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 infinitesimal 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 $0 \leq x \leq 1$, 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 $x \leq 0.5$, 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 potantial 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/TR288, 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 $\langle E^M \rangle = \operatorname{Tr} H^M$ 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 impor-

tant 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.