TT 21: Correlated Electrons: Poster Session

In case the presenters cannot be present at their posters for the full duration of the poster session, they are kindly requested to leave a note at their poster indicating when they will be available for discussion.

Time: Wednesday 15:00–18:00 Location: P1

TT 21.1 Wed 15:00 P1

Single crystal growth and characterization of $CeCoIn_5$ and $GdCoIn_5$ — •Leonard Essich, Anja Philipp, Alexej Kraiker, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main

The family of 115 rare-earth compounds $RTIn_5$ (T = Co, Rh, Ir) with tetragonal crystal structure received growing attention over the past decades. Low-temperature phenomenologies associated with the strong correlations of the 4f-electrons of the rare-earth element and the quasi-two-dimensionality of the Fermi surface such as spin and valence fluctuations [1], heavy fermions [2], and anisotropic superconductivity [3] are observed for the Ce-based compounds. The $GdTIn_5$ series show magnetic ordering of local 4f-moments with a reduced interplane coupling for $GdCoIn_5$ [3].

In this contribution, we show our results of the self-flux growth of $CeCoIn_5$ and $GdCoIn_5$ single crystals. The crystallographic orientation was determined using microscopy and Laue X-ray diffraction along with the characterization by powder X-ray diffraction, magnetization, specific-heat and specific-resistivity measurements for both compounds.

[1] D. Betancourth et al., JMMM **375**, 744 (2015)
[2] Y. Onuki et al., J. Phys. Soc. Jpn. **71**, 162 (2002)
[3] J.I. Facio et al., PRB **91**, 014409 (2015)

TT 21.2 Wed 15:00 P1

Single crystal growth and characterization of $Eu(Pd_{1-x}Au_x)_2Si_2$ — •Robert Möller, Marius Peters, Cornelius Krellner, and Kristin Kliemt — Physikalisches Institut, Goethe-Universität Frankfurt, Germany

In a general phase diagram for Eu compounds [1], the intermediate valent $EuPd_2Si_2$, T_V ~ 150 K, is located very close, but slightly at the high-pressure side of a second order critical endpoint [2]. The analysis of polycrystalline samples of $Eu(Pd_{1-x}Au_x)_2Si_2$ revealed that in this series a critical endpoint can be found which separates the region of continuous from first order transitions. It was shown that the valence state of the material can be tuned via Au substitution and that for x between 0.05 and 0.2 the transition becomes a first order phase transition [3]. In this contribution, we present the Czochralski growth and the characterization of $Eu(Pd_{1-x}Au_x)_2Si_2$ single crystals. Using magnetization and heat capacity measurements, we study the changes in the nature of the phase transition in detail.

[1] Y. Onuki et al., Philosophical Magazine 97, 3399 (2017)
[2] B. Batlogg et al., in: Wachter, Boppart (eds.): Valence Instabilities, North-Holland publishing company (1982)
[3] C. U. Segre et al., Physical Review Letters 49, 1947 (1982)

TT 21.3 Wed 15:00 P1

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

The study of collective phenomena raising from enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both, electronic and lattice-degrees of freedom. One system providing such a strongly coupled phase transition is $EuPd_2Si_2$ crystallizing in the $ThCr_2Si_2$ structure type. Because of the the high vapor pressure of Eu, high-quality single crystals of EuT_2X_2-compounds are very challenging to grow in larger size. One way to prevent Eu from evaporating out of the melt, is growing the crystals in argon overpressure. In this contribution, we present the crystal growth of $EuPd_2Si_2$ single crystals with a 20 bar Czochralski-furnace as well as the commissioning of a 150 bar high-pressure furnace which will provide the possibility of both the growth by the Czochralski and the Bridgman method.

TT 21.4 Wed 15:00 P1

$YbIn_{1-x}Ag_xCu_4$: single crystal growth and characterisation — •Michelle Ocker, Bereket Ghebretinsae, Kristin Kliemt und Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

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

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

TT 21.5 Wed 15:00 P1

Elastoresistance of $Eu_2T_2P_2$ (T=Fe, Ru, Co) systems close to a collapsed tetragonal phase transition — •Teslin Rose Thomas[1], N. S. Sangeetha[1], Thanh Duc Nguyen[2], Julian Reusch[2], Marius Peters[2], Kristin Kliemt[2], Cornelius Krellner[2], and Anna E. Böhmer[1] — [1]Lehrstuhl für Experimentalphysik IV, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum — [2]Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main

Manipulation of the properties of materials by applying anisotropic strain is an increasingly common method used in the study of correlated electron materials. In particular, the nematic state of several unconventional superconductors has been studied intensively using elastoresistance as a probing tool. In the current project, we employ elastoresistance to study the state close to the uncollapsed to collapsed-tetragonal transitions in $Eu_2T_2P_2$ (T=Fe, Ru, Co) and $CaCo_2As_2$ 122 systems. In contrast to investigations of nematicity, where the response to uniaxial strain is studied, we apply bi-axial strain which is by symmetry well suited. The corresponding elastoresistance is compared for the different compounds and at different temperatures. The results are then compared with the temperature and pressure dependence of lattice constants, which show the tetragonal collapse.

We acknowledge support from the German Research Foundation (DFG) under CRC/TRR 288 (Project A02).

TT 21.6 Wed 15:00 P1

Valence fluctuations and structural collapse in Eu-based phosphides EuT_2P_2 — Marius Peters[1], •Kristin Kliemt[1], Julian Dominik Reusch[1], Thanh Duc Nguyen[1], Franziska Walther[1], Michael Merz[2], Gaston Garbarino[3], Sofia Michaela Souliou[2], Matthieu Le Tacon[2], Amir-Abbas Haghighirad[2], and Cornelius Krellner[1] — [1]Kristall- und Materiallabor, Physikalisches Institut, Goethe University Frankfurt, Max-von-Laue-Str. 1, D-60438 Frankfurt — [2]Karlsruhe Institute of Technology, Institute for Quantum Materials and Technology, D-76021 Karlsruhe — [3]European Synchrotron Radiation Facility (ESRF), F-38043 Grenoble

Studies of enhanced coupling between electrons and phonons is focussed on materials exhibiting phase transitions involving both electronic and lattice degrees of freedom. Europium in intermetallic systems can exhibit different magnetic ground states: If the ground state is Eu^{2+}, the system shows long range magnetic order; if the ground state is Eu^{3+}, no magnetic order is observed. Instead, valence fluctuations occur in intermediate valent states [1].

In this work, we report on the structural collapse in divalent europium systems EuT_2P_2 (T = Fe, Co, Ru), which is connected to a change of europium's ground state by using single crystal diffractometry at pressures up to 15 GPa at 15 K and 300 K. Additionally, we show characterizations of the electronic and structural contributions to valence fluctuations in $EuNi_2P_2$.

[1] Y. Onuki et al., Philos. Mag. 97, 3399 (2017).

TT 21.7 Wed 15:00 P1

Crystal growth and characterization of $LnCo_2P_2$ (Ln = Pr, Nd) — •Fabian Fiedler, Marius Peters, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/Main, Germany

In condensed matter systems, the 4f-driven temperature scales at the surfaces of correlated materials have increasingly come into the focus of research efforts. Here, we present the crystal growth of $LnCo_2P_2$ (Ln = Pr, Nd) in tin flux and the corresponding structural/physical characterization.
Using temperatures of up to 1400°C and a vertical temperature-gradient, we optimized the growth, resulting in large high-quality single crystals, allowing for physical characterization, especially by means of thermodynamic measurements and angle-resolved photoemission spectroscopy.
The structural and chemical characterization is performed by X-ray powder diffractometry, energy-dispersive X-ray spectroscopy and the Laue-method.
Magnetic properties of these systems, arising from the combination of the 4f-moments of Ln^{3+}-ions and the 3d-moments of Co^{3+}, are investigated by measurements of magnetization, heat capacity and resistivity.

TT 21.8 Wed 15:00 P1

Growth and characterization of $KFe_{1-x}Ag_{1+y}Ch_2$ — •Jutta Püttmann, N. S. Sangeetha, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Universitätstraße 150, 44801 Bochum

Iron-based 122-compounds with $ThCr_2Si_2$ structure have been intensely studied over the past decades. K-based chalcogenides, such as $K_xFe_{2-\delta}Se_2$ have attracted attention due to their high-temperature superconductivity, their strong electronic correlations, and their complex microstructure dominated by vacancies and phase separation. Recently, $KFe_{0.8}Ag_{1.2}Te_2$ has been found to provide the possibility to study an iron chalcogenide 122-systems without vacancies on the alkali site and to investigate a superstructure in the Fe/Ag plane with an interesting magnetic and nematic ordering [1, 2].

The growth of K-based single crystals is challenging due to the high vapor pressure and reactivity of potassium. We developed a new, affordable and efficient growth technique using containers made from high-temperature resistant stainless steel that can be sealed without any air-exposure of the starting materials. The growth of $KFe_{1-x}Ag_{1+y}Ch_2$-crystals by self-flux was optimized with respect to the starting material composition. The obtained crystals were characterized by EDX and XRD. The XRD patterns were analyzed for signs of superstructure in the Fe/Ag plane. Additionally, low-temperature measurements were carried out to confirm the magnetic transitions.
[1] Yu Song et al., Phys. Rev. Lett. 122, 087201 (2019)
[2] Yu Song et al. Phys. Rev. Lett. 123, 247205 (2019)

TT 21.9 Wed 15:00 P1

Classical Ising-like dipolar antiferromagnet $DyScO_3$ with slow spin dynamics — •Nikita Andriushin[1], Stanislav Nikitin[2,3], and Andrey Podlesnyak[4] — [1]TU Dresden, Germany — [2]MPI CPfS, Dresden, Germany — [3]PSI, Villigen, Switzerland — [4]ORNL, Tennessee, USA

The usual timescale of the spin flip process in common magnetic systems is femto- to picoseconds. In this work we show with the help of both AC and DC magnetization measurements and classical Monte-Carlo calculations that the spin dynamics in $DyScO_3$ can be slowed down to milliseconds and further. The orthorhombic $DyScO_3$ has a large uniaxial anisotropy caused by the strong crystalline electric field (CFT), which freezes magnetic moments below a certain temperature. Large anisotropy and long-range dipolar interaction result in an Ising-like antiferromagnetic ordering with critical temperature $T_C = 3.14$ K. Magnetization and susceptibility measurements revealed a magnetization relaxation on a timescale of minutes, which is unexpected for an antiferromagnet. As a classical approach for modeling Ising-like spin systems, the Monte-Carlo calculations with Metropolis algorithm were used. Our calculations, taking into account the dipole-dipole interaction energy, comprehensively reproduce the observed magnetic behavior, correctly predict the ground state, critical temperature and capture slow magnetization dynamics.

TT 21.10 Wed 15:00 P1

Hierarchical equations of motion approach to open quantum dynamics: Matrix product state formulation in twin space — •Yaling Ke[1], Raffaele Borrelli[2], and Michael Thoss[1] — [1]Institute of Physics, Albert-Ludwig University Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]DISAFA, Università di Torino, I-10095 Grugliasco, Italy

The hierarchical equations of motion (HEOM) is a numerically exact approach to studying open quantum dynamics with strong non-perturbative and non-Markovian system-environment interactions at finite temperatures. Although considerable progress has been made over the past few decades to extend the applicability of the HEOM approach, the numerical cost is still very expensive for reasonably large systems.

In this contribution, we present the twin-space formulation of the HEOM approach in combination with the matrix product state representation for an open quantum system coupled to a hybrid fermionic and bosonic environment. The key ideas are a reformulation of a set of differential equations for the auxiliary density matrices into a time-dependent Schroedinger-like equation for an augmented multi-dimensional wave function as well as its tensor decomposition into a product of low-rank matrices. The new approach facilitates accurate simulations of non-equilibrium quantum dynamics in larger and more complex open quantum systems with both factorized and correlated initial condition.

TT 21.11 Wed 15:00 P1

Quantum criticality of $2k_F$ density wave order in two-dimensional metals — •Lukas Debbeler and Walter Metzner — Max Planck Institute for Solid State Research

We analyze the quantum critical point at the transition towards incommensurate charge or spin density wave order with a $2k_F$ wave vector that connects a single pair of hot spots on the Fermi surface. Perturbative renormalization group (RG) calculations confirm non-Fermi liquid behavior with anomalous frequency scaling and renormalization of the Fermi surface in proximity to the hot spots. Employing a functional RG approach we treat frequency and momentum dependence as well as fermionic and bosonic degrees of freedom on equal footing. This approach does not lead to a self consistent solution with a peak of the static polarization function at the $2k_F$-vector. We explore the possibility of a self consistent quantum critical solution via a scaling ansatz.

TT 21.12 Wed 15:00 P1

Field dependence of the low-energy magnon modes and a spin-cholesteric phase in $Sr_3Fe_2O_7$ — •Nikolai Pavlovskii[1], Yuliia Tymoshenko[1], Darren C. Peets[1], Alexandre Ivanov[2], Jacques Ollivier[2], Bernhard Keimer[3], and Dmytro Inosov[1] — [1]TU Dresden, Germany — [2]ILL, Grenoble, France — [3]MPI for Solid State Research, Stuttgart, Germany

We systematically studied low-energy magnon excitations in the helimagnetically ordered bilayer perovskite $Sr_3Fe_2O_7$. The magnetic ground state was previously believed to be characterized with a single-q magnetic order parameter that results from a frustration of exchange interactions, resulting in two types of equivalent helimagnetic domains. Our present results suggest that it could be instead a double-q state. Our elastic neutron-scattering measurements in a magnetic field applied along one of the (110) crystal directions further reveal an additional phase transition within the magnetic phase, associated with the destruction of long-range order along the direction orthogonal to the field, leading to an unusual spin-cholesteric magnetic phase that breaks both chiral symmetry and translational symmetry along only one of the crystal directions. In the orthogonal direction, we observe only short-range quasielastic spin dynamics. Across the transition from the magnetically ordered to the spin-cholesteric phase, these slow spin fluctuations fill in the spin gap in the spin-wave spectrum, as we can see in the high-resolution inelastic neutron-scattering spectra, and ultimately dominate the low-energy magnetic excitation spectrum after the long-range magnetic order is destroyed.

TT 21.13 Wed 15:00 P1

Crystal Growth and Characterization of $ZrFe_4Si_2$ — •Katharina M. Zoch, Isabel Reiser, Alexander Bodach, Kristin Kliemt, and Cornelius Krellner — Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

The $ZrFe_4Si_2$-structure consists of edge-linked Fe-tetrahedra along the crystallographic c-direction. This type of arrangement is prone to show frustration and low dimensional fluctuations. First results on polycrystalline samples indicate that $ZrFe_4Si_2$ displays some sort of weak

magnetic order, for an Fe-based compound, unusual low temperatures as well as deviant behavior in specific heat and resistivity compared to normal metals [1,2]. To investigate these features further, we are in need of single crystals. The crystal growth is a challenging subject. The compound is strongly peritectic melting and its elements are reactive with common crucible materials. Crystal growth experiments utilizing the Czochralski methods were performed, and the structure as well as magnetic, thermodynamic and electrical transport properties of the material were analyzed.

[1] M. O. Ajeesh et al., Phys. Rev. B, **102**, 184403 (2020)
[2] K. Weber, PhD thesis Technische Universität Dresden (2017)

TT 21.14 Wed 15:00 P1

Magnetic properties of monocrystalline euchroite $Cu_2(AsO_4)(OH)_3(H_2O)$ — •Yannis Hilgers, Leonie Heinze, Dirk Menzel, and Stefan Süllow — IPKM, TU Braunschweig, Braunschweig, Germany

Previous studies of magnetic susceptibility and magnetisation on a natural polycrystalline sample of euchroite ($Cu_2(AsO_4)(OH)_3(H_2O)$) suggested that euchroite may be understood as a representation of a delta spin chain and exhibits a spin gap of about 50 K. In order to test this notion, we have performed a corresponding study on a monocrystalline sample, determining these properties along the three crystallographic axes. Magnetic susceptibility from 2 K to 300 K and magnetisation for magnetic fields up to 5 T were measured on a natural monocrystalline sample, previously characterized for crystallinity by Laue diffraction, of euchroite. From our data, we establish Curie-Weiss temperatures $\Theta_{CW,a}$ = -150(20) K, $\Theta_{CW,b}$ = -140(10) K, $\Theta_{CW,c}$ = -140(10) K, significantly larger in value than Θ_{CW} = -50 K by Kikuchi et al. Moreover, we find that at low temperatures, magnetic susceptibility exhibits a spin gap, and a residual magnetisation at low temperatures can be understood in terms of about 1 % free magnetic impurity (S = 1/2) moments. Fitting a Brillouin-function to the magnetisation data with S = 1/2 results in saturation magnetisations of $M_{s,a}$ = 89,2(2,1) emu mol^{-1}, $M_{s,b}$ = 94,0(1,7) emu mol^{-1}, $M_{s,c}$ = 108,2(5,8) emu mol^{-1}. From this, the minimal length l_{min} of the delta spin chain segments can be estimated to l_{min} = 350(50) Å. Altogether, our data are consistent with euchroite as a delta spin chain material with a spin gap of about 50 K.

TT 21.15 Wed 15:00 P1

Bond-directional nearest-neighbor excitations in the proximate Kitaev spin liquid Na_2IrO_3 probed by RIXS — •Marco Magnaterra[1], Alessandro Revelli[1], Karolin Hopfer[1], Christoph Sahle[2], Marco Moretti Sala[3], Giulio Monaco[4], Jan Attig[5], Ciarán Hickey[5], Anton Jesche[6], Philipp Gegenwart[6], Simon Trebst[5], Paul H. M. van Loosdrecht[1], Jeroen van den Brink[7], and Markus Grüninger[1] — [1]II. Physikal. Inst., Universität zu Köln — [2]ESRF, Grenoble, France — [3]Dip. di Fisica, Politecnico di Milano, Italy — [4]Dip. di Fisica, Università di Padova, Italy — [5]Inst. für Theo. Physik, Universität zu Köln — [6]Exp. Physics VI, University of Augsburg — [7]Inst. for Theo. Solid State Physics, IFW Dresden

The Kitaev model hosts a spin-liquid ground state with Majorana fermion excitations. It is based on bond-directional exchange, i.e. Ising-like interactions that couple different spin components on different bonds. In Na_2IrO_3, resonant inelastic x-ray scattering (RIXS) revealed fingerprints of Kitaev physics in the magnetic excitations [1]. In fact, the RIXS intensity shows a sinusoidal **q** dependence that proves the nearest-neighbor or single-bond character of the excitations. We report on refined RIXS measurements where we exploit the polarization dependence of the different spin channels and the **q** dependence of the different bonds to demonstrate the direct connection between spin component and bond direction. Our results establish the bond-directional nearest-neighbor character of magnetic excitations in Na_2IrO_3.

[1] A. Revelli *et al.*, Phys. Rev. Research 2, 043094 (2020).

TT 21.16 Wed 15:00 P1

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

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

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

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

TT 21.17 Wed 15:00 P1

Berry Phases of Vison Transport in $\mathbb{Z}_2$ Topological Ordered States from Exact Fermion-Flux Lattice Dualities — Chuan Chen[1,2], •Peng Rao[2], and Sodemann Inti[2,3] — [1]Institute for Advanced Study, Tsinghua University, 100084 Beijing, China — [2]Max-Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Institut für Theoretische Physik, Universität Leipzig, 04103 Leipzig, Germany

We develop an exact map of all states and operators from 2D lattices of spins-1/2 into lattices of fermions and bosons with mutual semionic statistical interaction that goes beyond previous dualities of $\mathbb{Z}_2$ lattice gauge theories because it does not rely on imposing local conservation laws and captures the motion of 'charges' and 'fluxes' on equal footing. This map allows to explicitly compute the Berry phases for the transport of fluxes in symmetry enriched topologically ordered states that can be either chiral, non-chiral, abelian or non-abelian, and whose numerical complexity reduces to diagonalizing free-fermion Hamiltonians. Among other results, we establish numerically the conditions under which the Majorana-carrying flux excitation in Ising-Topologically-Ordered states enriched by translations acquires 0 or π phase when moving around a single plaquette.

TT 21.18 Wed 15:00 P1

Linked cluster expansions for a perturbed topological phase — •Viktor Kott, Matthias Mühlhauser, and Kai Phillip Schmidt — Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

We investigate the robustness of Kitaev's toric code in a uniform magnetic field on several two-dimensional lattices by perturbative linked cluster expansions using a full graph decomposition. In particular, the full graph decomposition allows to correctly take into account the non-trivial mutual exchange statistics of the anyonic elementary excitations. This allows us to calculate the ground-state energy and excitation energies of the topological phase which are then used to study the quantum phase transitions out of the topologically ordered phase as a function of the field direction.

TT 21.19 Wed 15:00 P1

Linked-cluster expansions for Rydberg atom arrays on the Kagome lattice — •Antonia Duft, Matthias Mühlhauser, Patrick Adelhardt, and Kai Phillip Schmidt — Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Deutschland

We investigate a model of hardcore bosons on the links of a Kagome lattice subject to a long-range decaying van-der-Waals interaction. This model is known to be the relevant microscopic description of Rydberg atom arrays excited by a detuned laser field which has been realized in experiments recently. We apply high-order linked cluster expansions about different limits to investigate the quantum phase diagram. One particular interest is to find further evidence for the proposed topological phase in this quantum platform.

TT 21.20 Wed 15:00 P1

Fractal quantum criticality in the Newman-Moore model in a transverse field investigated by linked cluster expansions — •Raymond Wiedmann, Matthias Mühlhauser, and Kai Phillip Schmidt — Friedrich-Alexander-Universität, Erlangen-Nürnberg, Germany

The zero-temperature phase transition in the two-dimensional self-dual quantum Newman-Moore model is investigated using perturbative linked cluster expansions. The model exhibits type-II fracton excitations that have a highly restricted mobility on the lattice. High-order series expansions of the energy gap for different quasi-particle sectors as well as the vacuum energy are calculated using perturbative continuous unitary transformations and matrix perturbation theory, respectively. Our results indicate a first-order phase transition between the fractal

phase and the polarized phase at the self-dual point in the model.

TT 21.21 Wed 15:00 P1

Improved EPR spectroscopy on single molecular magnets — •Michael Schulze[1], Daniel Schroller[1], Gheorghe Taran[1], Eufemio Pineda[3], Mario Ruben[2], Christoph Sürgers[1], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut, KIT, Karlsruhe — [2]Institut für Nanotechnologie, KIT, Karlsruhe — [3]Departamento de Química, Universidad de Panamá, Panama City

The quantum nature and large magnetic anisotropies in lanthanide-based single molecular magnets (SMMs) provides potential for interesting applications in quantum computing and information storage. The development of the micro-SQUID technique provides a tool for high-resolution magnetization measurements of SMM single crystals from the mK-range up to several Kelvin. EPR spectroscopy, where different spin states are excited by resonant absorption of radiofrequency radiation, serves as a powerful extension of the micro-SQUID technique to gain further insight into the magnetic properties of SMMs. This project strives to improve various features of this combined setup, such as higher coupling strengths, better thermalization, and coherent spin manipulation of SMMs.

TT 21.22 Wed 15:00 P1

Electrical read out of the nuclear spin and implementation of quantum algorithms on Tb_2Pc_3 triple decker — •Luca Kosche[1], Franck Balestro[2], Mario Ruben[3,4,5], and Wolfgang Wernsdorfer[1,2,3,4] — [1]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), Karlsruhe — [2]CNRS, Institut Néel, Univ. Grenoble Alpes, France — [3]Institute of Nanotechnology (INT), KIT — [4]Institute for Quantum Materials and Technology (IQMT), KIT — [5]Centre Européen de Sciences Quantiques (CESQ) , Strasbourg Cedex, France

Single-molecular magnets (SMMs) have emerged as an excellent link between the two disciplines of spintronics and molecular electronics. Their ultimate small size, excellent single spin characteristics, and long coherence times at low temperatures make them promising candidates for fundamental quantum operations. In this project we investigate spin-transistors comprising a SMM trapped in a nanometer sized gap coupled to a back gate thereby forming a quantum dot. The gap is achieved by electromigration of a gold constriction. Low-noise electrical transport measurements enable the read out of the four nuclear spin states of a single terbium ion in a $TbPc_2$ double decker. First quantum algorithms, most importantly the Grover's algorithm, have been implemented on this system. Recent measurements of more complex multi-state systems such as the Tb_2Pc_3 triple decker showed that the interactions between the two terbium nuclear spins can be detected. Here we pursue to use the increased Hilbert space dimension of coupled molecular spins for more complex quantum algorithms.

TT 21.23 Wed 15:00 P1

Synthesis, structure and property investigations of low-dimensional magnetism in double perovskite variants — •Anastasiia Smerechuk, Sabine Wurmehl, Bernd Büchner, and Ryan Morrow — Leibniz Institute for Solid-State and Materials Research, IFW-Dresden, 01069 Dresden, Germany

For many years perovskites in various modifications have been occupying a significant place in solid-state physics. The main feature of these materials is a large number of possible permutations of the structure. Although perovskites are mostly three-dimensional materials, low-dimensional magnetism can also be achieved in the special case. Current research is focused on two different approaches for that purpose. Experiments with the substitution of various compounds in double perovskites with Cu^{2+} were conducted at ambient and high pressure to acquire the magnetic interactions on a square lattice. Also, our research was concentrated on defect double perovskites, where vacancies have been ordered along with the ordering of cations. Then the hexagonal phases of perovskite can be transformed into triangular frustrated two-dimensional magnets. New inorganic transition metal oxides were synthesized. The crystallographic and magnetometry data will be discussed in detail in the poster.

TT 21.24 Wed 15:00 P1

Electronic properties of strongly correlated ruthenates — •Neda Riahisamani and Eva Pavarini — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425, Germany

We study the electronic properties of strongly correlated ruthenates by using the LDA+DMFT method. We construct materials-specific models for the t_{2g} bands via maximally localized Wannier functions. We solve the DMFT quantum impurity problem by adopting as solver the weak coupling continuous-time Quantum Monte Carlo approach, in the implementation of Refs. [1, 2, 3]. General trends will be discussed.

[1] E. Gorelov, M.Karolak, T. O. Wehling, F. Lechermann, A. I. Lichtenstein, E. Pavarini, Phys. Rev. Lett. **104**, 226401 (2010)
[2] G. Zhang, E. Gorelov, E. Sarvestani, E. Pavarini, Phys. Rev. Lett. **116**, 106402 (2016)
[3] E. Sarvestani, G. Zhang, E. Gorelov, E. Pavarini, Phys. Rev. B **97**, 085141 (2018)

TT 21.25 Wed 15:00 P1

Magnetic quantum oscillations in the molecular conductor κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl near and away from the Mott transition — •Shamil Erkenov[1,2], Sebastian Oberbauer[1,2], Vladimir Zverev[3], Werner Biberacher[1], Natalia Kushch[1], and Mark Kartsovnik[1] — [1]Walther-Meißner-Institut, Garching, Germany — [2]Technische Universität München, Garching, Germany — [3]Chernoglovka, Russia

Magnetic quantum oscillations have been extensively used for exploring correlated-electron materials near various correlation-driven instabilities of the normal metallic state. Applying this technique to the quasi-two-dimensional bandwidth-controlled Mott insulator κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl, we have recently disclosed several anomalies in the behavior of the effective mass and scattering rate, apparently inconsistent with theoretical predictions. For clarifying the role of the proximity to the Mott transition in these anomalies it is instructive to track their evolution in a broader range of the phase diagram, both very close to and far away from the metal-insulator phase boundary. To this end, we have measured quantum oscillations of magnetoresistance in the pressure interval 20 to 1000 MPa, which drives the system from the very edge of stability of the metallic phase to a "good metal" region of the phase diagram by means of the conducting bandwidth variation. We have also studied the possibility of changing the balance between the charge correlations and magnetic interactions governing the insulating instability by applying a strong magnetic field.

TT 21.26 Wed 15:00 P1

Building Blocks for Cluster Mott Insulators — •Vaishnavi Jayakumar and Ciarán Hickey — Institute for Theoretical Physics, University of Cologne, Germany

The Hubbard model provides a rich playground for investigating the physics of a wide range of strongly correlated systems. An important limit in the model is the Mott insulating regime, where, at half-filling, electrons get localized on single atomic sites. In this work, we investigate extensions of the idea to cluster Mott insulators– where electrons are now localized on clusters of sites. To that end, we study the Hubbard model on a plethora of different clusters, at different integer fillings, by constructing a general Hamiltonian for each cluster. This allows us to explore different regimes of the interplay of strong correlations and hopping within these clusters, and their respective emergent effective degrees of freedom. We then go beyond the single-orbital "cluster" Hubbard model and include multiple orbitals and interactions between them. Once these building blocks have been established, it is possible to introduce inter-cluster hopping terms into the picture; depending on the nature of the resulting effective interactions, they can give rise to novel Hamiltonians, which might possibly host highly correlated and/or frustrated phases.

TT 21.27 Wed 15:00 P1

Chern insulators in twisted bilayer graphene under hydrostatic pressure — •Israel Díaz[1], José González[2], and Tobias Stauber[1] — [1]Materials Science Factory, Instituto de Ciencia de Materiales de Madrid, CSIC, E-28049, Madrid, Spain — [2]Instituto de Estructura de la Materia, CSIC, E-28006, Madrid, Spain

It is well-known that high hydrostatic pressures can be used to induce flat bands in twisted bilayer graphene, at twist angles larger than those realizing the usual magic-angle condition. We show that these twisted graphene bilayers, tuned at such larger magic angles, are prone to fall into Chern insulator phases. We characterize such states by relying on a self-consistent real-space Hartree-Fock approach that accounts for the long-range Coulomb interaction between all the carbon atoms in the moiré unit cell, and which is exact at the Hartree-Fock level as we incorporate all the moiré minibands in the calculation. In our flat-band models with twist angles between 2 and 4 degrees, we show that a gap opens up at the charge neutrality point due to the dynamical

breakdown of time-reversal invariance. At 2 hole-doping, the dominant order parameter corresponds instead to valley symmetry breaking, but there is a critical coupling of the interaction above which a gap opens up due to the condensation of the Haldane mass. These Chern insulator phases seem to be absent in twisted bilayer graphene at the usual small magic angle, probably because they are hindered by the effects of in-plane relaxation, but they become manifest at the larger twist angles we study, leading to interesting phenomena like dissipationless edge states and anomalous Hall effect.

TT 21.28 Wed 15:00 P1

Calculating moments for many-electrons systems — •Elaheh Adibi and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a technique for computing the moments $\langle E^M \rangle = \mathrm{Tr}\, H^M$ of the many-electron spectrum. Taking the trace over a basis of Slater determinants $|I\rangle$ and expressing the Hamiltonian in the same orbital basis, matrix elements $\langle I|H^M|I\rangle$ can only be non-zero when the orbital indices of the creation operators are a permutation of those of the annihilation operators. Writing the permutations in cycle notation and realizing that the trace over a cycle with different orbital indices only depends on the number of descends, we can write the trace as a sum over products of Eulerian numbers times binomial factors involving the number of orbitals and electrons. For non-interacting electrons this further simplifies to a sum over Bell polynomials.

TT 21.29 Wed 15:00 P1

Multiloop fRG analysis of the attractive Hubbard model — •Aiman Al-Eryani[1], Sarah Heinzelmann[1], Anna Kauch[2], Alessandro Toschi[2], and Sabine Andergassen[1] — [1]University of Tuebingen — [2]TU Wien

We analyse the effect of multiloop corrections in the 2D Attractive Hubbard Model. In a TU-fRG scheme where the conventional multiloop self-energy flow equations are replaced with a Schwinger-Dyson flow, we demonstrate the importance of self-energy iteration in the convergence to reference Parquet results. Furthermore, we study the feedback of the s-wave pairing fluctuations on the charge density wave order.

TT 21.30 Wed 15:00 P1

Single-boson exchange fRG application to the two-dimensional Hubbard model at weak coupling — Kilian Fraboulet[1], •Sarah Heinzelmann[1], Pietro Bonetti[2], Aiman Al-Eryani[1], Demetrio Vilardi[2], Alessandro Toschi[3], and Sabine Andergassen[1] — [1]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [3]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria

The functional renormalization group (fRG) is one of the most modern implementation of the renormalization group and has proven successful in the description of various many-body quantum systems, in condensed matter theory and beyond (quantum chromodynamics, nuclear physics, ...). We illustrate in this work the computational advantages of the recently introduced single-boson exchange (SBE) formulation for the one-loop fRG applied to the two-dimensional Hubbard model.

We present a detailed analysis of the physical susceptibilities and their evolution with temperature and interaction strength, both at half filling and finite doping. We find that the rest functions describing the corrections beyond the SBE contributions play a negligible role in the weak coupling regime. The SBE formulation of the fRG flow hence allows for a substantial reduction of the numerical effort in the treatment of the two-particle vertex function, paving a promising route for future multiboson and multiloop extensions.

TT 21.31 Wed 15:00 P1

Linked cluster expansions via hypergraph decompositions — •Matthias Mühlhauser and Kai Phillip Schmidt — Institute for Theoretical Physics I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We present a hypergraph expansion which facilitates the direct treatment of quantum-spin-models with effective many-site interactions via perturbative linked cluster expansions. The main idea is to generate all relevant subclusters and sort them into equivalence classes essentially governed by hypergraph isomorphism. Concretely, a reduced König representation of the hypergraphs is used to make the equivalence relation accessible by graph isomorphism.

[1] M. Mühlhauser and K. P. Schmidt, arXiv:2202.03366 (2022)

TT 21.32 Wed 15:00 P1

Efficient and flexible approach to simulate low-dimensional quantum lattice models with large local Hilbert spaces at the example of the Holstein model — •Thomas Köhler[1], Jan Stolpp[2], and Sebastian Paeckel[3] — [1]Uppsala University, Sweden — [2]Georg-August-Universität Göttingen, Germany — [3]University of Munich, Germany

Quantum lattice models with large local Hilbert spaces emerge across various fields in quantum many-body physics. Problems such as the interplay between fermions and phonons, the BCS-BEC crossover of interacting bosons, or decoherence in quantum simulators have been extensively studied both theoretically and experimentally. In recent years, tensor network methods have become a successful tool to treat such lattice systems numerically. Nevertheless, systems with large local Hilbert spaces remain challenging. Here, we introduce a mapping that allows to construct artificial $U(1)$ symmetries for any type of lattice model. Exploiting the generated symmetries, numerical expenses that are related to the local degrees of freedom decrease significantly. Based on an intimate connection between the Schmidt values of the corresponding matrix-product-state representation and the single-site reduced density matrix, this allows for an efficient treatment of systems with large local dimensions. We demonstrate this new mapping, provide an implementation recipe, and perform example calculations for the Holstein model at half filling. We studied systems with a very large number of lattice sites up to $L = 501$ while accounting for $N_{\mathrm{ph}} = 63$ phonons per site with high precision in the CDW phase.

TT 21.33 Wed 15:00 P1

Electronic correlations in inhomogeneous model systems: Numerical simulation of spectra and transmission — •Andreas Weh[1], Wilhelm H. Appelt[1], Andreas Östlin[2], Liviu Chioncel[2], and Ulrich Eckern[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg — [2]EKM & ACIT, Institute of Physics, University of Augsburg, 86135 Augsburg

We investigate the effects of electronic correlations on the spectral and transport properties of inhomogeneous model systems. The models are based on the single-band Hubbard Hamiltonian, and electronic correlations are treated within dynamical mean-field theory (DMFT). In particular, continuous-time quantum Monte Carlo (CT-QMC) as well as the more recent tensor network methods (DMRG+TDVP) are employed as impurity solvers to study the spectral function of half-metallic ferromagents; a Bethe lattice as well as layered square-lattice structures are considered [1]. The transport properties through a barrier made of such a single interacting half-metallic layer is studied [2] employing the Meir–Wingreen formalism. In particular, we demonstrate that even for a single half-metallic layer, highly polarized transmissions are achievable.

[1] A. Weh, J. Otsuki, H. Schnait, H. G. Evertz, U. Eckern, A. I. Lichtenstein, L. Chioncel, Phys. Rev. Res. 2, 043263 (2020)
[2] A. Weh, W. H. Appelt, A. Östlin, L. Chioncel, U. Eckern, Phys. Status Solidi B 259, 2100157 (2021)

TT 21.34 Wed 15:00 P1

Fifth harmonic generated currents in conventional s-wave superconductor — •Pascal Derendorf and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum, Germany

Recent advances in the field of THz spectroscopy allow for controlled experiments to measure the Higgs modes signature in the Fifth Harmonic Generation (FHG), which was first measured by Z. X. Wang et al [1]. Here, we analyze a periodic multicycle pulse setup, where the driving electromagnetic field solely points into the direction of a lattice vector. We investigate the role of the Higgs mode in the clean-limit FHG of a s-wave superconductor and compare it to other contributing mechanisms, such as charge density fluctuations (CDF) and the phase mode. Further, we show that the signal in the FHG is dominated by the CDF, similar to the third harmonic generated currents. We predict a double peak signature in the frequency resolved intensity amplitude of the FHG for all three mechanisms with one peak being located at $2\Omega = 2\Delta$ and the other one at $2\Omega = \Delta$. The resonant enhancement at $2\Omega = \Delta$ is indicative of the next higher order coupling to the Higgs mode implying that it carries 4Ω. The other resonance at $2\Omega = 2\Delta$ is reminiscent of the Third Harmonic Generation and could therefore

describe e.g. the Higgs mode interacting with 3 single photons.
[1] Z. X. Wang et al., arXiv: 2107.07488

TT 21.35 Wed 15:00 P1

Transfer-matrix summation of path integrals for transport through nanostructures — •Alexander Hahn, Simon Mundinar, Jürgen König, and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

We develop a transfer-matrix style approach based on the numerical iterative summation of path integrals (ISPI) scheme [1,2] to solve non-equilibrium quantum transport. The usage of a transfer-matrix approach combined with further simplifications allows for the development of a method able to work in the stationary limit (TraSPI). Additionally, using the numerical properties of the transfer-matrix element calculation and Gray code, one can use the Woodbury formula to move inside the configuration space. Afterwards, the method is applied to a single-electron transistor with a single-level quantum dot as a central island.
[1] S. Mundinar *et al.*, Phys. Rev. B **99**, 195457 (2019)
[2] S. Mundinar *et al.*, Phys. Rev. B **102**, 045404 (2020)

TT 21.36 Wed 15:00 P1

Driven magnets: Domain wall motion in ferrimagnets in an oscillating magnetic field — •Dennis Hardt and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Germany

Transition regions between two magnetic domains are described by domain walls (DWs).

In this work, we numerically study a 1D ferrimagnet with anisotropy term given by a symmetric double-well potential in magnetization in z-direction. This establishes a Goldstone mode as rotation in the x-y-plane which can be activated by driving the system with an oscillating magnetic field in z-direction.

At $T = 0$ (noise-free case) this leads to a spontaneous symmetry breaking visible in the collective movement of all DWs in one direction (left or right). We also found an analytical description for this limit.

At finite temperature, DW-pairs can also be created meaning that there is a competition between the annihilation (2 DWs meet due to diffusion and driving) and the creation (due to noise).

The noise-created domain walls are driven randomly in left or right direction. This leads to a suppression of the total number of DWs compared to the non-driven thermal case.

TT 21.37 Wed 15:00 P1

Rate functions and quantum adiabatic theorem in many-body systems — •Vibhu Mishra — Institute for Theoretical Physics, Georg-August-Universität Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

We investigate the quantum adiabatic theorem in many body systems for XXZ and ANNNI spin chains. In order to have a well-defined quantitative measure of adiabacity in the thermodynamic limit we calculate a rate function defined via the overlap between the ground state of the final Hamiltonian and the time evolved initial state. The parameters in the Hamiltonian are varied with a linear ramp and we investigate how the rate function behaves with decreasing ramping speed (adiabatic limit). Our main tool is exact diagonalization, which is complemented by bosonization in the XY phase of the XXZ spin chain.

TT 21.38 Wed 15:00 P1

Pump-probe AC susceptibility of $\mathbf{LiHo_xY_{1-x}F_4}$ ($x = 4.5\,\%$) — •Michael Lampl, Andreas Wendl, Markus Kleinhans, Laura Stapf, Marc A. Wilde, and Christian Pfleiderer — Physik Department, Technical University of Munich, 85748 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 subject to intense experimental and theoretical studies [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.*, Nat. Commun. **10**, 4001 (2019)