shown to be fragmented and composed of partial condensates located on the stripes. The fragments of the condensates hybridize to form an extended macroscopic wave function across the system. The results are obtained from evaluating the singlet-pairing two-particle density matrix of the ground state on finite cylinders computed via the density matrix renormalization group method. Our results shed light on the intricate relation between stripe order and superconductivity in systems of strongly correlated electrons.

TT 63.9 Fri 11:45 HSZ 103

Superconductivity on the honeycomb lattice: A truncated unity perspective — •Matthew Bunney[1,2], Jacob Beyer[1,2], Carsten Honerkamp[2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Melbourne, Australia — [2]Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

The honeycomb lattice provides one of the simplest scenarios with sublattice degrees of freedom. For Cooper pairing of electrons on this lattice, this opens extensive and intricate opportunities of interplay between the momentum space wavefunction, the electron spins and the orbital (sublattice) dependencies. Recent advances and improvements in truncated unity versions of the functional renormalization group allows us to fully capture these phenomena. We thus revisit the honeycomb Hubbard model and its electron pairing and density wave instabilities. A particular emphasis is placed on the formation of sublattice singlets and the resulting exotic pairing states.

TT 63.10 Fri 12:00 HSZ 103

A low-dimensional ML Surrogate Model for Critical Temperature Prediction of Superconductors — •Angel Diaz Carral[1], Martin Roitegui Alonso[1], and Maria Fyta[2] — [1]Institute for Computational Physics, Universität Stuttgart, Allmandring 3, 70569, Stuttgart, Germany — [2]Computational Biotechnology, RWTH-Aachen University, Worringerweg 3, 52074, Aachen, Germany

A general theory of superconductivity has been the focus of research over the last decades. Machine learning (ML) approaches based on chemical and structural features have been developed in order to predict both the critical temperature (Tc) and potential novel superconducting structures. Nevertheless, the applied ML models lack interpretability; either the feature matrix is reduced via SVD/PCA transformations or augmented with statistical feature generation. Here, we introduce a ML model based only on electronic descriptors derived from the composition formula and the individual elements. We reach a very high accuracy (R2 over 91%) using a considerably reduced descriptor dimensionality, while retaining the physical meaning of the feature space. Our active learning model is efficiently tested in predicting critical temperatures and links to the discovery of new superconducting structures.

TT 63.11 Fri 12:15 HSZ 103

Ab initio study of magnetic doping in an Ising superconductor — •Mohammad Hemmati[1], Philipp Rüssmann[1,2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]University of Würzburg, Germany

The transition-metal dichalcogenide $NbSe_2$ is a layered superconducting material that exhibits unconventional Ising superconductivity that is particularly robust to certain directions of external magnetic fields [1]. We combined the Bogoliubov-de-Gennes formalism in the Korringa-Kohn-Rostoker Green function method with the Coherent Potential Approximation [2,3], to study superconducting $NbSe_2$ in the presence of dilute concentrations of magnetic transition-metal impurities. The ab initio results show a suppression of superconductivity at higher magnetic impurity concentration, which is in agreement with the Abrikosov-Gorkov theory.

*This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy * Cluster of Excellence Matter and Light for Quantum Computing (ML4Q) EXC 2004/1 * 390534769.*

[1] K. S. Novoselov *et al.*, Science **353**, aac9439 (2016)
[2] https://jukkr.fz-juelich.de
[3] P. Rüßmann and S. Blügel, PRB **105**, 125143 (2022)

TT 63.12 Fri 12:30 HSZ 103

Chiral surface superconductivity in half-Heusler semimetals — •Tilman Schwemmer[1], Domenico Di Sante[2,3], Jörg Schmalian[4], and Ronny Thomale[1] — [1]Institute for Theoretical Physics, University of Wuerzburg, D-97074 Wuerzburg, Germany — [2]Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy — [3]CCQ, Flatiron Institute, New York, NY 10010, USA — [4]Institute for Theory of Condensed Matter and Institute for Quantum Materials and Technologies, KIT, Karlsruhe 76131, Germany

We propose the metallic and weakly dispersive surface states of half-Heusler semimetals as a possible domain for the onset of unconventional surface superconductivity ahead of the bulk transition. Using density functional theory (DFT) calculations and the random phase approximation (RPA), we analyse the surface band structure of LuPtBi and its propensity towards Cooper pair formation induced by screened electron-electron interactions in the presence of strong spin-orbit coupling. Over a wide range of model parameters we find a chiral superconducting condensate featuring Majorana edge modes to be favoured energetically, while low-dimensional order parameter fluctuations trigger time-reversal symmetry breaking preceding the superconducting transition.

TT 63.13 Fri 12:45 HSZ 103

Transport in superconducting heterostructures: Quasiclassical theory and finite element method — •Kevin Marc Seja and Tomas Löfwander — Department of Microtechnology and Nanoscience - MC2, Chalmers University of Technology, Gothenburg, Sweden

We present results on steady-state transport in mesoscopic conventional and unconventional superconductors coupled to either normal-metal or superconducting reservoirs. Our self-consistent simulations are using nonequilibrium quasiclassical theory in the Eilenberger formulation which allows different order parameter symmetries at arbitrary mean free path. Previously we investigated the thermoelectric effect[1] and spectral rearrangements due to a voltage bias[2] in d-wave superconductors. These studies on nonequilibrium effects assumed translational invariance normal to the transport direction.

This talk will address the question of how to go beyond such quasi one-dimensional models and study superconducting hybrid structures in realistic device geometries. To this end we present a finite element method[3] for the self-consistent solution of the underlying quasiclassical transport equations in dimensions larger than one, and give examples of its application.

[1] Seja & Löfwander, Phys. Rev. B 105, 104506 (2022)
[2] Seja & Löfwander, J. Phys.: Condens. Matter 34, 425301 (2022)
[3] Seja & Löfwander, Phys. Rev. B. 106, 144511 (2022)

TT 63.14 Fri 13:00 HSZ 103

Nonlinear response of diffusive superconductors to ac electromagnetic Fields — •Pascal Derendorf, Anatoly Volkov, and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Using the generalized Usadel equation, we theoretically study the nonlinear response of a diffusive BCS superconductor to the action of electromagnetic fields. The response is found in the second order of the perturbation in the amplitude of the field E for the superconducting order parameter Δ and in the third order for the current j. We represent the matrix Keldysh function $\hat{g}^K$ as the sum of a regular function $\hat{g}^{reg}$ and an anomalous function $\hat{g}^{an}$. On the basis of this approach, general formulas for deviations of the retarded (advanced) Green's functions, as well as the Keldysh function for an arbitrary number of harmonics of the incident field are explicitly obtained. The frequency and temperature dependencies of zero harmonic $\delta\Delta_0$ (Eliashberg effect) and the second harmonic $\delta\Delta_{2\Omega}$ under action of a monochromatic irradiation are analyzed. We also study the third harmonic $j_{3\Omega}$ and the possibility of parametric amplification of a signal with a frequency Ω_x in the presence of a pumping with a frequency Ω which excites the Higgs (amplitude) mode.

TT 64: Topology: Other Topics

Time: Friday 9:30–11:30 Location: HSZ 201

TT 64.1 Fri 9:30 HSZ 201

Fermi arc reconstruction in synthetic photonic lattice — •Duy Hoang Minh Nguyen[1], Chiara Devescovi[1], Dung Xuan Nguyen[2], Hai Son Nguyen[3,4], and Dario Bercioux[1,5] — [1]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain — [2]Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), Daejeon, 34126, Republic of Korea — [3]Univ Lyon, Ecole Centrale de Lyon, CNRS, INSA Lyon, Universite Claude Bernard Lyon 1, CPE Lyon, CNRS, INL, UMR5270, Ecully 69130, France — [4]Institut Universitaire de France (IUF), F-75231 Paris, France — [5]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

The chiral surface states of Weyl semimetals are known for having an open Fermi surface called Fermi arc. At the interface between two Weyl semimetals, these Fermi arcs are predicted to potentially deform into unique interface states. In this work, we numerically study a one-dimensional (1D) dielectric trilayer grating where the relative displacements between adjacent layers play the role of two synthetic momenta. The lattice is described by an effective Hamiltonian whose spectral properties coincide closely with rigorous electromagnetic simulations. Our trilayer system is a simple but versatile platform that emulates 3D crystals without time-reversal symmetry, including Weyl semimetal, nodal line semimetal, and 3D Chern insulator. It allows us to not only observe phenomena such as the phase transition between Weyl semimetal and Chern insulator but also confirm the Fermi arc reconstruction between two Weyl semimetals.

[1] arXiv:2211.07230

TT 64.2 Fri 9:45 HSZ 201

Electronic correlations and pseudo Fermi arcs due to geometry of the Fermi surface in semimetals — •Elena Derunova — IFW, Helmholz str.20, Dresden

Moving forward from topological theory I present a geometrical approach to analyze the bandstructures and Fermi surfaces. Particularly, the effect of hyperbolic geometry of the Fermi surface on the Fermi liquid breakdown and correlated transport effects will be presented. As a mechanism for realizing these correlations, I introduce pseudo Fermi arcs connecting separate pockets of hyperbolic Fermi surface. A breakdown of time-reversal symmetry via tunneling through those pseudo arcs is referred as Fermi Surface Geometry Effect (FS-GE). The predictable power of FS-GE is tested on the spin and anomalous Hall effects, traditionally associated with intrinsic time-reversal symmetry breaking. An index, H_F, quantifying FS-GE in a particular direction, shows a universal correlation ($R^2 = 0.97$) with the experimentally measured intrinsic anomalous Hall conductivity in that direction, of 16 different compounds spanning a wide variety of crystal, chemical, and electronic structure families, where the topological methods give just $R^2 = 0.52$. This raises a question about the principal limits of topological physics, dominating now the predictions of non-trivial electron transport, and its transformation into a wider study of bandstructures' and Fermi surfaces' geometries, opening a horizon for the prediction of phenomena beyond topological understanding.

TT 64.3 Fri 10:00 HSZ 201

Markers in Landau levels for topological transitions in Bernal bilayer graphene — •Nils Jacobsen[1], Anna Seiler[1], Zhiyu Dong[2], Thomas Weitz[1], and Leonid Levitov[2] — [1]1st Physical Institute, Faculty of Physics, University of Göttingen, Göttingen, Germany — [2]Department of Physics, Massachusetts Institute of Technology, Cambridge, USA

This talk will discuss Landau levels in an electron band that exhibits the topological Lifshitz transition. We focus on Bernal-stacked bilayer graphene, a system that has drawn a lot of attention recently. A dual gated experimental setup allows to tune the out-of-plane displacement field and the charge carrier density independently, giving insights in exotic correlation effects [1]. Depending on the charge carrier density its Fermi surface changes its topology, that is, four disconnected pockets merge together to form one connected Fermi sea [2].

This topological transition results in a complex series of Landau levels which are not valley-symmetric and, as a result, change their order and degeneracy when the magnetic field is varied. These effects are added to the degeneracies that are already present due to valley and spin degrees of freedom. By virtue of numerical diagonalization methods based on a realistic tight binding model, we extract this Landau level sequence and directly relate it to transport measurements. Our model allows us to access the range of parameters of interest where the topological Lifshitz transition can occur.

[1] A. M. Seiler et al., Nature 608, 298 (2022)
[2] E. McCann et al. Rep. Prog. Phys. 76, 056503 (2013)

TT 64.4 Fri 10:15 HSZ 201

Topological classification of single-particle Green functions and effective Hamiltonians for interacting systems — Maximilian Kotz[1] and •Carsten Timm[1,2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

The single-particle Green function for any interacting-electron system can be written as the resolvent of a generally frequency-dependent and non-Hermitian effective Hamiltonian. Both these properties together allow for 54 instead of ten global-symmetry classes. The absence of Hermiticity also requires to reconsider the concept of a spectral gap. If the limits of the effective Hamiltonian for frequency $\omega \to \pm\infty$ coincide one can compactify the frequency axis and consider winding in $(d+1)$-dimensional momentum-frequency space. We derive a complete list of the homotopy groups for the 54 classes and spatial dimensions d, for the cases without and with frequency dependence.

TT 64.5 Fri 10:30 HSZ 201

Solitons and topology: Observation of cnoidal wave localization in non-linear topolectric circuits — •Hendrik Hohmann[1], Tobias Hofmann[1], Tobias Helbig[1], Hauke Brand[2], Lavi K. Upreti[1], Alexander Stegmaier[1], Alexander Fritzsche[1], Tobias Müller[1], Ching Hua Lee[3], Martin Greiter[1], Laurens W. Molenkamp[2], Tobias Kiessling[2], and Ronny Thomale[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany — [3]Department of Physics, National University of Singapore, Singapore, 117542

Topological phases have been realized in a variety of classical metamaterials. They provide easily accessible platforms to study topology in regimes beyond experimental limitations of real materials.

While most implementations are limited to the linear regime, investigating non-linear effects promises to reveal a plethora of new phenomena, such as solitons and chaos.

To study the intertwining of topology and non-linearity we engineered a topolectric circuit reminiscent of the Su-Schrieffer-Heeger (SSH) model with added tunable onsite non-linearity. We observe the localized cnoidal (LCn) state which maintains the spatial exponential localization of the SSH edge mode while distorting a sinusoidal input into eccentric waves in time domain.

In this talk, we complement the non-linear differential equations with the theory of topological localization and develop an analytic description of the LCn state.

TT 64.6 Fri 10:45 HSZ 201

Non-Hermitian diamond chain — •Carolina Martinez Strasser[1], Miguel Ángel Jimenez Herrera[1], and Dario Bercioux[2] — [1]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, Plaza Euskadi 5 48009 Bilbao, Spain

We investigate the spectral properties of a non-Hermitian quasi-one-dimensional lattice in several possible dimerization configurations. Specifically, we focus on a non-Hermitian diamond chain that presents a zero-energy flat band. In the Hermitian case, this flat band originates from wave interference and results in a wave function localized only on a subset of sites on the unit cell [1]. We transform the system into a non-Hermitian one by considering asymmetric hopping terms between some of the lattice sites of the chain. This leads to the accumulation of eigenstates, known as the skin effect. Despite this accumulation of eigenstates, we can characterize the presence of non-trivial edge states at zero energy by a real-space topological invariant known as biorthogonal polarization. We show that this invariant, evaluated using the destructive interference method, can also characterize the non-trivial phase of the non-Hermitian diamond chain [2].

[1] D. Bercioux, O. Dutta, and E. Rico, Ann. Phys. (Berl.) 529, 1600262 (2017)
[2] F. K. Kunst *et al.*, Phys. Rev. Lett. 121, 026808 (2018)

TT 64.7 Fri 11:00 HSZ 201

Direct optical probe of magnon topology in two-dimensional quantum magnets — •Michael Sentef[1], Emil Boström[1], Tahereh Parvini[2], James McIver[1], Angel Rubio[1], and Silvia Viola Kusminskiy[3] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [2]University of Greifswald — [3]RWTH Aachen

Controlling edge states of topological magnon insulators is a promising route to stable spintronics devices. However, to experimentally ascertain the topology of magnon bands is a challenging task. Here we derive a fundamental relation between the light-matter coupling and the quantum geometry of magnon states. This allows to establish the two-magnon Raman circular dichroism as an optical probe of magnon topology in honeycomb magnets, in particular of the Chern number and the topological gap. Our results pave the way for interfacing light and topological magnons in functional quantum devices.
arXiv:2207.04745

TT 64.8 Fri 11:15 HSZ 201

Inelastic topological light scattering in chiral liquids — Silvia Müllner[1], Florian Büscher[1], Angela Möller[2], and •Peter Lemmens[1] — [1]IPKM, TU Braunschweig — [2]Anorg. Chemie, JGU Mainz

Vortex beams of light contain spin (SAM, helicity) and angular momentum (OAM, chirality). However, there is a long debate whether OAM can couple to a topological system. In a recent experimental study of chiral liquid crystals we demonstrate the effect of vortex light with different topological charge. We give evidence for roton like quasiparticles with a dispersion that dominates the scattering at small and intermediate scattering vectors [1].

*Work supported by DFG LE967/16-1, GrK 1952/2, Metrology for Complex Nanosystems*NanoMet, and DFG EXC-2123 QuantumFrontiers - 390837967.*

[1] S. Müllner, F. Büscher, A. Möller, and P. Lemmens, Phys. Rev. Lett. 129, 207801 (2022)

TT 65: Correlated Electrons: Other Theoretical Topics

Time: Friday 9:30–12:15 Location: HSZ 204

TT 65.1 Fri 9:30 HSZ 204

Quantum oscillations beyond the Onsager relation in a doped Mott insulator — •Valentin Leeb[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, Germany; TUM School of Natural Sciences, Department of Physics, TQM — [2]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The kinetic energy of electrons in a magnetic field is quenched resulting in a discrete set of highly degenerate Landau levels (LL). This gives rise to fascinating phenomena like quantum oscillations or the integer and fractional quantum Hall effect. The latter is a result of interactions partially lifting the degeneracy within a given LL while inter-LL interactions are usually assumed to be unimportant. Here, we study the LL spectrum of the Hatsugai–Kohmoto model, a Hubbard-like model which is exactly soluble on account of infinite range interactions. For the doped Mott insulator phase in a magnetic field we find that the degeneracy of LLs is preserved but inter-LL interactions are important leading to a non-monotonous reconstruction of the spectrum. As a result, strong interactions lead to aperiodic quantum oscillations of the metallic phase in contrast to Onsager's famous relation connecting oscillation frequencies with the Fermi surface areas at zero field. In addition, we find unconventional temperature dependencies of quantum oscillations and effective mass renormalizations. We discuss the general importance of inter-LL interactions for understanding doped Mott insulators in magnetic fields.

TT 65.2 Fri 9:45 HSZ 204

Non-Fermi-liquid behavior from critical electromagnetic vacuum fluctuations — •Peng Rao and Francesco Piazza — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study two-dimensional materials where electrons are coupled to the vacuum electromagnetic field of a cavity. We show that, at the onset of the superradiant phase transition towards a macroscopic photon occupation of the cavity, the critical electromagnetic fluctuations, consisting of photons strongly overdamped by their interaction with electrons, can in turn lead to the absence of electronic quasiparticles. Since transverse photons couple to the electronic current, the appearance of non-Fermi-Liquid behavior strongly depends on the lattice. In particular, we find that in a square lattice the phase space for electron-photon scattering is reduced in such a way to preserve the quasiparticles, while in a honeycomb lattice the latter are removed due to a non-analytical frequency dependence of the damping $\propto |\omega|^{2/3}$. Standard cavity probes could allow to measure the characteristic frequency spectrum of the overdamped critical electromagnetic modes responsible for the non-Fermi-liquid behavior.

TT 65.3 Fri 10:00 HSZ 204

Collapse of fermionic quasiparticles upon coupling to local bosons — Adam Kłosiński, Piotr Wrzosek, Krzysztof Wohlfeld, and •Cliò Efthimia Agrapidis — Insitute of Theoretical Physics, Faculty of Physics, University of Warsaw, Poland

We study the stability of the fermionic quasiparticle in a fermion-boson model on a Bethe lattice, with fermions interacting with local bosons thorough a Peierls coupling. We solve the model by mapping it onto a non-interacting chain with a site-dependent potential. We show that the model does not support a quasiparticle solution – provided that a finite number of local bosonic excitations cost zero energy. The quasiparticle disappearance becomes easier with an increase in: (i) the total number of bosons with zero energy, and (ii) the relative strength of the coupling between bosons and fermions. The postulated model can be applied to study systems in which fermions are coupled to condensed bosons or magnons in spin stripes embedded in hole-doped 2D antiferromagnets or Ising-like magnetic interfaces (ferromagnetic-antiferromagnetic). Finally, we show how this model leads to an in-depth understanding of the onset of quasiparticles in the 1D and 2D t-J^z model.

TT 65.4 Fri 10:15 HSZ 204

Breakdown of the many-electron perturbation expansion beyond particle-hole symmetry — •Herbert Essl, Matthias Reitner, and Alessandro Toschi — Institute of Solid State Physics, TU Wien

The breakdown of the self-consistent perturbation theory for many-electron systems has several physical and formal manifestations. Among the latter, one of the most studied is the divergence of two-particle irreducible vertex functions. Hitherto most investigations of the divergences appearing in the irreducible vertex functions of many-electron systems have been restricted to the particle hole symmetric cases and the calculations were performed at finite temperatures. This work is a first step beyond such restrictions. To this aim we investigate the two particle properties of the Hubbard Atom, both for positive (repulsive) and negative (attractive) on-site interaction. As a main result a *universal phase-diagram* of vertex divergences, valid for arbitrary (finite) temperatures, has been determined. Using this result as a "compass", the T=0 limit has been investigated, in order to unveil possible connections between the vertex divergences and the validity or the violation of the Luttinger Theorem. We also study the convergence of the self-consistent perturbation series beyond the particle-hole symmetry condition, determining specific constraints for the convergence of the series to the physical solution at arbitrary electronic densities.

TT 65.5 Fri 10:30 HSZ 204

Cooling and heating in the Bose-Hubbard model by parameter tuning — •Sebastian Eggert, Sven Stawinski, and Axel Pelster — University of Kaiserslautern

We investigate short-range interacting Bosons in an optical lattice at finite temperature. It is well known that the system shows a Mott-Superfluid transition when changing the repulsion U, the hopping t and/or the filling. However, it is much less clear how the temperature is affected by those changes, assuming the parameters U and/or t are tuned adiabatically. We now present higher order calculations for the full Free energy and derive the temperature and entropy in a large parameter space. We discuss where significant heating or cooling effects can be expected in the superfluid phase, in the Mott region and near the phase transition lines.

15 min. break

TT 65.6 Fri 11:00 HSZ 204

Fixed-point annihilation and duality in the SU(2)-symmetric spin-boson model — •Manuel Weber[1,2] and Matthias Vojta[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [2]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

The annihilation of two intermediate-coupling renormalization-group (RG) fixed points is of interest in diverse fields from statistical mechanics to high-energy physics, but has so far only been studied using perturbative techniques. Using the recently developed wormhole quantum Monte Carlo method, we present high-accuracy results for the SU(2)-symmetric $S = 1/2$ spin-boson (or Bose-Kondo) model. We study the model with a power-law bath spectrum $\propto \omega^s$ where, in addition to a critical phase predicted by perturbative RG, a stable strong-coupling phase is present. Using a detailed scaling analysis, we provide direct numerical evidence for the collision and annihilation of two RG fixed points at $s^* = 0.6540(2)$, causing the critical phase to disappear for $s < s^*$. In particular, we uncover a surprising duality between the two fixed points, corresponding to a reflection symmetry of the RG beta function, which we utilize to make analytical predictions at strong coupling which are in excellent agreement with numerics. Our work makes phenomena of fixed-point annihilation accessible to large-scale simulations, and we comment on the consequences for impurity moments in critical magnets.

TT 65.7 Fri 11:15 HSZ 204

Thermodynamics properties of interacting Dirac fermion with SO(3) symmetry — •Zihong Liu[1], Matthias Vojta[2], Fakher F. Assaad[1], and Lukas Janssen[2] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden,

Germany

In the previous work[Physical Review Letters, 128(8):087201, 2022], we figure out the zero temperature phasediagram of a interacting Dirac fermion model processed explicit SO(3) symmetry with unbias quantum Monte Carlo(QMC) method. By threading size dependent magnetic flux ($B \sim 1/L^2$) across two dimensional honeycomb lattice, we reduce the finite size effect in the QMC simulation and suppress the superconductivity in the strong coupling region. In this scenario, the ground state phase diagram of the model is splitted by two phase transitions. In this talk, we implement the QMC simulation by turning off the magnetic flux. Without the externel magnetic field, the model recover to a higher symmetry and the superconductivity emergence in the strong coupling region on the ground state. In addition, we investigate the thermodynamics properties near the second transition point, where the finite temperature phase boundary are determined by the Ising type particle-hole order parameter and the Kosterlitz-Thouless transition govered by the U(1) symmetry breaking.

TT 65.8 Fri 11:30 HSZ 204

Long-term memory magnetic morrelations driven by local electronic repulsion — •Emin Moghadas[1], Matthias Reitner[1], Clemens Watzenböck[1], Giorgio Sangiovanni[2], and Alessandro Toschi[1] — [1]TU Wien — [2]University of Würzburg

We investigate the onset of non-decaying temporal magnetic correlations in simple electronic models with on-site (Hubbard) electrostatic repulsion U. This effect[1] corresponds to the existence of a finite difference between the static/isothermal and the zero-frequency limit of the dynamical Kubo (magnetic) susceptibility. The long-term behavior is studied, on the one hand, analytically for the non-interacting Bethe lattice case in infinite dimensions and, on the other hand, for finite-size Hubbard ring-molecules by means of exact diagonalization. This way, we can directly observe and investigate the link between the emergence of infinitely long-lived temporal correlations and the degeneracies of the exact many-body eigenspectrum, possibly inferring underlying relations with the entropic properties of the system. Our findings also pave the way to study the enhancement of the static/isothermal density response in the proximity of metal-insulator transitions [2] and, in particular, of its possible impact on the renormalization of electron-phonon coupling.

[1] C. Watzenböck et al., Sci. Post Phys. (2022)
[2] M. Reitner et al., PRL (2020) and references therein.

TT 65.9 Fri 11:45 HSZ 204

Simulation of anyonic tight-binding Hamiltonians — •Nico Kirchner[1], Adam Smith[2,3], Babatunde Ayeni[5], Frank Pollmann[1,4], and Joost Slingerland[5,6] — [1]Department of Physics, TFK, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — [2]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK — [3]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, NG7 2RD, UK — [4]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [5]Department of Mathematical Physics, National University of Ireland, Maynooth, Ireland — [6]Dublin Institute for Advanced Studies, School of Theoretical Physics, 10 Burlington Rd, Dublin, Ireland

Anyons are quasiparticles with exotic exchange statistics that can be supported in two-dimensional systems such as quantum spin liquids and fractional quantum Hall systems. In general, even effective models for such systems are not exactly solvable, which leads to numerical approaches to study the properties of anyons. In this talk, I will discuss how to numerically simulate anyonic tight-binding Hamiltonians for general abelian and non-abelian anyon models using the formalism of fusion diagrams. The presented results for such tight-binding Hamiltonians include energy level spacing statistics, which reveal level repulsion for all considered anyons. Further, it is observed that the density distribution following a quench becomes homogeneous at large times for these systems, which indicates thermalization.

TT 65.10 Fri 12:00 HSZ 204

Absence of fractal quantum criticality in the quantum Newman-Moore model — •Raymond Wiedmann[1,2], Lea Lenke[1], Matthias Mühlhauser[1], and Kai Phillip Schmidt[1] — [1]Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany — [2]MPI-FKF, Stuttgart, Germany

The quantum phase transition between the high-field polarized phase and the low-field fracton phase with type-II fracton excitations is investigated in the two-dimensional self-dual quantum Newman-Moore model. We apply perturbative and numerical linked cluster expansions to calculate the ground-state energy per site in the thermodynamic limit revealing a level crossing at the self-dual point. In addition, high-order series expansions of the relevant low-energy gaps are determined using perturbative continuous unitary transformations indicating no gap-closing. Our results therefore predict a first-order phase transition between the low-field fracton and the high-field polarized phase at the self-dual point.

TT 66: Cryogenic Detectors

Time: Friday 9:30–11:30 Location: HSZ 304

Invited Talk TT 66.1 Fri 9:30 HSZ 304

Towards ultrasensitive calorimetric detection in superconducting quantum circuits — •Bayan Karimi[1,2], Kuan-Hsun Chiang[2], Yu-Cheng Chang[2], Danilo Nikolic[3], Joonas T. Peltonen[2], Wolfgang Belzig[3], and Jukka P. Pekola[2] — [1]QTF Centre of Excellence, Department of Physics, Faculty of Science, University of Helsinki, Finland — [2]Pico group, QTF Centre of Excellence, Department of Applied Physics, Aalto University, Finland — [3]Fachbereich Physik, Universität Konstanz, D-78467, Germany

We demonstrate experimentally an ultra-sensitive thermal detector formed of an electronic absorber coupled to a phonon bath, which reaches the ultimate noise level dictated by the fundamental thermal fluctuations [1]. A scheme of coupling a superconducting qubit to this calorimeter is presented and we conclude positively about sufficient signal-to-noise ratio (SNR) in detecting a microwave photon emitted by it [2,3,4]. Recently this scheme was applied to the thermal detection of quantum phase slips in a Josephson junction [5], and currently we are performing experiments on the proposed qubit calorimetry.

[1] J. P. Pekola and B. Karimi, Rev. Mod. Phys. 93, 041001 (2021)
[2] B. Karimi and J. P. Pekola, Phys. Rev. Lett. 124, 170601 (2020)
[3] B. Karimi, D. Nikolic, T. Tuukkanen, J. T. Peltonen, W. Belzig, and J. P. Pekola, Phys. Rev. Applied 13, 054001 (2020)
[4] J. P. Pekola and B. Karimi, Phys. Rev. X 12, 011026 (2022)
[5] E. Gumus, D. Majidi, D. Nikolic, P. Raif, B. Karimi, J. T. Peltonen, E. Scheer, J. P. Pekola, H. Courtois, W. Belzig, and C. B. Winkelmann, arXiv:2202.08726 [cond-mat.mes-hall]

TT 66.2 Fri 10:00 HSZ 304

Novel concept for a superconducting microcalorimeter with tunable gain — •Constantin Schuster, Gabriel Jülg, and Sebastian Kempf — Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Karlsruhe, Germany

Cryogenic microcalorimeters such as metallic magnetic calorimeters (MMC) or transition edge sensors (TES) are becoming a mature technology and are hence presently used in various applications requiring an excellent energy resolution. They rely on transducing the temperature rise upon the absorption of an energetic particle into a change of magnetic flux (MMC) or electrical current (TES) which is measured using a SQUID. Despite the overall great success, it turns out that the resolving power still lacks behind the fundamental limit set by fluctuations of thermal energy among different degrees of freedom of the detector. Against this background, we present a novel detector concept which may help to improve the energy resolution. It is based on the strong temperature dependence of the magnetic penetration depth of a superconductor close to its critical temperature. By embedding a properly chosen superconductor directly into the SQUID loop and using a special input circuit configuration, a change in temperature is transduced into a change in magnetic flux threading the SQUID loop. Moreover, it turns out that the temperature to flux transfer coefficient can be tuned in-situ. We present our detector concept and gauge the possible performance and energy resolution of this novel detector concept by discussing simulating results and and first experimental data.

TT 66.3 Fri 10:15 HSZ 304

Advances in microwave SQUID multiplexing of magnetic microcalorimeters — •Martin Neidig, Alexander Maatz, Felix Schuderer, Marvin Völlinger, Mathias Wegner, Stefan Wünsch, and Sebastian Kempf — Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Karlsruhe, Germany.

The excellent energy resolution, very fast signal rise time and almost ideal linear detector response over a wide energy range makes magnetic microcalorimeters (MMCs) an exceedingly attractive detector technology for applications in various fields of science. The increasing necessity to operate large-scale detector arrays consisting of thousands to millions of individual detectors inherently poses the challenge of developing a suitable multiplexing technique. The presently most promising one is microwave SQUID multiplexing. Here, each individual detector is inductively coupled to a non-hysteretic, unshunted rf-SQUID that, in turn, is inductively coupled to a superconducting microwave resonator having a unique resonance frequency. In this configuration, an actual detector event results in a change of the effective SQUID inductance and hence in the resonance frequency of the related resonator. Moreover, capacitively coupling many of such readout channels to a single transmission line ultimately allows to read out hundreds to thousands of detectors simultaneously. In this contribution, we summarize our latest developments regarding the implementation of a microwave SQUID multiplexer for MMC readout. This includes aspects regarding to microfabrication as well as device characterization using software defined radio based readout electronics.

TT 66.4 Fri 10:30 HSZ 304

Design, fabrication and characterization of magnetic microcalorimeters for radionuclide metrology within the EMPIR project PrimA-LTD — •Michael Müller, Fabienne Bauer, Ria-Helen Zühlke, Trung Duc Tran, Alex Mocanu, and Sebastian Kempf — Institute of Micro- and Nanoelectronic Systems, Karlsruhe Institute of Technology, Karlsruhe.

The EMPIR project "PrimA-LTD" aims to provide ultra-precise measurements of the decay spectra of several radionuclides to enable activity standardization for medicine and industry. As the measurements require an outstanding energy resolution and great linearity over a wide energy range, magnetic microcalorimeters (MMCs) are used as detector technology. The latter are cryogenic particle detectors that make use of a paramagnetic temperature sensor linked to a particle absorber in which the radionuclide is embedded. The sensor is biased by a magnetic field to create a temperature dependent sensor magnetization which is altered by the temperature rise upon a radioactive decay within the absorber and measured using a SQUID. To provide a flexible detector platform, we designed three optimized MMC layouts allowing for different methods of source preparation. For in-house microfabrication of the detectors, we established deposition processes for the various materials needed. This particularly includes an electroplating process for thick, highly conductive absorbers made of gold that are free-standing on stems having a diameter of only $5\,\mu$m. We summarize the detector layouts as well as the fabrication status of the detectors and discuss characterization measurements of detector prototypes.

TT 66.5 Fri 10:45 HSZ 304

Fluxon counters and velocimeters at superconducting strips — •Oleksandr Dobrovolskiy — University of Vienna, Faculty of Physics, Nanomagnetism and Magnonics, SuperSpin Laboratory

Thin strips with large critical current Ic are required for superconducting microstrip single-photon detectors (SMSPDs) [1] and Cherenkov generators/detectors of spin waves by ultra-fast moving fluxons [2]. In this regard, high Ic implies blocking of the penetration of vortices via the strip edges and their control via material and edge-barrier engineering [3]. Thus, at sufficiently large transport currents Itr, a slit at the edge of a superconducting strip acts as a gate for the vortices entering into it. These vortices form a jet, which is narrow near the slit and expands due to the repulsion of vortices as they move to the opposite edge of the strip, giving rise to a transverse voltage Vp. In my talk, I will present our experimental results on voltage kinks in the I-V curves which occur each time the number of fluxons crossing the strip is increased by one [4]. I will also dwell on the appearance of the non-monotonic Vp in MoSi strips with slits milled by FIB at various distances from the transverse voltage leads [5]. Our findings are relevant for the performance of SMSPDs and superconducting devices operated in the single-fluxon regime.

[1] Korneeva et al., PRAppl. 13, 024011 (2020)
[2] Dobrovolskiy et al., arXiv:2103.10156
[3] Budinska et al., PRAppl. 17, 034072 (2021)
[4] Bevz et al., submitted
[5] Bezuglyj et al., PRB 105, 214507 (2022)

TT 66.6 Fri 11:00 HSZ 304

Superconducting 3D-cavity architecture for microwave single-photon detection — •Yuki Nojiri[1,2], Kedar E. Honasoge[1,2], Daniil Bazulin[1,2], Florian Fesquet[1,2], Maria-Teresa Handschuh[1,2], Fabian Kronowetter[1,4], Michael Renger[1,2], Achim Marx[1], Kirill G. Fedorov[1,2], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institute, Bavarian Academy of Sciences and Humanities, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 Munich, Germany — [4]Rohde & Schwarz GmbH & Co. KG, Mühldorfstraße 15, 81671 München

Microwave single-photon detectors (SPDs) are essential quantum devices required in a large variety of quantum communication and quantum computation protocols. First microwave SPDs have been realized with the help of superconducting qubits and resonators. Here, we experimentally study an SPD design compatible with the superconducting 3D cavity architecture. We exploit the multimode nature of horseshoe aluminum cavities in combination with transmon qubits to experimentally realize efficient detection of single microwave photons. We analyze the performance of such devices and discuss possible ways to improve it.

TT 66.7 Fri 11:15 HSZ 304

Novel susceptibility thermometer for mK-temperatures based on Au:Er micro-fabricated on a copper substrate — •Nathalie Probst, Andreas Fleischmann, Andreas Reifenberger, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

There are not too many options for fast, highly sensitive and reliable thermometers for use at low and ultra-low temperatures. Here, we present a novel concept of a susceptibility thermometer based on the paramagnetic alloy Au:Er that has the potential to meet these requirements. To ensure very good thermal contact, the superconducting readout coils and the paramagnetic materials are micro fabricated on a polished copper wafer. In this concept, four planar meander-shaped niobium coils each with a width of 5μm and a total length of 20m, are arranged as a Wheatstone bridge. Two opposite coils are covered with sensor material. The inductances of the covered and uncovered coils were chosen so that the bridge is balanced at a certain temperature, as indicated by the zero detector. This temperature can be conveniently set by the erbium concentration and the design of the coils. For certain applications, this can serve as an individual fixed point for precise temperature stabilization. The imbalance due to the paramagnetic contribution of the Au:Er at different temperatures is used to establish a temperature scale by calibration with another thermometer. We will discuss the design, fabrication, function and readout of this novel susceptibility thermometer.

TT 67: Dynamics and Chaos in Many-Body Systems II (joint session DY/TT)

Time: Friday 9:30–12:30 Location: MOL 213

TT 67.1 Fri 9:30 MOL 213

Towards a more fundamental understanding of eigenstate thermalization — •Tobias Hofmann, Tobias Helbig, Ronny Thomale, and Martin Greiter — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We explore several venues how eigenstate thermalization may be understood on a more fundamental level. In particular, we report on extensive numerical work in spin systems with random interactions, where a small subsystem is subject to thermalization. We discuss possible directions towards an understanding of our numerical results.

TT 67.2 Fri 9:45 MOL 213

Spectral Response of Disorder-Free Localized Lattice Gauge Theories — •Nilotpal Chakraborty[1], Markus Heyl[1,2], Petr Karpov[1], and Roderich Moessner[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden — [2]University of Augsburg

We show that certain lattice gauge theories exhibiting disorder-free localization have a characteristic response in spatially averaged spectral functions: a few sharp peaks combined with vanishing response in the zero frequency limit. This reflects the discrete spectra of small clusters of kinetically active regions formed in such gauge theories when they fragment into spatially finite clusters in the localized phase due to the presence of static charges. We obtain the transverse component of the dynamic structure factor, which is probed by neutron scattering experiments, deep in this phase from a combination of analytical estimates and a numerical cluster expansion. We also show that local spectral functions of large finite clusters host discrete peaks whose positions agree with our analytical estimates. Further, information spreading, diagnosed by an unequal time commutator, halts due to real space fragmentation. Our results can be used to distinguish the disorder-free localized phase from conventional paramagnetic counterparts in those frustrated magnets which might realize such an emergent gauge theory.

TT 67.3 Fri 10:00 MOL 213

Chaos in the three-site Bose-Hubbard model - classical vs quantum — •Goran Nakerst[1] and Masudul Haque[1,2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, D-01187 Dresden, Germany

We consider a quantum many-body system - the Bose-Hubbard system on three sites - which has a classical limit, and which is neither strongly chaotic nor integrable but rather shows a mixture of the two types of behavior. We compare quantum measures of chaos (eigenvalue statistics and eigenvector structure) in the quantum system, with classical measures of chaos (Lyapunov exponents) in the corresponding classical system. As a function of energy and interaction strength, we demonstrate a strong overall correspondence between the two cases. In contrast to both strongly chaotic and integrable systems, the largest Lyapunov exponent is shown to be a multi-valued function of energy.

TT 67.4 Fri 10:15 MOL 213

Many-Body Dwell-time and Density of States — •Georg Maier, Carolyn Echter, Juan-Diego Urbina, and Klaus Richter — Universität Regensburg, Regensburg, Germany

Many body systems with a large number of degrees of freedom are usually described by statistical physics on the theoretical side while experiments usually relay on scattering (e.g. particle physics). Is it possible to relate scattering and statistical physics, or to measure scattering-related observables which directly relate to quantities of statistical physics? At least for single particle systems a close relation exists between the well known Wigner-Smith delay time in scattering theory and the density of states of the scattering system.

I will present a novel ansatz relating a many-body version of dwell-/Wigner-Smith delay time and many body density of states based on the famous Birman-Krein-Friedel-Loyd formula connecting scattering theory and statistical observales in the many-body context. This formalism could provide answers to a wide variety of interesting questions, e.g. can we observe the effect of interactions (or even the emergence of chaos) through the lens of the dwell-time? Another interesting point is the roll of particle statistics on dwell-time meaning e.g. does it take longer for a particle to leave a fermionic or bosonic system?. I will present our analytical and numerical results on these questions.

TT 67.5 Fri 10:30 MOL 213

Dynamical correlations and domain wall relocalisation in transverse field Ising chains — •Philippe Suchsland[1], Benoît Douçot[2], Vedika Khemani[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]LPTHE, UMR 7589, CNRS and Sorbonne Université, 75252 Paris Cedex 05, France — [3]Department of Physics, Stanford University, Stanford, California 94305, USA

We study order parameters and out-of-time-ordered correlators (OTOCs) for a wide variety of transverse field Ising chains: classical and quantum, clean and disordered, integrable and generic. The setting we consider is that of a quantum quench. We find a remarkably rich phenomenology, ranging from stable periodic to signals decaying with varying rates. This variety is due to a complex interplay of dynamical constraints (imposed by integrability and symmetry) which thermalisation is subject to. In particular, a process we term dynamical domain wall relocalisation provides a long-lived signal in the clean, integrable case, which can be degraded by the addition of disorder even without interactions. Our results shed light on a proposal to use an OTOC specifically as a local dynamical diagnostic of a quantum phase transition even when evaluated in a state with an energy density corresponding to the paramagnetic phase.

15 min. break

TT 67.6 Fri 11:00 MOL 213

Time evolution at the quantum-critical point of the sawtooth chain — •Jannis Eckseler, Florian Johannesmann, and Jürgen Schnack — Fakultät für Physik, Universität Bielefeld, Postfach 100131, D-33501 Bielefeld, Germany

It is known for the antiferromagnetic sawtooth chain with Heisenberg interactions to develop a flat band at the quantum-critical point of $J_1 = 2J_2$, where J_1 is the exchange interaction between nearest neighbors and J_2 the interaction at the base of the triangles [1]. We investigate the time evolution of several observables of the sawtooth chain, especially near that point and in particular in view of their equilibration properties. [1] J. Schulenburg, A. Honecker, J. Schnack, J. Richter, H.-J. Schmidt, Phys. Rev. Lett. 88 (2002) 167207

TT 67.7 Fri 11:15 MOL 213

Quantum Noise as a Symmetry-Breaking Field — •Paul McClarty[1], Beatriz Dias[2], Domagoj Perkovic[3], Masudul Haque[4], and Pedro Ribeiro[5] — [1]MPI PKS, Dresden, Germany — [2]TU Munich, Garching, Germany — [3]Cavendish Lab, University of Cambridge, UK — [4]TU Dresden, Germany — [5]IST, Lisbon, Portugal

We investigate the effect of quantum noise on the measurement-induced quantum phase transition in monitored random quantum circuits. Using the efficient simulability of random Clifford circuits, we find that the transition is broadened into a crossover and that the phase diagram as a function of projective measurements and noise exhibits several distinct regimes. We show that a mapping to a classical statistical mechanics problem accounts for the main features of the random circuit phase diagram. The bulk noise maps to an explicit permutation symmetry breaking coupling; this symmetry is spontaneously broken when the noise is switched off. These results have implications for the realization of entanglement transitions in noisy quantum circuits.

TT 67.8 Fri 11:30 MOL 213

Finite-size prethermal behavior at the chaos-to-integrable transition — •Johannes Dieplinger[1] and Soumya Bera[2] — [1]Institute of Theoretical Physics, University of Regensburg, D-93040 Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

We investigate the dynamics of the complex Sachdev-Ye-Kitaev model complemented with a single particle hopping term, leading to a chaos-to-integrable transition of the eigenstates. We determine the dynamics close to the transition via the density-density correlator, where we observe a prethermal plateau in the ergodic phase. This indicates a finite time localised behavior up to an interaction-dependent thermalization time scale. This time scale is quantified as $t_{th} \propto 2^{\alpha/\sqrt{\lambda}}$ as a function of the relative interaction strength λ. The results are validated by investigating the time-dependent structure of the time-evolved wave functions in the Fock space.

TT 67.9 Fri 11:45 MOL 213

Quasiparticle Description of Entanglement Growth — •Molly Gibbins, Bruno Bertini, and Adam Smith — University of Nottingham

The quasiparticle picture of entanglement is a novel way to describe a feature unique to quantum many-body systems. Recent research has found excellent agreement of this description with numeric results: a description that had been shown to hold for the general family of Rényi entanglement entropies, for different classes of quench and different geometries of the boundary across which entanglement develops.

The aim of this project is to develop a quasiparticle description of the entanglement growth in free-fermionic systems with translational invariance in both 1D and 2D. The propagation of quasiparticles across this cut will respect this translational invariance and it is expected that the entanglement generated between these particles will be in very good agreement with the exact solution for these systems.

TT 67.10 Fri 12:00 MOL 213

Excitation Transport in Molecular Aggregates with Thermal Motion — •Ritesh Pant and Sebastian Wüster — Indian institute of science education and research, Bhopal, India

Molecular aggregates can under certain conditions transport electronic excitation energy over large distances due to the long range dipole-dipole interactions. These interactions are also the characteristics of Rydberg aggregates which have been proved as the quantum simulators for molecular aggregates. An idea that naturally arises in Rydberg aggregates, is adiabatic excitation transport through atomic motion, where slow motion of the atoms combined with excitation transport can result in efficient and guided transport of the excitation from one end of an atomic chain to the other. Based on the analogy between Rydberg and Molecular aggregates, in ref. [1] we explore whether the adiabatic excitation transport can play a functional role in molecular aggregates in the absence of intra-molecular vibrations. But because the transport is partially adiabatic and because it involves transitions between non-eigenstates, it is challenging to estimate the adiabaticity of transport in molecular aggregates. Hence, in ref [2] we established a measure to quantify the adiabatic character of quantum transitions in general. Next, the effect of intramolecular vibrations is included by extending our calculation for excitation transport to an open-quantum-system technique [3].

[1] R. Pant and S. Wüster, Physical Chemistry Chemical Physics 22, 21169 (2020). [2] R. Pant, et al., https://arxiv.org/abs/2007.10707. [3] R. Pant, et al., (Manuscript in preparation)

TT 67.11 Fri 12:15 MOL 213

Tailoring the Phonon Environment of Embedded Rydberg Aggregates — •Sidharth Rammohan[1], Sebastian Wüster[1], and Alexander Eisfeld[2] — [1]IISER Bhopal, Madhya Pradesh, India — [2]MPIPKS, Dresden, Germany

State-of-the-art experiments can controllably create Rydberg atoms inside a Bose-Einstein condensate (BEC) such that the Rydberg electron orbital volume contains many neutral atoms, which can be tuned, resulting in electron-atom scattering events [1]. In my talk, I will discuss the physics of the interaction and corresponding dynamics of a single or multiple Rydberg atoms in two internal electronic states embedded inside a BEC, to assess their utility for controlled studies of decoherence and quantum simulations of excitation transport similar to photosynthetic light-harvesting. We initially developed a theoretical framework to calculate the open quantum system input parameters for a single Rydberg atom, possibly in two internal states, in BEC and then for a chain of Rydberg atoms, forming an aggregate [2]. The electron-atom interactions lead to Rydberg-BEC coupling, creating phonons in the BEC. Using the spin-boson model with the calculated parameters, we then examine the decoherence and the Non-Markovian features of a Rydberg atom in a superposition, resulting from the interaction with the environment [3]. The scenario with a single Rydberg atom is then extended to the aggregate case, allowing us to set up dynamics similar to those found in light-harvesting complexes. Ref:1. J. B. Balewski, et.al; Nature 502 664 (2013).2. S. Rammohan, et.al; PRA 103, 063307 (2021).3. S. Rammohan, et.al; PRA 104, L060202 (2021).

TT 68: Focus Session: Making Experimental Data F.A.I.R. – New Concepts for Research Data Management II (joint session O/TT)

Time: Friday 9:30–12:45 Location: WIL A317

Topical Talk TT 68.1 Fri 9:30 WIL A317

FAIRifying ARPES: a Route to Open Data & Data Analytics — •Ralph Ernstorfer[1,2], Tommaso Pincelli[1,2], Patrick R. Xian[2], Abeer Arora[2], Florian Dobener[3], Sandor Brockhauser[3], and Laurenz Rettig[2] — [1]TU Berlin, Germany — [2]Fritz-Haber-Institut Berlin, Germany — [3]HU Berlin, Germany

While angle-resolved photoemission spectroscopy (ARPES) is the most direct probe of crystals' electronic structure, the globally collected ARPES data have not been merged into an open experimental electronic structure database in equivalence to well-established atomic structure databases. We discuss a data format based on NeXus [1] as a concept for unifying the data structure for all types of photoemission experiments including time-, spin-, and time-resolved ARPES [2]. The aim is to immediately enable preprocessed data and metadata shareability according to FAIR data principles, employing existing public storage and archiving research data infrastructures such as Zenodo, OpenAIRE, and Nomad/FAIRmat. Ultimately, the multidimensional photoemission spectroscopy (MPES) format is designed to allow high-performance automated access, providing experimental databases for high-throughput material search [3]. References: [1] https://www.nexusformat.org/ [2] https://mpes.science/; https://fairmat-experimental.github.io/nexus-fairmat-proposal/ [3] R. P. Xian et al., Scientific Data 7, 442 (2020); R.P. Xian et al., Nat. Comp. Sci, in print, arXiv:2005.10210

TT 68.2 Fri 10:00 WIL A317

A FAIR data infrastucture for photoemission experiments — •Marten Wiehn[1], Tobias Eul[1], Benjamin Stadtmüller[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Recent trends toward data-driven, high-tech experimental research and the growing volumes of data associated with it show the increasing importance of comprehensive data acquisition and management. We present an automated workflow for well-described photoemission data from experiment to archive and publication. Utilizing a powerful experiment control software to capture essential metadata for each measurement enables the collection of FAIR-ready data (Findable, Accessible, Interoperable, Reusable). In addition, using an electronic lab notebook pushes our lab further toward a FAIR data infrastructure that supports researchers in their daily work.

TT 68.3 Fri 10:15 WIL A317

Multi-Dimensional Photoemission Spectroscopy: a concept for FAIR photoemission data — •Florian Dobener[1], Tommaso Pincelli[2,3], Abeer Arora[2,4], Steinn Ymir Augustsson[5], Dmytro Kutnyakhov[6], Michael Hartelt[7], Laurenz Rettig[1], Martin Aeschlimann[2], Ralph Ernstorfer[7], and Sandor Brockhauser[2,3] — [1]Department of Physics, HU Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Institut für Optik und Atomare Physik, TU Berlin, Germany — [4]FU Berlin, Fachbereich Physik, Berlin, Germany — [5]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [6]DESY, Hamburg, Germany — [7]Department of Physics and OPTIMAS, University of Kaiserslautern, Germany

The complexity and size of photoemission data is rapidly increasing as new technological breakthroughs have enabled multidimensional parallel acquisition. However, most of the community is currently using heterogeneous data formats and workflows. We propose a new data format based on NeXus, a hierarchically organized hdf5 structure. This multidimensional photoemission spectroscopy format is designed to allow high-performance automated access, enabling experimental databases for high-throughput material search. Our approach involves reaching out to the community using a website with extensive documentation of our proposed standard. As a demonstrator of the potential of our approach we present a workflow and data pipeline integrated into the NOMAD research data management solution, which provides powerful analysis and search functionalities.

TT 68.4 Fri 10:30 WIL A317

Towards an Infrastructure for FAIR Synthesis Data — •Sebastian Brückner[1,2], Andrea Albino[1], Jose Marquez[1], Florian Dobener[1], Hampus Näsström[1], Markus Scheidgen[1], Claudia Draxl[1], and Martin Albrecht[2] — [1]HU Berlin, Zum Großen Windkanal 2, 12489 Berlin — [2]IKZ Berlin, Max-Born-Straße 2, 12489 Berlin

A data infrastructure based on the FAIR (findable, accessible, interoperable and reusable) principles promises a new way of sharing and exploring data by using highly efficient data analysis and artificial intelligence tools. This also applies to data related to sample synthesis. At present, most synthesis data are not structured comprehensively or not even stored digitally but in handwritten lab books. There hardly exists any data standards in synthesis, which is in contrast to data from characterization techniques. The FAIRmat project (https://FAIRmat-NFDI.eu) is building a FAIR data infrastructure for condensed-matter physics and the chemical physics of solids. In FAIRmat's Area A, we focus on synthesis data to make sample synthesis reproducible, accelerate the development of novel materials, and make characterization data of synthesized materials assessable. Here we summarize our ongoing work and progress including: providing a general data model for synthesis which is harmonized with data from measurements and theory (ontologies); implementation of our data model in use cases and electronic laboratory notebooks; developing tools for data acquisition and analysis; data governance guidelines to enable a sustainable change of research data management at the institute/university level.

TT 68.5 Fri 10:45 WIL A317

FAIRifying Material Synthesis with the NOMAD Electronic Laboratory Notebook (ELN) — •Andrea Albino[1], Hampus Näsström[1], Florian Dobener[1], Jose Marquez Prieto[1], Lauri Himanen[1], David Sikter[1], Mohammad Nakhaee[1], Amir Golparvar[1], Sebastian Brückner[1], Martin Albrecht[2], Markus Scheidgen[1], and Claudia Draxl[1,3] — [1]Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany. — [2]Leibniz-Institut für Kristallzüchtung, Berlin, Germany. — [3]The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany.

Approaching the era of big data-driven materials science, one crucial step to collecting, describing, and sharing experimental data is the adoption of ELNs. The project FAIRmat (fairmat-nfdi.eu) is offering such tools by developing and operating the open-source software NOMAD. The NOMAD ELN aims at offering a secure environment to protect the integrity of both data and metadata, whilst also affording the flexibility to adopt new synthetic processes or changes to existing ones without recourse to further software development.

We find that to promote an early adoption, it is important to adapt to a single user's needs and workflows. An inductive approach, going from a particular set of experiments to a general description of the similarities recurring in each of them, led us to adopt a common data structure as a standard. The state-of-the-art ELN features for a synthetic process will be shown in the talk, highlighting the development of both data modeling and specific implementation solutions.

TT 68.6 Fri 11:00 WIL A317

FAIR Data Infrastructure for Computation: Classical Simulations and Multiscale Modeling — •Joseph F. Rudzinski[1,2], José M. Pizarro[1], Nathan Daelman[1], Luca M. Ghiringhelli[1], Karsten Reuter[3], Kurt Kremer[2], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [4]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena

The emergence of the (big-)data-centric techniques as a fundamental paradigm of science calls for the development of infrastructure for ensuring FAIR—findable, accessible, interoperable, reusable—data management. The FAIRmat consortium aims to build extensive infrastructure for a wide variety of materials-science data, including soft matter simulations [1], by expanding upon the success of the NOMAD Laboratory—a repository for atomistic calculations in materials science [2]. Both the large volume and heterogeneous nature of classical molecular-dynamics simulation data presents a number of distinct challenges. In this talk, we present FAIRmat's progress in developing infrastructure for molecular-dynamics simulations, including metadata for molecular topologies and tools for workflow management. We will also discuss the need for standardization of metadata schemas and ontologies within the community, and planned collaborations with other open science initiatives and software developers.

[1] Scheffler, M. et al. Nature 2022, 604, 635-642.
[2] Draxl, C.; Scheffler, M. JPhys Materials 2019, 2, 036001.

Topical Talk TT 68.7 Fri 11:15 WIL A317

Electronic Lab Notebooks in Teaching and Implications on Science — •Michael Krieger — Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

In our department, we have recently introduced Electronic Lab Notebooks (ELN) in the obligatory electronic lab course in the 4th semester of the physics curriculum. Immediate advantages for the students are obvious: all data, raw data and metadata including experiment description and experimental observations, are digitally stored at the same place. Moreover, student teams share and actively work in their group ELN with access at the university as well as at home, and script-based evaluations can be performed directly in the ELN.

The introduction of ELNs in teaching has also implications on science. Students carry their ELN experience and data competences into all research groups. There, however, modern research data management is much more complex. According to the FAIR principles, it requires structured, machine-readable data using open formats and vocabularies that meet community standards. The development of such standards is in many cases still to be done and is the core of the Nationale Forschungsdateninfrastruktur (NFDI). Here, ELNs in teaching provide a sandbox with short learning and innovation cycles for testing structured schemas. The experience helps to develop and establish sustainable and FAIR documentation of research workflows in science.

TT 68.8 Fri 11:45 WIL A317

A step towards predicting synthesis conditions of metal-organic frameworks — •Dinga Wonanke[1], Thomas Heine[2], and Christof Wöll[1] — [1]Institut für Funktionelle Grenzflächen (IFG), Karlsruher , Germany — [2]Faculty of Chemistry and Food Chemistry,Dresden, Germany

The process of synthesising metal-organic frameworks (MOFs) falls under a branch of chemistry known as reticular chemistry. Here, well defined crystalline compounds are synthesised from a well thought out design principle by linking predefined building blocks under specific conditions. Although, this approach appears to be intuitive, the synthesis of any novel MOF still follows the conventional approach that begins with a thorough literature survey to explore reagents, calculations of aliquots and finally a series of time consuming and stressful trial-and-error syntheses. Consequently, although millions of stable hypothetical MOFs with interesting properties have been predicted, only approximately 100 thousand crystal structures of MOFs currently exist in the Cambridge Structural Database (CSD). Indicating a significant bottleneck in the intelligent design of novel stable MOFs with targeted properties.

In this talk, we will present an overview of our journey to design a new machine learning algorithm for predicting the synthesis condition of existing and hypothetical MOFs. We will discuss our experiences and challenges in mining and curating the MOF subset in the CSD. Finally, we will present our new MOF database that maps every MOF to its experimental synthetic conditions.

TT 68.9 Fri 12:00 WIL A317

Deep learning surface scattering data analysis for processing large synchrotron datasets — •Vladimir Starostin, Valentin Munteanu, Linus Pithan, Alexander Gerlach, Alexander Hinderhofer, and Frank Schreiber — Institute of Applied Physics, University of Tübingen, Germany

In situ real-time surface scattering experiments such as grazing-incidence wide-angle X-ray scattering (GIWAXS) produce large amounts of data, frequently exceeding the capabilities of traditional data processing methods. Here we demonstrate an automated pipeline for the analysis of GIWAXS images, based on a machine learning architecture for object detection, designed to conform to the specifics of the scattering data [1]. Our pipeline enables real-time GIWAXS analysis and is designed to be employed at synchrotron facilities. We also present FAIR data strategies and traceable data resources from the raw data to the corresponding scientific publication and vice versa [2] including intermediate processing steps.

We demonstrate our method on real-time tracking of lead halide perovskite structure crystallization processes, which are relevant for hybrid solar cell applications. However, our approach is equally suitable for other crystalline thin-film materials by design. In general, the solution substantially accelerates the analysis process of GIWAXS images, potentially boosting the speed of scientific discoveries in material science.

[1] V. Starostin et al. *npj Comput Mater* **8**, 101 (2022)
[2] V. Starostin et al. *Synch Rad News* **13**, 31–37 (2022)

TT 68.10 Fri 12:15 WIL A317

FAIR Data Infrastructure for Computation: Mapping out the Space of Density Functionals — •Nathan Daelman[1], Joseph F. Rudzinski[1,2], José M. Pizarro[1], Luca M. Ghiringhelli[1], Miguel A. L. Marques[3], Silvana Botti[4], and Claudia Draxl[1] — [1]Institut für Physik und IRIS-Adlershof, Humboldt-Universität zu Berlin, Berlin — [2]Max-Planck-Institut für Polymer Forschung, Mainz — [3]Institut für Physik, Martin-Luther-University Halle-Wittenberg, Halle — [4]Friedrich Schiller Universität Jena, Jena

The NOMAD Laboratory [1] holds over 135 million computational results, the vast majority of which stem from density-functional theory (DFT). The platform provides adequate querying and data analytics tools (e.g., machine-learning modelling) for processing such Big Data. However, the exchange-correlation (xc) functional with which the data was generated, limits the analysis scope of most thermodynamic and kinetic properties. Here, we present a strategy rooted in semantics for extending method interoperability. We will showcase our map of the entire xc-functional space that, in the context of the FAIRmat consortium [2], is built to be widely accessible and facilitate findability. Lastly, we will discuss the integration of this xc-functionals map into the NOMAD data platform, as well as its publication in ontology format as an effort towards a community-wide vocabulary standard.

[1] C. Draxl and M. Scheffler, MRS Bulletin 43, 676-682 (2018).
[2] M. Scheffler, M. et al., Nature 604, 635-642 (2022).

TT 68.11 Fri 12:30 WIL A317

OpenSemanticLab: Towards Open Semantic Research — •Simon Stier and Matthias A. Popp — Fraunhofer ISC, Neunerplatz 2, 97082 Würzburg, Germany

In materials science, complex relationships exist between the properties of materials and their composition and processing. Therefore, digital transformation and acceleration in this domain represents a particularly important challenge. Although it is generally agreed that data must be linked by means of semantics and ontologies to form holistic data spaces, there is still a lack of suitable tools for integrating the necessary structures into the everyday work of scientists.

Fraunhofer ISC addresses this challenge with a broad-based strategy that closely links activities at all relevant levels. The goal hereby is the development towards Lab 4.0, the machine-readable documentation of scientific processes and the harmonization of data structures in accordance with international standards.

Core of the resulting OpenSource solution architecture is the central web data platform OpenSemanticLab [1] that links people (knowledge), machines (data) and algorithms (AI) equally. As an open system, this platform is easily adaptable even without programming knowledge and without losing the uniform structure. In this way, OpenSemanticLab enables us as scientists to contribute individually and yet in a standardized fashion to future digital materials research.

[1] https://github.com/OpenSemanticLab