TT 9: Poster Session: Correlated Electrons

Time: Tuesday 13:30–16:00 Location: P

TT 9.1 Tue 13:30 P

Electronic Nematicity in 4f electron systems — •Mario Malcolms de Oliveira[1], Pascoal Pagliuso[2], and Eduardo Miranda[2] — [1]Max Planck Institute for Solid State Research — [2]Unicamp

In this work, we show that the interplay between the Neel order and the spin-orbit coupling present in 4f electron systems are key ingredients to give rise to the emergence of an electronic nematic state in this kind of system. Our result can shed light on the understanding of the experimental results observed for the heavy-fermion compound $CeRhIn_5$.

TT 9.2 Tue 13:30 P

Spin excitations in the fully gapped hybridized two band superconductor — •Alireza Akbari and Peter Thalmeier — Max Planck Institute for the Chemical Physics of Solids, D-01187 Dresden, Germany

In f-electron heavy fermion superconductors, the presence of a spin resonance in the inelastic magnetic response is commonly associated with an unconventional nodal gap function that is not fully symmetric. However, it appears possible that the resonance is still observed even when the low-temperature thermodynamic behavior suggests a fully gapped state. We investigate such possibility within a two-dimensional toy model of a hybridized superconductor with a fully symmetric unconventional symmetry with a different sign of the gap function on disjoint Fermi surface sheets. We compute the collective magnetic response function in the hybridized superconducting state of the two-band model and show that the appearance of the resonance is also possible for the fully gapped state.[1]
[1] A. Akbari, P. Thalmeier, Annals of Physics 428, 168433 (2021)

TT 9.3 Tue 13:30 P

Probing the electron-lattice coupling near the valence transition of $EuPd_2Si_2$ — •Jan Zimmermann, Steffi Hartmann, Bernd Wolf, Marius Peters, Cornelius Krellner, and Michael Lang — PI, SFB/TR288, Goethe Univ., Frankfurt/M., Deutschland

The thermodynamic properties of materials close to a second-order critical endpoint in strongly correlated electron systems are a field of high interest. Within the strong-coupling regime, it is expect to find cross-correlations between electronic and lattice properties like the recently proposed phenomena of critical elasticity, which implies a strong lattice softening and strongly nonlinear strain-stress relations. [1] Intermetallic compounds from the EuT_2X_2 family show various types of phase transitions such as valence- or structural instabilities that make it possible to study collective phenomena resulting from such a particularly strong coupling of electrons to phonons [2]. In this work electron lattice coupling near the second-order critical endpoint of the valence transition in $EuPd_2Si_2$ is investigated via thermodynamic methods. Recently published measurements [2] indicate the unique possibility of experimental access to the critical endpoint of the valence transition using helium gas pressure. We present measurements of thermal expansion and compressibility in a pressure range from 0 MPa up to 40 MPa and temperatures from 90 K to 210 K. Results are compared to specific heat measurements and analyzed for sample-to-sample variations.
[1] E. Gati *et al.*, Sci. Adv. **2**, e1601646 (2016)
[2] Y. Onuki *et al.*, Philosophical Magazine **97**, 3399 (2017)

TT 9.4 Tue 13:30 P

Magnetic and electronic phases of $U_2Rh_3Si_5$ — •Jannis Willwater[1], Nico Steinki[1], Dirk Menzel[1], Ricarda Reuter[1], Hiroshi Amitsuka[2], Vladimír Sechovsky[3], Michal Valiska[3], Marcelo Jaime[4], Franziska Weickert[5], and Stefan Süllow[1] — [1]TU Braunschweig, Braunschweig, Germany — [2]Hokkaido University, Sapporo, Japan — [3]Charles University, Prague, Czech Republic — [4]Los Alamos National Laboratory, Los Alamos, USA — [5]Florida State University, Tallahassee, USA

It has been demonstrated that the intermetallic uranium compound $U_2Rh_3Si_5$ exhibits a unique first-order antiferromagnetic transition accompanied by a structural transition. This was explained with the so-called bootstrapping effect. Here, we present a detailed study of the magnetic and electronic properties of this compound.

Based on the results of magnetization and magnetostriction measurements in high magnetic fields, we establish the complex magnetic phase diagram of $U_2Rh_3Si_5$ up to 60 T. For the first time, various steps in the high-field magnetization of the a axis have been observed. These effects are probably due to several metamagnetic transitions. In addition, the electrical resistivity exhibits a unique anomaly in a narrow temperature range above the Néel temperature. Since there is no associated signature in the magnetic susceptibility or the structural parameters for all three crystallographic axes, this anomaly in the resistivity cannot be caused by a magnetic, but rather by an electronic phase transition.
[1] J. Willwater et al., Phys. Rev. B **103**, 054408 (2021)

TT 9.5 Tue 13:30 P

Anisotropic magnetic and thermodynamic properties of single crystals of antiferromagnetic $CePdAl_3$ — •Vivek Kumar[1], Andreas Bauer[1], Christian Franz[2,3], Rudolf Schönmann[1], Michal Stekiel[1], Astrid Schneidewind[1], and Christian Pfleiderer[1] — [1]Physik-Department, Technische Universität München, D-85748 Garching, Germany — [2]JCNS at MLZ, FZ Jülich GmbH, Lichtenbergstr. 1, D-85747 Garching — [3]TUM at MLZ, Technische Universität München, D-85748 Garching, Germany

Recently, the class of $CeTAl_3$ (T is a transition metal) attracted considerable scientific attention when strong coupling between phonons and crystal electric field excitations was demonstrated in $CeCuAl_3$ and $CeAuAl_3$ [1,2]. Here, we report on the magnetic and thermodynamic properties of single-crystalline $CePdAl_3$ studied by means of ac susceptibility, magnetization, and specific heat measurements. The compound crystallizes in an orthorhombic crystal structure and displays antiferromagnetic order below $T_N = 5.6$ K. A strong anisotropy was observed in magnetic properties. We obtained a large electronic specific heat coefficient, $\gamma = 121$ mJ K^{-2} mol^{-1}, characteristic of heavy-fermion behavior. Field-driven magnetic transitions were detected for fields applied along the easy basal plane, which leads to a complex magnetic phase diagram.
[1] Franz *et al.*, J. Alloys Compd. **688**, 978 (2016).
[2] Čermák *et al.*, Proc. Natl. Acad. Sci. U.S.A. **116**, 6695 (2019).

TT 9.6 Tue 13:30 P

Low-Temperature Properties of the Non-Centrosymmetric Heavy-fermion Compound $CeAl_2$ — •Christian Oberleitner, Alexander Regnat, Christian Franz, Jan Spallek, Georg Benka, Michael Petrov, Marc Andreas Wilde, Andreas Bauer, and Christian Pfleiderer — Physik-Department, Technische Universitaet Muenchen, 85748 Garching, Germany

We report a comprehensive study of the non-centrosymmetric heavy-fermion compound $CeAl_2$ with $T_N = 3.8$ K. The metallurgical characterization by Laue x-ray scattering and powder x-ray diffraction shows the excellent crystalline quality, which is confirmed by very high residual-resistivity ratios (RRR). Magnetization, specific heat, torque magnetometry, resistivity, and Hall-effect measurements down to 50 mK and up to 18 T were carried out. The low-temperature measurements in the antiferromagnetic regime show complex magnetic behavior. The Hall-effect cannot be explained by a superposition of anomalous and normal Hall-effect.

TT 9.7 Tue 13:30 P

Robust hybridization gap in the Kondo insulator YbB_{12} probed by femtosecond optical spectroscopy — •Amrit raj Pokharel[1], Steinn y. Agustsson[1], Viktor v. Kabanov[2], Fumitoshi Iga[3], Toshiro Takabatake[4], Hidekazu Okamura[5], and Jure Demsar[1] — [1]JGU Mainz, Mainz, Germany — [2]Jozef Stefan Institute, Ljubljana, Slovenia — [3]Ibaraki University, Mito, Japan — [4]Hiroshima University, Higashi-Hiroshima, Japan — [5]Tokushima University, Tokushima, Japan

Carrier relaxation dynamics is susceptible to subtle changes in the low energy electronic structure. In heavy fermions the dynamics is shown to be governed by the low energy indirect gap, E_g, resulting from interplay/hybridization between localized moments and conduction band electrons. Here, carrier relaxation dynamics in a prototype Kondo insulator YbB_{12} is studied over large temperature range and over three orders of magnitude in excitation density. We utilize the intrinsic non-

linearity of dynamics to quantitatively determine microscopic parameters, such as electron-hole recombination rate. The extracted value reveals that hybridization is accompanied by a strong charge transfer from localized 4f levels. Furthermore, results suggest hybridization gap to be present up to temperatures of the order of $E_g/k_B \approx 200$ K, and is extremely robust against electronic excitation. Finally, the results imply further changes in the low energy electronic structure below 20 K, attributed to short-range antiferromagnetic correlations between the localized levels [1].
[1] A. R. Pokharel, et. al., Phys. Rev. B 103, 115134 (2021)

TT 9.8 Tue 13:30 P

Floquet renormalization group approach to the periodically driven Kondo model — •Valentin Bruch[1], Mikhail Pletyukhov[1], Herbert Schoeller[1], and Dante Kennes[1,2] — [1]Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany and JARA-FIT, 52056 Aachen — [2]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany

We study the interplay of strong correlations and coherent driving by considering the Kondo model driven by a time-periodic bias voltage. By combining a recent nonequilibrium renormalization group method with Floquet theory, we find that the coherent dressing of the driving field leads to side-replicas of the Kondo resonance in the conductance, which are not completely washed out by the decoherence induced by the driving. We show that to accurately capture the interplay of driving and strong correlations one needs to go beyond simple phenomenological pictures, which underestimate decoherence, or adiabatic approximations, highlighting the relevance of memory effects. Within our method the differential conductance shows good quantitative agreement with experimental data in the full crossover regime from weak to strong driving. In the time-resolved current and differential conductance we identify nonlinear memory effects and time scales of the relaxation to the ground state.

TT 9.9 Tue 13:30 P

Quadrature Magnetoresistance from Impeded Cyclotron Motion — •Roemer Hinlopen[1], Stijn Hinlopen[2], Jake Ayres[1], and Nigel Hussey[1,3] — [1]University of Bristol, United Kingdom — [2]Fudura B.V., Netherlands — [3]High Field Magnet Laboratory (HFML-EMFL), Netherlands

Recently, quadratic to linear magnetoresistance (MR) as a function of magnetic field has emerged as a pervasive phenomenon among strange and quantum critical metals. Examples are the antiferromagnetic quantum critical metal $BaFe_2(As,P)_2$ (1), heavy fermion $(Yb,La)Rh_2Si_2$ (2) and optimally and overdoped cuprates (Nd-)LSCO (3,4), Tl-2201 and Bi-2201 (5) as well as electron doped LCCO (6). Given the variety of Fermi surface topologies, dominant interactions and energy scales in these systems, the striking similarity of their magnetic-field response suggests some universal, but as yet unidentified, organizing principle. Here, we propose a new, simple theory to explain this phenomenology based on impeded cyclotron motion. We reproduce the quadrature form and show a high level of robustness to scattering and correlation effects. The unsaturating nature of the MR is found even in the high field limit. We predict this model also explains the magnetoresistance observed in charge density wave systems such as the dichalcogenides.
[1] Nat. Phys. 12:916-919 (2016)
[2] Physica B: Cond. Matt. 378-380:72-73 (2006)
[3] Science 361:6401 (2018)
[4] G. Grissonnanche arXiv:2011.13054 (2020)
[5] J. Ayres et al. Nature (in press)
[6] Sci. Adv. 5:5, eaav6753 (2019)

TT 9.10 Tue 13:30 P

Possible superconductivity from incoherent carriers in overdoped cuprates — •Caitlin Duffy[1], Matija Čulo[1,2], Jake Ayres[1,3], Maarten Berben[1], Yu-Te Hsu[1], Roemer Hinlopen[3], Bence Bernáth[1], and Nigel Hussey[1,3] — [1]High Field Magnet Laboratory (HFML-EMFL), Netherlands — [2]Institut za fiziku, Zagreb, Croatia — [3]University of Bristol, United Kingdom

The non-superconducting normal state of the overdoped, hole-hoped cuprates is formed of two distinct charge sectors: one coherent with quasiparticle excitations, the other incoherent and governed by non-quasiparticle Planckian dissipation (1). From $p^* = 0.19$ to the end of the superconducting dome, a decrease in the superfluid carrier density $n_s(0)$ concurrent with an increase in the Hall (coherent) carrier density $n_H(0)$ from p to $1 + p$ is found; this striking anti-correlation contradicts the expectations of conventional BCS theory (2, 3). Here, we demonstrate that in two families of cuprates - $La_{2-x}Sr_xCuO_4$ and $Tl_2Ba_2CuO_{6+\delta}$ - the loss of carriers in the coherent sector is entirely compensated for by the growth in $n_s(0)$ with decreasing p. This implies that superconductivity in the overdoped cuprates stems from the sector that displays incoherent transport properties (4).
[1] J. Ayres *et al.*, *Nature*, (in press)
[2] I. Božović *et al.*, *Nature* **536**, 309*311 (2016)
[3] C. Putzke *et al.*, *Nat. Phys.* **17**, 826 (2021)
[4] M. Čulo, C. Duffy *et al.*, *SciPost Phys.* **11**, 012 (2021)

TT 9.11 Tue 13:30 P

Emergence of a fluctuating magnetic ground state in $Mn_{1-x}Fe_xSi$ — Andreas Bauer[1], Jonas Kindervater[1], •Johanna K. Jochum[2], Wolfgang Häussler[1,2], Nicolas Martin[3], Markus Garst[4], and Christian Pfleiderer[1] — [1]Physik Department, Technische Universität München, D-85748 Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum, Technische Universität München, D85748 Garching, Germany — [3]Université Paris-Saclay, CNRS, CEA, Laboratoire Léon Brillouin, 91191 Gif-sur-Yvette, France — [4]Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, D-76131 Karlsruhe, Germany

Substitutional doping of the cubic chiral magnet MnSi results in a suppression of magnetic order and quantum critical behavior that is masked by the influence of disorder. Combining measurements of the ac susceptibility and specific heat with elastic neutron scattering and neutron resonance spin-echo spectroscopy on single-crystal $Mn_{1-x}Fe_xSi$ in zero magnetic field, we show that up to $x = 0.10$ static helimagnetic order emerges through a Brazovskii-type fluctuation-induced first-order phasetransition. For $x = 0.12$, the signatures in the susceptibility are reminiscent of helimagnetic order, while the specific heat indicates the absence of a first-order transition and neutron spectroscopy unambiguously establishes the dynamic character down to temperatures of 50 mK, suggesting a magnetic ground state that is dominated by interacting chiral fluctuations.

TT 9.12 Tue 13:30 P

Orientation dependence of the transverse-field Ising transition in $LiHoF_4$ — •Andreas Wendl[1], Heike Eisenlohr[2], Felix Rucker[1], Christopher Duvinage[1], Markus Kleinhans[1], Matthias Vojta[2], and Christian Pfleiderer[1,3,4] — [1]Physik Department, TU München, Garching, Germany — [2]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany — [3]Centre for QuantumEngineering (ZQE), TU München, Garching, Germany — [4]Munich Centre for Quantum Science and Technology (MCQST), TU München, Garching, Germany

The perhaps best understood example of a quantum critical point is the response of the dipolar Ising ferromagnet $LiHoF_4$ to a transverse field [1-3]. We report an investigation of the AC susceptibility of $LiHoF_4$ as a function of the magnetic field direction relative to the hard magnetic axis, deriving the evolution of the magnetic-phase-diagram as a function of field orientation. We discuss our findings in terms of a theoretical model taking quantiatively into account the non-Kramers nature of the Ho ions, the effects of hyperfine coupling and the presence of magnetic domains.
[1] D. Bitko et al., Phys. Rev. Lett. **77**, 940 (1996)
[2] H. M. Rønnow et al., Science **308**, 389 (2005)
[3] P. B. Chakraborty et al., Phys. Rev. B **70**, 144411 (2004)

TT 9.13 Tue 13:30 P

Pump-Probe AC Susceptibility of $LiHo_xY_{1-x}F_4$ (x = 4.5 %) — •Michael Lampl, Andreas Wendl, Markus Kleinhans, Laura Stapf, Marc A. Wilde, and Christian Pfleiderer — Physik-Department Technical University of Munich, Garching, Germany

$LiHoF_4$ under a transverse magnetic field exhibits one of the best understood examples of a quantum critical point. Substitutional doping of Ho with non-magnetic Yttrium may be used to study the effects of disorder [1]. In the highly diluted system $LiHo_xY_{1-x}F_4$ (x = 4.5 %), investigated in our study, the nature of the ground state is still unresolved [2]. To explore the ground state properties of this system, multiple studies employed so-called pump-probe susceptibility measurements [3-5]. We revisit this question and report a study of the pump-probe susceptibility as a function temperature and field orientation, covering a wide parameter range.
[1] J. P. Gingras and P. Henelius, J. Phys.: Conf. Ser. **320**, 012001

(2011).
[2] J. A. Quilliam *et al.*, Phys. Rev. Lett. **101**, 187204 (2008).
[3] S. Ghosh *et al.*, Science **296**, 2195 (2002)
[4] M. A. Schmidt *et al.*, Proc. Natl. Acad. Sci. USA **111**, 3689 (2014)
[5] D. M. Silevitch *et al.*, Nature Com. **10**, 4001 (2019)

TT 9.14 Tue 13:30 P

Gross-Neveu-Heisenberg criticality from competing nematic and antiferromagnetic orders in bilayer graphene — Shouryya Ray and •Lukas Janssen — TU Dresden, Germany

The nature of the ground state of Bernal-stacked bilayer graphene has received significant attention in the last ten years, but still represents an open problem both experimentally and theoretically. The two most promising scenarios feature nematic and antiferromagnetic orders. We have studied theoretically the competition between these two orders, revealing that they allow a coexistence phase characterized by both nematicity and antiferromagnetism. This leads to interesting quantum phase transitions, including weak first-order transitions and continuous Gross-Neveu-type transitions that feature emergent Lorentz invariance. Implications for experiments in bilayer graphene are discussed.

[1] S. Ray, L. Janssen, Phys. Rev. B 104, 045101 (2021)

TT 9.15 Tue 13:30 P

Terahertz conductivity of heavy-fermion systems from time-resolved spectroscopy — •Chia-Jung Yang[1], Shovon Pal[1], Farzaneh Zamani[2], Kristin Kliemt[3], Cornelius Krellner[3], Oliver Stockert[4], Hilbert v. Löhneysen[5], Johann Kroha[2], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]University of Bonn, Germany — [3]Goethe-University Frankfurt, Germany — [4]MPI CPfS Dresden, Germany — [5]KIT Karlsruhe, Germany

Ultrafast terahertz (THz) spectroscopy has recently been introduced as a novel tool to investigate the quasiparticle dynamics across the quantum phase transition in heavy-fermion compounds [1,2]. The incident THz pulse with a spectral range of 0.1–3 THz creates collective intraband excitations within the heavy band as well as resonant interband transitions between the hybridizing heavy and light parts of the conduction band. The former leaves the heavy quasiparticles intact, while the latter breaks the Kondo-singlet and leads to a time-delayed echo-like response [1,2]. In this contribution, we expand our investigations towards the individual transport properties of strongly and weakly correlated electrons. We utilize the time-resolved, phase-sensitive THz spectroscopy to separate two types of excitations and derive the associated optical conductivity. We find that the Kondo-singlet-breaking interband transitions do not create a conventional metallic Drude peak, while the Kondo-retaining intraband excitations yield the Drude response as expected [3].

[1] C. Wetli *et al.*, Nat. Phys. **14**, 1103 (2018)
[2] S. Pal *et al.*, PRL **122**, 096401 (2019)
[3] C.-J. Yang *et al.*, PRR **2**, 033296 (2020)

TT 9.16 Tue 13:30 P

Multifractality at the spin quantum Hall (class C) transition — •Martin Puschmann[1], Daniel Hernangómez-Pérez[2], Bruno Lang[3], Soumya Bera[4], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany — [2]Department of Molecular Chemistry and Material Science, Weizmann Institute of Science, Rehovot 7610001, Israel — [3]IMACM and Institute of Applied Computer Science, Bergische Universität Wuppertal, D-42119 Wuppertal, Germany — [4]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

Recent analytical work on the integer quantum Hall transition (class A) predicts a parabolic dependency of the exponents τ_q, that describe the system-size scaling of wavefunction moments $|\psi|^{2q}$. [1] The prediction has raised attention, since it contradicts numerical observations [2]. The arguments of [1] rely on conformal invariance and therefore are believed to carry over also to class C. Since in class C corrections to scaling are under control, it provides an excellent laboratory for testing the salient concepts numerically. Thus motivated, we investigate τ_q in class C and eliminate subleading powers guided by finite-size corrections of distribution functions. Thereby, we demonstrate unambiguously the presence of quartic terms in τ_q [3], inconsistent with the predicted parabolic shape but in agreement with [4].

[1] M. R. Zirnbauer, Nucl. Phys. B 941, 458 (2019)
[2] e.g. K. Slevin and T. Ohtsuki, Phys. Rev. B 80, 041304 (2009)
[3] M. Puschmann et al., Phys. Rev. B 103, 235167 (2021)
[4] J. Karcher et al., arXiv:2107.06414

TT 9.17 Tue 13:30 P

Spin-phonon interaction and tunnel splitting in single-molecule magnets — •Kilian Irländer[1], Jürgen Schnack[1], and Heinz-Jürgen Schmidt[2] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany — [2]Fachbereich Physik, Universität Osnabrück, Osnabrück D-49069, Germany

Quantum tunneling of the magnetization is a phenomenon that impedes the use of small anisotropic spin systems for storage purposes even at the lowest temperatures. Phonons, usually considered for temperature dependent relaxation of magnetization over the anisotropy barrier, also contribute to magnetization tunneling for integer spin quantum numbers. In this context, it is not viable to consider phonons perturbatively but to treat spins and phonons on the same footing by performing quantum calculations of a Hamiltonian where the single-ion anisotropy tensors are coupled to harmonic oscillators. We demonstrate the ability of phonons to induce a tunnel splitting of the ground doublet which then reduces the required bistability due to Landau-Zener tunneling of the magnetization [Phys. Rev. B 102, 054407]. We also present the unexpected observation that certain spin-phonon Hamiltonians are robust against the opening of a tunneling gap, even for strong spin-phonon coupling. The key to understanding this phenomenon is provided by an underlying supersymmetry that involves both spin and phonon degrees of freedom.

[1] Eur. Phys. J. B 94, 68

TT 9.18 Tue 13:30 P

NMR investigations of the 2D Heisenberg system CuPOF under pressure — •F. Bärtl[1,2], D. Opherden[1,2], C. P. Landee[3], S. Molatta[1,2], J. Wosnitza[1,2], M. Baenitz[4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA — [4]MPI for Chemical Physics of Solids, Dresden, Germany

The molecular-based material CuPOF ($[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$) is an excellent realization of a two-dimensional square-lattice quantum $S = 1/2$ Heisenberg antiferromagnet, with an intralayer exchange coupling $J/k_B = 6.8$ K and an interlayer coupling $J' \approx 10^{-4}J$. Previously reported nuclear magnetic resonance (NMR) data revealed a low-temperature transition to commensurate antiferromagnetic (AF) quasistatic long-range order (LRO), with a preceding crossover from isotropic Heisenberg to anisotropic XY behaviour. We present further NMR studies of the low-temperature correlations in magnetic fields up to 7 T and temperatures down to 0.3 K. The application of hydrostatic pressure up to 10 kbar leads to a change of the interlayer coupling and, therefore, the magnetic correlations in the critical regime. The transition regime is probed by ^{1}H and ^{31}P spectroscopy and relaxometry, revealing a non-monotonic change of T_N with increasing pressure. The commensurate AF LRO below T_N still persists at high pressures, as revealed by a splitting of the ^{1}H NMR lines, stemming from the broken symmetry of the local spin polarizations in the LRO regime.

TT 9.19 Tue 13:30 P

Magnetic heat transport and strong magneto-elastic coupling in the frustrated spin-chain mineral linarite — •Matthias Gillig[1,2], Xiaochen Hong[1,3], Piyush Sakrikar[4], Gaël Bastien[5], Anja Wolter[1], Leonie Heinze[6], Satoshi Nishimoto[1,2], Bernd Büchner[1,2], and Christian Hess[1,3] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Bergische Universität Wuppertal, Germany — [4]IISER Mohali, India — [5]Charles University, Prague, Czech Republic — [6]TU Braunschweig, Germany

Motivated by recent theoretical results predicting a finite thermal Drude weight in frustrated spin chains, we have studied the thermal conductivity of the mineral Linarite $PbCuSO_4(OH)_2$ at low temperature. In this well-studied material the Cu-ions form a s=1/2 spin chain with competing FM nearest-neighbor and AFM next-nearest-neighbor interactions, creating a magnetically frustrated system which orders below $T_N = 2.8$ K in an elliptical spiral ground state. In a magnetic field along the spin chain, other magnetically ordered phases can be induced. Our results reveal that the thermal conductivity κ in zero field is dominated by a phononic contribution. As a function of magnetic field κ shows a peculiar non-monotonic behavior. Whenever the magnetic field value approaches a critical field, κ is highly suppressed. This trend can be explained by magnetic fluctuations which are expected near a phase boundary and which reduce thermal conductivity due to

strong phonon scattering. Furthermore, a magnon thermal transport channel was verified in the spiral phase.

TT 9.20 Tue 13:30 P

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

Magnetic frustration attracts great interest since it leads to exotic magnetic orders like spin liquids, spin glasses and spin ice all associated with the geometric frustration of magnetic spins. We report vibrating coil magnetometry down to mK temperatures [2] of the frustrated system $Gd_2Ga_5O_{12}$[1,3,4]. Based on the magnetization measured in a spherical sample for field along $\langle 100\rangle$, $\langle 110\rangle$, and $\langle 111\rangle$ we track the magnetic phase diagram as a function of field orientation in great detail.

[1] P. P. Deen textitet al., PRB **91**, 014419 (2015)
[2] S. Legl *et al.*, RSI **81**, 043911 (2010)
[3] S. Hov. *et al.*, JMMM **455-456**, 15-18 (1980)
[4] P. Schiffer and A.P. Ramirez *et al.*, PRL **2500**, 73 (1994)

TT 9.21 Tue 13:30 P

Low-temperature investigation of thermodynamic properties on the spin-liquid candidate system $PbCuTe_2O_6$ in various finite fields. — •Paul Eibisch[1], Christian Thurn[1], Ulrich Tutsch[1], Arif Ata[1], Abanoub R. N. Hanna[2,3], A. T. M. Nazmul Islam[3], Shravani Chillal[3], Bella Lake[3], Bernd Wolf[1], and Michael Lang[1] — [1]PI Goethe-University Frankfurt — [2]IFKP, TU Berlin — [3]HZ Berlin

The quantum spin liquid is an exotic state of magnetic systems which shows no long-range order down to $T = 0\,\mathrm{K}$ but instead exhibits persistent spin dynamics with highly entangled spins fluctuating between various degenerate configurations. A favourable route to realize this state is to use geometric frustrations for instance in 2D materials where the spins interact on top of a kagome lattice. In this study we present low-temperature thermodynamic measurements in various fields on the spin-liquid candidate system $PbCuTe_2O_6$ showing a Hyper-kagome lattice, a 3D adaptation of the 2D kagome lattice. First investigations on polycrystalline samples supported the spin-liquid character [1], whereas more recent studies revealed an even more exotic behaviour i.e. a ferroelectric phase transition around $T = 1\,\mathrm{K}$ together with a diverging thermal Grüneisen parameter, indicating proximity to a quantum critical point [2]. Here we show that the magnetic Grüneisen parameter diverges as well, supporting zero-field-quantum-critical behaviour. Further focus of our investigations lies on the field dependence of the ferroelectric transition.

[1] S.Chillal *et al.*, Nat. Commun. **11**, 2348 (2020)
[2] C.Thrun *et al.*, arXiv:2103.17175

TT 9.22 Tue 13:30 P

Nesting instability of gapless U(1) spin liquids with spinon Fermi pockets in two dimensions — •Wilhelm Krüger and Lukas Janssen — TU Dresden, 01062 Dresden, Germany

Quantum spin liquids are exotic states of matter that may be realized in frustrated quantum magnets and feature fractionalized excitations and emergent gauge fields. Here, we consider a gapless U(1) spin liquid with spinon Fermi pockets in two spatial dimensions. Such a state appears to be the most promising candidate to describe the exotic field-induced behavior observed in numerical simulations of the antiferromagnetic Kitaev honeycomb model. A similar such state may also be responsible for the recently-reported quantum oscillations of the thermal conductivity in the field-induced quantum paramagnetic phase of α-$RuCl_3$. We consider the regime close to a Lifshitz transition, at which the spinon Fermi pockets shrink to small circles around high-symmetry points in the Brillouin zone. By employing renormalization group and mean-field arguments, we demonstrate that interactions lead to a gap opening in the spinon spectrum at low temperatures, which can be understood as a nesting instability of the spinon Fermi surface. This leads to proliferation of monopole operators of the emergent U(1) gauge field and confinement of spinons. While signatures of fractionalization may be observable at finite temperatures, the gapless U(1) spin liquid state with nested spinon Fermi pockets is ultimately unstable at low temperatures towards a conventional long-range-ordered ground state, such as a valence bond solid. Implications for Kitaev materials in external magnetic fields are discussed.

TT 9.23 Tue 13:30 P

Magnetostriction in the J-K-Γ-model on the honeycomb lattice — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Using the numerical linked cluster expansion (NLCE) [1], we investigate thermodynamic and magnetoelastic properties of the J-K-Γ spin-$\frac{1}{2}$ model on the honeycomb lattice in the presence of a magnetic field $\vec{B}$, for field orientations both in-plane and out-of-plane.

Apart from the specific heat and the magnetization, we focus in particular on the linear magnetostriction coefficient $\lambda(B,T)$. As a prime result and based on expansions up to order $\sim \mathcal{O}(11)$, we find clear indications for a field-induced transition in $\lambda(B,T)$.

Employing exchange parameters as proposed for $\alpha - RuCl_3$, our results are very similar to recently observed experimental data [2] on this proximate quantum spin-liquid candidate material.

[1] M. Rigol et al., Phys. Rev. Lett. 97, 187202 (2006)
[2] S. Gass et al., Phys. Rev. B 101, 245158 (2020)

TT 9.24 Tue 13:30 P

Glass-like transitions in the frustrated charge system θ-(BEDT-TTF)$_2$CsM(SCN)$_4$ (M = Cs and Co) revealed by thermal expansion measurements — •Yohei Saito[1], Tatjana Thomas[1], Steffi Hartmann[1], Tim Thyzel[1], Yassine Agarmani[1], Hungwei Sun[1], Jens Müller[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2], Hiroshi Yamamoto[3], and Michael Lang[1] — [1]Institute of Physics, Goethe University Frankfurt, Frankfurt (M), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan — [3]Institute for Molecular Science, Okazaki, Japan

Geometrical frustration causes degenerate states, giving rise to intriguing quantum phenomena such as a spin liquid. In addition to a frustrated spin system, a frustrated charge system is proposed in organic conductors called θ-type BEDT-TTF salts. It is expected that charge ordering is suppressed and is possibly replaced by a charge glass state. In organic charge-ordered salts, the charge order transition accompanies a structural transition. Therefore, investigating their elastic properties is of fundamental interest. We performed thermal expansion measurements on θ-(BEDT-TTF)$_2$CsM(SCN)$_4$ (M = Cs and Co) that does not show charge ordering. The thermal expansion coefficient 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. We also found another glassy transition at 120-130 K for both salts where the development of a superlattice structure was reported. These results point to the importance of the lattice degrees of freedom in the frustrated charge system.

TT 9.25 Tue 13:30 P

The one-dimensional Long-Range Falikov-Kimball Model: Thermal Phase Transition and Disorder-Free Localisation — •Thomas Hodson[1], Josef Willsher[2], and Johannes Knolle[2,3,1] — [1]Blackett Laboratory, Imperial College London, London SW72AZ, United Kingdom — [2]Department of Physics TQM, Technische Universit at Munchen,James-Franck-Strasse 1, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Disorder or interactions can turn metals into insulators. One of the simplest settings to study this physics is given by the FK model, which describes itinerant fermions interacting with a classical Ising background field. Despite the translational invariance of the model, inhomogenous configurations of the background field give rise to effective disorder physics which lead to a rich phase diagram in two (or more) dimensions with finite temperature charge density wave (CDW) transitions and interaction-tuned Anderson versus Mott localized phases. Here, we propose a generalised FK model in one dimension with long-range interactions which shows a similarly rich phase diagram. We use an exact Markov Chain Monte Carlo method to map the phase diagram and compute the energy resolved localisation properties of the fermions. We compare the behaviour of this transitionally invariant model to an Anderson model of uncorrelated binary disorder about a background CDW field which confirms that the fermionic sector only fully localizes for very large system sizes.

TT 9.26 Tue 13:30 P

Anisotropic Magnetoresistance in LAO/STO nanostructures — •Mithun S Prasad[1] and Georg Schmidt[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120 Halle, Germany — [2]Interdisziplinäres

Zentrum für Meterialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Straße 4, D-06120 Halle, Germany

The high-mobility two-dimensional electron gas (2DEG) confined at the interface LaAlO3 (LAO) and SrTiO3 (STO) provides new opportunities to explore Nanoelectronic devices. In our group, we have developed an industry-compatible Nanopatterning technique [1] for the LAO/STO interface. Recent studies on this interface have revealed that at low temperature the current is confined to filaments which are linked to structural domain walls in the STO[2] with drastic consequences for example for the temperature dependence of local transport properties [3]. We have investigated magneto-transport in nanostructures having a different crystalline orientation with respect to the lattice. Our experiments show that not only the resistance but also the magnetoresistance varies with orientation. The magnetoresistance can even change sign strongly supporting the model of filamentary charge transport. The angle of orientation of the domain walls can lead to various localization effects on the application of magnetic fields which can explain the anisotropy found in our experiments.

[1] M. Z. Minhas et.al, AIP Advances 6, 035002 (2016)
[2] Kalisky et.al, Nat. Mat. 12, 1091-1095 (2013)
[3] M. Z. Minhas et.al, Sci. Rep. 7, 5215(2017)

TT 9.27 Tue 13:30 P

Anisotropic metamagnetism in trilayer ruthenate $Sr_4Ru_3O_{10}$ — •Izidor Benedičič[1], Masahiro Naritsuka[1], Luke C. Rhodes[1], Rosalba Fittipaldi[2], Veronica Granata[3], Christopher Trainer[1], Antonio Vecchione[2], and Peter Wahl[1] — [1]School of Physics and Astronomy, University of St Andrews, North Haugh. St Andrews, Fife KY16 9SS, United Kingdom — [2]CNR-SPIN, UOS Salerno, Via Giovanni Paolo II 132, I-84084, Fisciano, Italy — [3]Dipartimento di Fisica "E.R.Caianiello", Universita di Salerno, I-84084 Fisciano, Salerno,Italy

The ground state of metamagnetic materials can be precisely controlled by application of magnetic field, making them exciting candidates for spintronic applications. In itinerant metamagnets, such as trilayer ruthenate $Sr_4Ru_3O_{10}$, understanding their electronic structure is crucial for successful manipulation and tuning of their magnetic properties. I will show measurements using quasiparticle interference imaging in a low temperature scanning tunneling microscope to study the electronic structure of $Sr_4Ru_3O_{10}$ in magnetic field. We find a strongly anisotropic response to the in-plane field, suggesting an unusually strong effect of the orthorhombic distortion on the electronic structure. Using DFT calculations, we can model the QPI signal and find the Fermi surface dominated by bands of spin-minority character, putting constraints on theories for the origin of the metamagnetic transition.

TT 9.28 Tue 13:30 P

Real-space cluster dynamical mean-field theory: Center focused extrapolation on the one- and two particle level — Marcel Klett[1], •Nils Wentzell[2], Thomas Schaefer[1], Fedor Simkovic[3], Olivier Parcollet[2], Sabine Andergassen[4], and Philipp Hansmann[5] — [1]Theory of strongly correlated quantum matter, Max Planck Institute for Solid State Research, Stuttgart — [2]Center for Computational Quantum Physics, Flatiron institute, NYC — [3]College de France, Paris — [4]Institut fuer Theoretische Physik and Center for Quantum Science, University Tuebingen — [5]Institut für Theoretische Physik, Friedrich-Alexander-University Erlangen-Nuernberg

We revisit the cellular dynamical mean-field theory (CDMFT) for the single band Hubbard model on the square lattice at half filling, reaching real-space cluster sizes of up to 9 x 9 sites. Using benchmarks against direct lattice diagrammatic Monte Carlo at high temperature, we show that the self-energy obtained from a cluster center focused extrapolation converges faster with the cluster size than the periodization schemes previously introduced in the literature. The same benchmark also shows that the cluster spin susceptibility can be extrapolated to the exact result at large cluster size, even though its spatial extension is larger than the cluster size.

We acknowledge financial support from the Deutsche Forschungsgemeinschaft (DFG) through ZUK 63 and Project No. AN 815/6-1

TT 9.29 Tue 13:30 P

Spectral function of the Hubbard model using cluster perturbation theory — •Nicklas Enenkel[1], Peter Schmitteckert[2], and Markus Garst[1] — [1]Karlsruher Institut für Technologie, Karlsruhe, Deutschland — [2]HQS - Quantum Simulations, Karlsruhe, Deutschland

The spectral function of the single band Hubbard model is calculated as part of a benchmark study using cluster perturbation theory (CPT). Within the framework of CPT, the Green function of a certain cluster of sites is first calculated numerically exactly, and, in a second step, the hopping of electrons between the clusters is treated in perturbation theory. Practically, however, a numerically reliable determination of the cluster Green function poses a challenge, and we compare various numerical approaches involving exact diagonalization, Chebychev expansion and equation of motion techniques. Results for the full spectral function are presented and discussed for the one- and two-dimensional Hubbard model.

TT 9.30 Tue 13:30 P

Four-point functions on the real-frequency axis – A spectral representation and its numerical evaluation — •Fabian B. Kugler[1,2], Seung-Sup B. Lee[2], and Jan von Delft[2] — [1]Rutgers University, USA — [2]LMU Munich, Germany

We present spectral representations for multipoint correlation functions for each of three widely-used formalisms: the imaginary-frequency Matsubara formalism and the real-frequency zero-temperature as well as Keldysh formalisms. The spectral representations separate information on the system's dynamics, encoded in universal partial spectral functions, from the correlators' analytical properties, encoded in formalism-dependent convolution kernels [1]. We present numerical results for the four-point vertex of the Anderson impurity model, obtained by a novel numerical renormalization group scheme [2]. In the imaginary-frequency Matsubara formalism, our approach allows us to compute the vertex at arbitrarily low temperatures and to follow the complete crossover from strongly interacting particles to weakly interacting quasiparticles. In the real-frequency Keldysh formalism, we first benchmark our method against analytical results at weak and infinitely strong interaction. Then, we consider the dynamical mean-field solution of the Hubbard model to reveal the rich real-frequency structure of the vertex in the metal-insulator coexistence regime.

[1] F. B. Kugler, S.-S. B. Lee, J. von Delft, arXiv:2101.00707, accepted in PRX
[2] S.-S. B. Lee, F. B. Kugler, J. von Delft, arXiv:2101.00708, accepted in PRX

TT 9.31 Tue 13:30 P

Accuracy of the typicality approach using Chebyshev polynomials — Florian Gayk[1], Heinz-Jürgen Schmidt[2], Andreas Honecker[3], Jürgen Schnack[4], and •Henrik Schlüter[4] — [1]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany — [2]Fachbereich Physik, Universität Osnabrück, Osnabrück D-49069, Germany — [3]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, Cergy-Pontoise Cedex F-95302 — [4]Fakultät für Physik, Universität Bielefeld, Postfach 100131, Bielefeld D-33501, Germany

Trace estimators allow us to approximate thermodynamic equilibrium observables with astonishing accuracy. A prominent representative is the finite-temperature Lanczos method (FTLM) which relies on a Krylov space expansion of the exponential describing the Boltzmann weights. Here we report investigations of an alternative approach which employs Chebyshev polynomials [1]. This method turns out to be also very accurate in general, but shows systematic inaccuracies at low temper- atures that can be traced back to an improper behaviour of the approximated density of states with and without smoothing kernel. Applications to archetypical quantum spin systems are discussed as examples.

[1] H. Schlüter, F. Gayk, H.-J. Schmidt, A. Honecker and J. Schnack, Zeitschrift für Naturforschung A, 2021 https://doi.org/10.1515/zna-2021-0116

TT 9.32 Tue 13:30 P

Inhomogeneous mean-field approach to collective excitations near the superfluid–Mott glass transition — •Martin Puschmann[1,2], João C. Getelina[1,3], José A. Hoyos[3], and Thomas Vojta[1] — [1]Department of Physics, Missouri University of Science and Technology, Rolla, Missouri, 65409, USA — [2]Institute of Theoretical Physics, University of Regensburg, D-93040, Regensburg, Germany — [3]Instituto de Física de São Carlos, Universidade de São Paulo, C.P. 369, São Carlos, São Paulo, 13560-970, Brazil

We develop an inhomogeneous quantum mean-field approach to the

behavior of collective excitations across the superfluid–Mott glass transition in two dimensions, complementing recent quantum Monte Carlo simulations [1,2]. In quadratic approximation, the Goldstone (phase) and Higgs (amplitude) modes completely decouple. Each is described by a disordered Bogoliubov Hamiltonian which can be solved by an inhomogeneous multi-mode Bogoliubov transformation. We find that the Higgs mode is spatially localized in both phases. The corresponding scalar spectral function shows a broad peak that is noncritical in the sense that its peak frequency does not soften but remains nonzero across the quantum phase transition. In contrast, the lowest-energy Goldstone mode delocalizes in the superfluid phase, leading to a zero-frequency spectral peak. We compare these findings to both the results of the quantum Monte Carlo simulations and the general knowledge on localization of bosonic excitations. We also show first results for three-dimensional systems.

[1] M. Puschmann et al., Phys. Rev. Lett. 125 (2020), 027002
[2] M. Puschmann et al., Ann. Phys. (2021), 168526

TT 9.33 Tue 13:30 P

Applications of real-space truncated unity functional RG — •Jonas B. Hauck[1], Carsten Honerkamp[2], and Dante M. Kennes[1,3] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen, 52074 Aachen,Germany and JARA - Fundamentals of Future Information Technology — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany and JARA - Fundamentals of Future Information Technology — [3]Max Planck Institute for the Structure and Dynamics of Matter and Center for Free Electron Laser Science, 22761 Hamburg, Germany

The discovery of superconductivity in a quasicrystalline material and its approximants lead to a plethora of theoretical predictions. Calculations in such systems are however computationally very heavy, rendering numerical verification of these hypotheses difficult. To resolve this issue we developed a real-space version of the truncated unity functional renormalization group. In this talk I will present this method and discuss its possible use when combining it with the momentum space TUfRG. I will give a short introduction into the derivation, the implementation and showcase the predictive power of the method by presenting our investigation of a penrose quasicrystal and the chiral edge modes in a $d + id$ superconductor.

TT 9.34 Tue 13:30 P

Tracking the footprints of spin fluctuations: a multi-method, multi-messenger study of the two-dimensional Hubbard model — •T. Schäfer[1], N. Wentzell[2], F. Šimkovic[3,4], Y.-Y. He[2], C. Hille[5], M. Klett[1], C. Eckhardt[6], B. Arzhang[7], V. Harkov[8], F.-M. Le Régent[4], A. Kirsch[4], Y. Wang[9], A. J. Kim[10], E. Kozik[10], E. A. Stepanov[8], A. Kauch[6], S. Andergassen[5], P. Hansmann[11], D. Rohe[12], Y. Vilk[9], J. P. F. LeBlanc[7], S. Zhang[2], A.-M. S. Tremblay[9], M. Ferrero[3,4], O. Parcollet[2], and A. Georges[2,3,4] — [1]MPI-FKF, Stuttgart — [2]CCQ, Flatiron Institute, New York — [3]Collège de France, Paris — [4]École Polytechnique, Palaiseau — [5]Universität Tübingen — [6]TU Wien — [7]Memorial University of Newfoundland — [8]University of Hamburg — [9]Université de Sherbrooke — [10]King's College London — [11]University of Erlangen-Nuremberg — [12]Forschungszentrum Juelich GmbH

This work represents an extensive multi-method, multi-messenger assessment of the wealth of computational methods that have been developed in recent years to determine the physical properties of the Hubbard model, the most fundamental model for electronic correlations, in two spatial dimensions. These methods range from simple mean-field theory to cutting-edge quantum-field theoretical approaches as dynamical mean field theory and its extensions. Each of these methods is compared to two numerically exact benchmarks and the role of magnetic fluctuations as well as their implications on the theory of metallic materials with strong magnetic correlations are elucidated.

TT 9.35 Tue 13:30 P

Enhancement of paring in asymmetric Hubbard ladder model — •Anas Abdelwahab, Gökmen Polat, and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Germany

We investigate a ladder system with two inequivalent legs, namely two legs with two different Hubbard interaction and two different intra-leg hopping terms. We use exact diagonalization and the density matrix renormalization group method to determine ground-state properties of this system at half-filling and at various doping. We found strong enhancement of pairing correlations of dopped ladders at some ranges of model parameters. We discuss the behaviors of charge, spin and pairing correlations.

TT 9.36 Tue 13:30 P

Orientational order parameters for arbitrary quantum systems* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The concept of quantum-mechanical nematic order, which is important in systems such as superconductors, is based on an analogy to classical liquid crystals, where order parameters are obtained through orientational expansions [1]. We generalize this method to quantum mechanics based on an expansion of Wigner functions [2]. This provides a systematic framework for the derivation of quantum order parameters, which unifies all known types of quantum orientational order into one framework and has a natural connection to the classical case. The formalism recovers the standard definitions for spin systems. For Fermi liquids, the formalism reveals the nonequivalence of various definitions of the order parameter used in the literature.

Funded by the Deutsche Forschungsgemeinschaft (DFG) - WI 4170/3-1

[1] M. te Vrugt, R. Wittkowski, AIP Adv. 10, 035106 (2020)
[2] M. te Vrugt, R. Wittkowski, Ann. Phys. (Berl.) 532, 2000266 (2020)

TT 9.37 Tue 13:30 P

Electronic transport in molecular junctions: The generalized Kadanoff-Baym ansatz with initial contact and correlations — •Riku Tuovinen[1], Robert van Leeuwen[2], Enrico Perfetto[3], and Gianluca Stefanucci[3] — [1]University of Helsinki, Finland — [2]University of Jyväskylä, Finland — [3]Università di Roma Tor Vergata, Italy

The generalized Kadanoff-Baym ansatz (GKBA) offers a computationally inexpensive approach to simulate out-of-equilibrium quantum systems within the framework of nonequilibrium Green's functions. For finite systems, the limitation of neglecting initial correlations in the conventional GKBA approach has recently been overcome [1]. However, in the context of quantum transport, the contacted nature of the initial state, i.e., a junction connected to bulk leads, requires a further extension of the GKBA approach. In this work, we lay down a GKBA scheme that includes initial correlations in a partition-free setting [2]. In practice, this means that the equilibration of the initially correlated and contacted molecular junction can be separated from the real-time evolution. The information about the contacted initial state is included in the out-of-equilibrium calculation via explicit evaluation of the memory integral for the embedding self-energy, which can be performed without affecting the computational scaling with the simulation time and system size. We demonstrate the developed method in carbon-based molecular junctions.

[1] D. Karlsson et al., Phys. Rev. B 98, 115148 (2018)
[2] R. Tuovinen et al., J. Chem. Phys. 154, 094104 (2021)

TT 9.38 Tue 13:30 P

Luttinger liquids with inhomogeneous interactions — Sebastian Huber[1] and •Marcus Kollar[2] — [1]Theoretical Solid State Physics, Ludwig-Maximilians-University, Munich, Germany; current address: Institute for Solid-State Physics, TU Wien, Austria — [2]Theoretical Physics III, University of Augsburg, Germany

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

[1] S. Huber, M. Kollar, Phys. Rev. Research 2, 043336 (2020)

TT 9.39 Tue 13:30 P

RPA as exact high-density limit of 1D correlated electrons — •Klaus Morawetz[1,2], Vinod Ashokan[3], Renu Bala[4], and Kare Narain Pathak[5] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — [3]Department of Physics, Dr. B.R. Ambedkar NationalInstitute of Technology, Jalandhar (Punjab)

- 144 011, India — [4]Centre for Advanced Study in Physics, Panjab University, 160014 Chandigarh, India — [5]Department of Physics, MCM DAV College for Women, 160036 Chandigarh, India

It is shown that in d-dimensional systems, the vertex corrections beyond the random phase approximation (RPA) or GW approximation scales with the power $d-\beta-\alpha$ of the Fermi momentum if the relation between Fermi energy and Fermi momentum is $\epsilon_{\mathrm{f}} \sim p_{\mathrm{f}}^{\beta}$ and the interacting potential possesses a momentum-power-law of $\sim p^{-\alpha}$. The condition $d < \beta + \alpha$ specifies systems where RPA is exact in the high-density limit. The one-dimensional structure factor is calculated analytically and the ground-state energy is presented exactly in the high-density and Coulomb limit. The proposed high-density expansion agrees with diffusive Monte Carlo simulations which we performed for this purpose.

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

TT 9.40 Tue 13:30 P

Quantum friction in the hydrodynamic model — •Kunmin Wu, Thomas Schmidt, and María Farias — Campus Limpertsberg, University of Luxembourg Faculty of Science, Technology and Medicine 162 A, avenue de la Faïencerie L-1511 Luxembourg

We study the phenomenon of quantum friction in a system consisting of a polarizable atom moving at a constant speed parallel to a metallic plate. The plate is described using a charged hydrodynamic model for the electrons. This model featuring long-range, instantaneous interactions is appropriate for graphene or a clean metal in a temperature range where scattering due to Coulomb interactions dominates over the scattering of electron by impurities. We find that a quantum friction force between the atom and the metal surface exists even in the absence of intrinsic damping in the plate, but that it only starts once the velocity of the atom exceeds the effective speed of sound in the plate. We argue that this condition can be fulfilled most easily in metals with nearly empty or nearly filled bands. We make quantitative predictions for the friction force to the second and fourth order in the atomic polarizability, and show that the threshold behavior persists to all orders of the perturbation theory.

TT 9.41 Tue 13:30 P

Dicke transition in open many-body systems determined by fluctuation effects — •Alla Bezvershenko[1], Catalin-Mihai Halati[2], Ameneh Sheikhan[2], Corinna Kollath[2], and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [2]Physikalisches Institut, University of Bonn, Nussallee 12, 53115 Bonn, Germany

We develop an approach to describe the Dicke transition of interacting many-particle systems strongly coupled to the light of a lossy cavity. A mean-field approach is combined with a perturbative treatment of fluctuations beyond mean-field, which becomes exact in the thermodynamic limit. Fluctuations are crucial to determine the mixed state character of the transition and to unravel universal properties of the emerging self-organized states. A rate equation is used to calculate an effective temperature. We validate our results by comparing to time-dependent matrix-product-state calculations.

TT 9.42 Tue 13:30 P

Dynamical quantum phase transitions in a chiral p-wave superconductor upon chemical potential quenches — •Yuto Shibata[1,2], Chitra Ramasubramanian[2], and Aline Ramires[1] — [1]Condensed Matter Theory Group, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]Institute for Theoretical Physics, ETH Zürich, 8093 Zürich, Switzerland

Dynamical quantum phase transitions (DQPTs) have been shown useful to identify non-trivial topology of quantum systems [1,2]. However, most of the preceding works do not incorporate self-consistency conditions for order parameters, which leads to periodic DQPTs.

Here, we study the dynamics of a two-dimensional chiral p-wave superconductor upon a quantum quench in the sign of the chemical potential within the BCS weak-coupling limit. We solve the BdG equations using fourth-order Runge-Kutta methods self-consistently and observe the phase of order parameter persistently oscillates sinusoidally in time after the quench. Despite the imposition of self-consistent conditions, periodic DQPTs are observed. These are identified as cusps in Loschmidt echo and accompanied by simultaneous creation of topological defects in the Pancharatnam geometric phase over curves in momentum space. We also discuss the robustness of the persistent phase oscillation against deformation of the Fermi surface and introduction of asymmetry to the chemical potential quenches.

[1] M. Heyl, Rep. Prog. Phys. **81**, 054001 (2018).
[2] N. Fläschner *et al.*, Nature Physics **14**, 265-268 (2018).

TT 9.43 Tue 13:30 P

Localization dynamics in a centrally coupled system — •Sebastian Wenderoth[1], Nathan Ng[2], Michael Kolodrubetz[3], Eran Rabani[2], and Michael Thoss[1] — [1]University of Freiburg, Freiburg, Germany — [2]University of California, Berkeley, USA — [3]University of Texas, Dallas, USA

In recent years, locally interacting system with static disorder, such as e.g. a random-field Ising chain with nearest neighbor interactions, received much attention because they can exhibit many-body localization. Many-body localized systems fail to equilibrate locally under unitary time evolution due to the absence of transport and the emergence of quasi-local integrals of motions, and thus, retain information about the initial state in local observables.

In our work, we explore the dynamics of a spin chain with a local antiferromagnetic interaction, and non-local spin-flip interactions induced by coupling of the spins to a central d-level system (qudit). We employ the multilayer multiconfiguration time-dependent Hartree approach [2,3] to simulate the dynamics of moderately large spin chains in a numerically exact way. Using this approach, we examine dynamical properties of the spin chain and the qudit, with particular focus on the question whether the system retains information about the initial state in local observables.

[1] A. Pal *et al.*, Phys. Rev. B **82**, 174411 (2010)
[2] H. Wang *et al.*, J. Chem. Phys. **119**, 1289 (2003)
[3] O. Vendrell *et al.*, J. Chem. Phys. **134**, 044135 (2011)