TT 37: Correlated Electrons: Poster

Time: Wednesday 15:00–18:00 Location: P4

TT 37.1 Wed 15:00 P4

Unveiling the Origin of Magnetic Anisotropy in $CeSb_2$ — •Jan T. Weber[1,2], Kristin Kliemt[1], Sergey L. Bud'ko[2,3], Paul C. Canfield[2,3], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt am Main, Germany — [2]Ames National Laboratory, U.S. DOE, Ames, Iowa 50011, USA — [3]Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA

$CeSb_2$ is a well-established Kondo-lattice system, crystallizing in the orthorhombic $SmSb_2$ structure (space group 64) [1] and forming plate-like crystals. Extensive past studies have revealed a rich magnetic phase diagram for fields within the plane and a strong suppression of magnetization out of plane [2-5]. However, the in-plane magnetization anisotropy remains poorly understood. Nearly identical lattice parameters present challenges in aligning the crystals within the plane, and unexpected magnetization curves - seemingly inconsistent with symmetry arguments - pose additional questions.

In this contribution, we present rotational magnetization measurements together with magnetic measurements as a function of field, temperature and orientation, providing new insights into the in-plane anisotropy addressing these open questions.

[1] R. Wang et. al., Inorg. Chem. 6, 1685 (1967).
[2] S. L. Bud'ko et. al., Phys. Rev. B 57, 13624 (1998).
[3] Y. Zhang et al., Chin. Phys. B 26, 067102 (2017).
[4] B. Liu et al., J. Phys.: Condens. Matter 32, 405605 (2020).
[5] C. Trainer et al., Phys. Rev. B 104, 205134 (2021).

TT 37.2 Wed 15:00 P4

Single Crystal Growth and Characterisation of $EuMn_2Si_2$ and $EuMn_2Ge_2$ — •Janina Strahl, Kristin Kliemt, and Cornelius Krellner — Institute of Physics, Goethe University, Frankfurt (Main), Germany

$EuMn_2Si_2$ exhibits a thermally driven valence transition at around 530 K of the europium ions from Eu^{3+} at low temperatures to $Eu^{\sim 2.5+}$ at high temperatures [1]. The isoelectronic and isostructural substitution of silicon with germanium leads to a stabilization of the divalent state of Eu in $EuMn_2Ge_2$ with reported ferromagnetic Eu ordering below 13 K [2]. Both rare earth intermetallic 122 compounds crystallize in the tetragonal $ThCr_2Si_2$ structure type and show antiferromagnetic ordering of the manganese sublattices above room temperature. In literature [1,2], additional Mn spin-reorientation transitions in polycrystalline $EuMn_2Si_2$ samples at low temperatures were observed. In this contribution, we present the single crystal growth and magnetic properties of both compounds. We found antiferromagnetic ordering of the Eu ions in single crystalline $EuMn_2Ge_2$ below 8.5 K and evidence that previously reported Mn reorientation transitions are absent in pure $EuMn_2Si_2$ single crystals.

[1] M. Hofmann et al., Phys. Rev. B 69, 174432 (2004)
[2] I. Nowik et al., Phys. Rev. B 55, 3033 (1997)

TT 37.3 Wed 15:00 P4

Single Crystal Growth and Characterization of a New Yb-based Heavy Fermion Compound — •Fabian Fiedler[1], Florian Stoll[1], Kristin Kliemt[1], Manuel Brando[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]MPI CPfS, 01187 Dresden, Germany

A system near a quantum-critical point usually shows anomalous thermodynamic and transport properties at low temperatures [1,2].
Presently there are only rare cases of such systems with a ferromagnetic ground state together with pronounced Kondo interactions. Especially Yb-based intermetallic compounds with their possible unstable 4f-shell are of interest due to their low magnetic ordering temperatures.

We found a candidate system for Yb-based ferromagnetic quantum criticality with a large and diverging Sommerfeld coefficient below 10 K. We used substitution in order to manipulate the ground state. Here we report on the single crystal growth as well as the structural and physical characterization of these systems.

[1] Steppke et al., Science 331, 933 (2013);
[2] Shen et al., Nature 579, 51 (2020).

TT 37.4 Wed 15:00 P4

Negative Pressure Studies on $CeRh_2As_2$ with La Substitution — •Sushma Lakshmi Ravi Sankar[1,2], Arushi Yadav[1], Manual Brando[1], Joachim Wosnitza[2], and Seunghyun Khim[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden Germany

$CeRh_2As_2$ is a Kondo-lattice system with novel phase diagrams involving a superconducting and an unknown ordered state appearing below T_c and T_0, respectively. Recent observations of a suppression of T_c and T_0 under external pressure [1] motivated an investigation of a negative pressure study, which can be achieved by a La substitution with Ce. We have succeeded in growing single crystals of ($Ce_{1-x}La_xRh_2As_2$) up to $x \sim 0.1$. We found a negative pressure effect as the La substitution leads to an increase in the a- and c- lattice parameters (unit cell volume increase by $\sim 0.15\%$ with $x = 0.1$) while maintaining the $CaBe_2Ge_2$-type crystal structure. Resistivity measurements showed that both T_c and T_0 decrease with the La substitution to be almost suppressed at $x \sim 0.08$, while the resistivity maximum is slightly shifted to a lower temperature. At the same time, the residual resistivity ratio decreases from 2.24 at $x = 0$ to 1.46 at $x = 0.1$, indicating additional disorder introduced by the La substitution. This suggests that both the negative pressure effect and the increased disorder should be considered in understanding the evolution of T_c and T_0 with the La substitution.

[1] M. Pfeiffer et al., Phys. Rev. Lett. 133, 126506 (2024).

TT 37.5 Wed 15:00 P4

Terahertz Time-domain Spectroscopy on the Topological Kondo Insulator SmB_6 — •Zekai Chen, Debankit Priyadarshi, Erik de Vos, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

We present a terahertz time-domain spectroscopy (THz-TDS) measurement on the topological Kondo insulator samarium hexaboride (SmB_6). These results are aimed at providing insight into the coexistence of a topologically conductive surface state and the opening of a bandgap below the Kondo temperature. Previous work on Kondo insulators has shown that the Kondo quasiparticles disintegrate near a quantum critical point (QCP) in response to THz radiation, leading to a delayed echo-pulse-like response in the time domain [1]. In contrast to these materials, SmB_6 exhibits an additional in-gap state that could be related to its topological surface conductivity. In the presented experiment, this in-gap state is resonantly probed with THz radiation. Our measurement concentrates on studying the emergence of the in-gap state through correlated electron interaction.

[1] Nat. Phys. 14, 1103 (2018).

TT 37.6 Wed 15:00 P4

Cyclotron Resonance on SmB_6 Probed by Superconducting Coplanar Microwave Resonators — •Anastasia Bauernfeind and Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

Samarium hexaboride (SmB_6) is a homogeneously mixed-valent, narrow-gap semiconductor typically classified as a topological Kondo insulator. Its resistivity increases sharply as the temperature decreases, showing activated behavior that saturates below approximately 5 K. Experimental evidence suggests that topological surface states dominate low-temperature transport. Two notable studies on quantum oscillations in SmB_6 have sparked intense debate about their origin: one observes behavior consistent with a two-dimensional (2D) Fermi surface attributed to surface states, while the other reports a three-dimensional (3D) bulk Fermi surface, despite the insulating nature of the bulk at low temperatures. In our research, we perform cyclotron resonance experiments on SmB_6 using superconducting coplanar waveguides, a powerful method for investigating the Fermi surface of various materials. By tracing the evolution of the cyclotron frequency (up to 20 GHz) as a function of magnetic field, we can determine the type of charge carriers, the effective mass, and the properties of the associated electronic bands. Combined with temperature-dependent measurements (down to 20 mK) and power-dependent studies, this approach provides valuable insights into the electronic structure of the strongly correlated material SmB_6.

TT 37.7 Wed 15:00 P4

Bonding in UO_2^{2+} Dumbbell Structures: The Influence of a Non-Orthogonal Atomic Basis Set and the U 5f, 6d, 7s, and 6p Orbitals — •Henrik Hahn, Michelangelo Tagliavini, Kevin Ackermann, Sarah L. Goerlitz, Johann Collard, Ruth Kaiser, and Maurits W. Haverkort — Institute for Theoretical Physics (ITP), Heidelberg University, Philosophenweg 19, 69120, Heidelberg, Germany

Actinide compounds exhibit a wide range of complex properties, making their theoretical description a significant challenge. This complexity arises primarily from the open 5f shell, which introduces strong electronic correlations, as well as the close proximity of multiple subshells with different angular momentum (l) values due to the large principal quantum numbers (n) of actinides. In this study, we investigate the U-O bond in UO_2^{2+}, a well-known coordination structure of U^{2+} ($5f^0$). Notably, the stronger σ bond derived from the 5f z^3 orbital lies higher in energy than the weaker π bonds formed by the 5f xz^2 and yz^2 orbitals - an unusual ordering. Through a detailed analysis of the underlying LDA Hamiltonian in a non-orthogonal basis, we provide an explanation for this behavior. Our findings demonstrate that fully understanding the bonding and properties of actinides requires a many-orbital model that transcends the conventional assumption that the low-energy physics is governed solely by the 5f shell. This broader perspective is essential for capturing the intricate electronic structure and bonding characteristics of these materials.

TT 37.8 Wed 15:00 P4

Quantum-Spin Impurities Coupled to a Chern Insulator: Topological Remnants — •David Alan Krüger[1] and Michael Potthoff[1,2] — [1]University of Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Treating quantum-spin impurities as classical vectors is a frequently used approximation to study the impact of local magnetic impurities on the formation of subgap bound states in insulators. Recently, the classical-spin approximation has been exploited for a "local" topological characterization of the ground-state bundle over the manifold of impurity-spin configurations, as opposed to the bundle over the Brillouin zone. This has been achieved by computing spin-Chern numbers $C^{(S)}$ as the corresponding topological invariants.

Here, we numerically solve a system with a single or two quantum spin-$\frac{1}{2}$ locally exchange coupled to a Chern insulator given by the QWZ model. Via Lanczos tridiagonalization, the system is mapped onto a gapped Kondo-impurity model. Local ground-state properties and local single-particle as well as magnetic excitations spectra are obtained by means of an adaptive natural-orbital configuration-interaction technique.

We study the interplay of possible remnants of the classical-spin topology, the intrinsic QWZ topology, and the finite-size Kondo effect. To this end we trace subgap excitations as a function of the local exchange-coupling strength and the mass parameter.

TT 37.9 Wed 15:00 P4

Chiral Kondo Lattice Analyzed via Variational Cluster Approach — •Benjamin Heinrich and Maria Daghofer — Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany

Moiré systems composed of van der Waals heterostructures provide an experimentally accessible platform to realize a wide range of strongly correlated electron phenomena. Using transition metal dichalcogenide materials, such as an AB-stacked $MoTe_2/WSe_2$ bilayer, gives rise to an effective multi-orbital Hubbard model on the honeycomb lattice, which can be tuned via doping and the introduction of charge transfer energy through external voltages. Including strong Ising spin-orbit coupling leads to chiral Kondo exchange between localized and itinerant electrons in different layers near half-filling.[1]

To gain a better understanding of experimentally observed phenomena, including magnetic ordering, numerical modeling is performed using the variational cluster approach. This methodology, closely related to cluster dynamical mean-field theory, has been proven effective for studying analogous systems exhibiting Kondo lattice behavior.

[1] Guerci et al., Sci. Adv. 9, eade7701 (2023).

TT 37.10 Wed 15:00 P4

Influence of Band Mixing on FCI and CDW — •Marco Schönleber and Maria Daghofer — Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany

Fractional quantum hall physics with vanishing magnetic fields has become an increasingly important research topic in recent years due to new findings in the field of moiré materials. Experimental signatures of these phases are often observed in combination with signatures of charge ordered or other symmetry broken phases. This indicates that band mixing might play an elementary role in the complete description of this phase of matter. For this purpose, an extended Hubbard model on a triangular lattice with $\nu = 1/3$ and $\nu = 2/3$ is considered. This allows the formation of bands of non-trivial topology as well as the formation of commensurate charge density waves. The analysis is carried out by exact diagonalisation. By varying the band gap, it can be shown that the stability of the charge order depends on this, whereby the degree of filling plays a decisive role.

TT 37.11 Wed 15:00 P4

Quantum Monte Carlo simulations of generalized Dicke-Ising models — •Anja Langheld, Max Hörmann, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Recently, we introduced a wormhole algorithm for the paradigmatic Dicke-Ising model to gain quantitative insights on effects of light-matter interactions on correlated quantum matter [1]. This method enabled us to determine the quantum phase diagram for ferro- and antiferromagnetic interactions on the chain and square lattice alongside the criticality of its second order quantum phase transitions. The continuous superradiant phase transitions are in the same universality class as the Dicke model, leading to a well-known peculiar finite-size scaling which can be understood in terms of scaling above the upper critical dimension.

Going one step further we now introduce new ingredients to the matter Hamiltonian like geometric frustration, long-range interactions and disorder to study the interplay between a variety of correlated matter phenomena and light-matter interactions.

[1] A. Langheld et al., arXiv:2409.15082

TT 37.12 Wed 15:00 P4

Chiral quantum phase transition in moiré Dirac materials — •Ana García-Page[1] and Laura Classen[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart 70569, Germany — [2]Department of Physics, Technical University of Munich, Garching 85749, Germany

Strong enough interactions induce a semimetal-to-insulator transition in Dirac materials, which can be viewed as the solid-state analogue of the chiral phase transition in quantum chromodynamics1-4. Moiré Dirac materials such as twisted bilayer graphene offer a new opportunity to study this transition because they facilitate tuning the effective interaction via a twist angle5-6. Motivated by this, we explore the quantum phase transition of a 2D Dirac material which spontaneously develops a gap that breaks an Ising symmetry7. We model it via an effective Gross-Neveu-Yukawa theory and employ the functional renormalization group method to map out the phase diagram. We analyze the quantum critical behavior at the transition and investigate the effect of a chemical potential which introduces a finite charge density.

TT 37.13 Wed 15:00 P4

NMR in Pulsed Magnetic Fields - Recent Developments — •Hannes Kühne[1] and Yoshihiko Ihara[2] — [1]HLD-HZDR, Dresden — [2]Department of Physics, Hokkaido University

NMR measurements in the highest pulsed magnetic fields have been developed at dedicated large-scale research facilities for some time and are becoming increasingly available for user experiments. On the poster, I will give an overview of the current developments, possibilities and peculiarities of NMR experiments in pulsed magnetic fields. In particular, the implementation of NMR experiments with dynamically controlled flat-top field pulses has recently been reported, enabling the measurement of broadband NMR spectra and relaxation times up to the ms range [1]. Furthermore, through several examples on low-dimensional spin systems, I will present opportunities to work on scientific questions that can be uniquely addressed using this technique [2].

[1] Y. Ihara et al., Rev. Sci. Instrum. 92, 114709 (2021).
[2] H. Kühne and Y. Ihara, Contemp. Phys. 65, 40 (2024).

TT 37.14 Wed 15:00 P4

Magnetic Anisotropy and Low-Energy Spin Dynamics in van der Waals Magnets $M_2P_2S_6$ Probed by Electron Spin Resonance — Joyal J. Abraham[1,2], Yurii Senyk[1,2], Yuliia Shemerliuk[1], Sebastian Selter[1,2], Saicha-

ran Aswartham[1], Bernd Büchner[1,2,3], Vladislav Kataev[1], and •Alexey Alfonsov[1,3] — [1]Leibniz IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, 01062 Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden, Germany

In the past recent years magnetic van der Waals (vdW) materials have become increasingly attractive for the fundamental investigations since they provide immense possibility to study intrinsic magnetism in a low-dimensional limit. The weak vdW forces hold together the atomic monolayers in vdW crystals, which results in a poor interlayer coupling, and therefore renders these materials intrinsically two dimensional. That makes them particularly attractive for probing the low-dimensional physics while investigating bulk crystals. On the other hand, a remarkable success in exfoliation of this class of materials due to the lack of significant interlayer chemical bonds unlocks vast potential for applications in the fields of advanced electronics, optoelectronics, and spintronics. In this work we present the results of the electron spin resonance investigation of such magnetic vdW materials $M_2P_2S_6$ (M = Mn, Ni, Cu, Cr) performed in the broad range of temperatures, magnetic fields and excitation frequencies, and discuss their low-energy spin dynamics as well as magnetic anisotropy responsible for the stabilization of the magnetic order.

TT 37.15 Wed 15:00 P4

Magnetic Properties of a Trillium Lattice Compound $Li_2NiGe_3O_8$ — •Annarose Jose Palliyan[1,2], Nazmul Islam[2], Ralf Feyerherm[2], and Bella Lake[2,1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Frustrated magnets are interesting materials that exhibit exotic properties due to the competing localized spins [1]. Certain lattices are intrinsically predisposed to show frustration due to the arrangement of their magnetic ions and one such lattice is the trillium lattice [2]. The trillium lattice is composed of a three-dimensional chiral network of corner sharing equilateral triangles. $Li_2NiGe_3O_8$ is a trillium lattice candidate where each Ni^{2+} ion is shared between three equilateral triangles. Polycrystalline samples of $Li_2NiGe_3O_8$ were synthesized by solid - state reaction method. The magnetic properties of this complex spinel oxide were studied by magnetization, susceptibility and heat capacity measurements down to He-3 temperatures. Our studies shows the presence of weak antiferromagnetic interactions in this material with no long-range order. A three-level schottky anomaly was observed in this material because of the splitting of the S = 1 triplet state.

[1] J. M. Bulled et al., Phys. Rev. Lett. 128, 177201 (2022);
[2] N. Tristan et al., Phys. Rev. B 72, 174404 (2005).

TT 37.16 Wed 15:00 P4

Geometric Magnetic Frustration in $Mn_3Al_2Si_3O_{12}$ — •Marwa Abouelela[1,2], Nazmul Isalam[2], Ralf Feyerherm[2], and Bella Lake[1,2] — [1]Institut für Festkörperphysik, Technische Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Geometric magnetic frustration in triangular lattices has garnered significant interest in recent research [1]. $Mn_3Al_2Si_3O_{12}$ exhibits geometrical frustration, where Mn^{2+} ($3d^5$) ions form a hyperkagomé structure [2]. In this study, the spessartine was synthesized at high temperatures, and its magnetic susceptibilities and heat capacities were investigated at low temperatures. Temperature-dependent magnetic susceptibility measurements revealed an antiferromagnetic ordering of the Mn^{2+} ions below T_N=6.5K, with a Curie-Weiss temperature of -26.7K. The high ratio of Curie-Weiss temperature to Néel temperature suggests strong frustration in the system.

[1] A. P. Ramirez, Annu. Rev. Mater. Sci. 24, 453 (1994);
[2] G. C. Lau et al., Phys. Rev. B 80, 214414 (2009).

TT 37.17 Wed 15:00 P4

Static and Dynamic Properties of Quantum Magnets: Results from Numerical Linked Cluster Expansion — •Alexander Schwenke and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

We consider static and dynamic properties of two-dimensional frustrated quantum antiferromagnets utilizing the numerical linked cluster expansion (NLCE). In particular, we are interested in spin-$^1/_2$ models showing quantum phase transitions versus internal parameters, e.g., the J_1-J_2 model on the square lattice or the triangular lattice XXZ model in external magnetic fields.

For the NLCE, we employ a single-site representation focussing on three topics: First, we present results for thermodynamic quantities, namely the internal energy and the specific heat at finite temperature. Second, we study the ground-state energy per site as a function of competing exchange coupling constants focussing on its second derivative. Finally, we investigate the dynamics of the system following a quantum quench.

TT 37.18 Wed 15:00 P4

Magnetism in i-Tb-Cd Quasicrystals — •Andreas Kreyssig[1,2], P. Das[2], G. S. Tucker[2], A. Podlesnyak[3], Feng Ye[3], Masaaki Matsuda[3], T. Kong[2], S. L. Bud'ko[2], P. C. Canfield[2], R Flint[2], P. P. Orth[2,4], T. Yamada[5], and A. I. Goldman[2] — [1]Experimental Physics IV, Ruhr University Bochum, Bochum, Germany — [2]Ames Laboratory, U.S. DOE, and Department of Physics and Astronomy, Iowa State University, Ames, USA — [3]Neutron Scattering Division, Oak Ridge National Laboratory, USA — [4]Department of Physics, Harvard University, Cambridge, USA — [5]Department of Applied Physics, Tokyo University of Science, Tokyo, Japan

i-Tb-Cd orders as icoshedral quasicrystal with the magnetic Tb^{3+} ions arranged in Tsai-type clusters. We studied the magnetic correlations and excitations by elastic and inelastic neutron scattering on single-grain isotopically enriched samples. The measurements of the crystalline electric field excitations demonstrated that the Tb^{3+} moments are directed along the local fivefold axes of the Tsai-type clusters. We calculated the magnetic diffuse scattering for the low-energy configurations using an Ising-type model for the moment arrangements on a single Tb^{3+} icosahedron. By comparison with our diffuse neutron scattering signals, we identified the most likely moment configuration in a single cluster. We further studied the role of intercluster interactions for magnetic frustration and the magnetic scattering.

This work was supported by the U. S. DOE, BES, DMSE, Contract DE-AC02-07CH11358, and resources at HFIR and SNS, U. S. DOE.
[1] P. Das, A. Kreyssig et al., Phys. Rev. **B** 108, 134421 (2023).

TT 37.19 Wed 15:00 P4

Chiral spin liquid in external magnetic field: Phase diagram of the decorated-honeycomb Kitaev model — •Sabastian Granberg Cauchi and Matthias Vojta — TU Dresden, Germany

Studies of Kitaev models on different lattices have shown signatures of topological phase transitions as a function of external magnetic field direction and magnitude. These transitions are often accompanied by a change in the statistics of the low-energy anyonic excitations. In particular, the antiferromagnetic Kitaev system yields a field-induced spin liquid, of arguably gapless U(1) or Abelian character. The existence of field-induced spin liquids on different lattices has consequently been intensely investigated. Here, we determine the phase diagram of the decorated-honeycomb Kitaev model for different inter- and intra-triangle coupling ratios and magnetic fields using a mean-field theory derived from Kitaev's Majorana parton decomposition.

TT 37.20 Wed 15:00 P4

Low-energy description of the SU(3) Hubbard model on the triangular lattice — •Linus Hein — Ludwig-Maximilians-Universität München

It has been a longstanding goal to better understand strongly correlated fermionic systems. Extensive studies have been conducted on these systems, particularly on the square lattice Hubbard model. To find out which of the results are artefacts of this fine-tuned model, it is sensible to analyze slightly modified models with for instance enlarged symmetry. We consider an SU(3) antiferromagnet on a tripartite triangular lattice near one third filling. Previous works explored a non-linear sigma model and its emerging Goldstone modes. Building on these results, we derive a linear spin-wave description of the low-energy excitations. Furthermore, we consider the hole-doped system and derive an effective Hamiltonian to describe the emergent magnetic polarons. Thereby, we broaden our understanding of strongly correlated fermionic systems, in a setting that can be experimentally explored using e.g. ultracold atom experiments.

TT 37.21 Wed 15:00 P4

Temperature Dependent Infrared Spectroscopy on the Frustrated Spin-Ladder System $BiCu_2PO_6$ — •Johanna Strauss[1], Renjith Mathew Roy[1], Maxim Wenzel[1], Haidong Zhou[2], Martin Dressel[1], and Komalavalli Thirunavukkuarasu[3] — [1]1. Physikalisches Institute, University of Stuttgart, Germany —

[2]Department of Physics, University of Tennessee Knoxville, Knoxville, USA — [3]3. Department of Physics, Florida A and M University, Tallahassee, USA

Spin systems with frustrated geometries are of significant interest due to their potential to exhibit quantum spin liquid behaviour. This study focuses on $BiCu_2PO_6$ which exhibits no magnetic ordering down to 0.1 K. Various experimental studies on this zig-zag spin-ladder compound reveal that the magnetism in this material arise from complex exchange coupling mechanisms that are not completely understood yet. However, it is clear that the magneto-structural correlations play a major role. Here, we present our attempt to employ infrared spectroscopy to determine the optical conductivity and phonons along planes parallel and perpendicular to the spin-ladders at temperatures ranging from 300 K to 10 K and look for signatures on the nature of spin-phonon coupling.

TT 37.22 Wed 15:00 P4

Magnetic Phase Diagrams of the Frustrated Langbeinite Material $Tl_2Mn_2(SO_4)_3$ — •Manuel Tönnissen[1], Alexander Bäder[1], Ladislav Bohatý[2], Petra Becker-Bohatý[2], Oliver Breunig[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Kristallographie, Universität zu Köln

Antiferromagnetic Heisenberg spins on the so-called trillium lattice form a highly frustrated 3-dimensional spin system [1]. This theoretical model can be realizied in cubic, low-symmetry space group $P2_13$ materials. One family of materials that partially crystallizes in this space group are langbeinites. Recent studies report that the langbeinite $K_2Ni_2(SO_4)_3$ with S=1 Ni^{2+} ions show close proximity to a field-driven quantum spin-liquid behavior, although there is magnetic order in zero field [2] [3]. Here we focus on the different magnetic phases of the related langbeinite $Tl_2Mn_2(SO_4)_3$ with S=5/2 Mn^{2+} ions. By conducting specific-heat, magnetocaloric-effect, and magnetization measurements, we derive B-T phase diagrams for different orientations of the magnetic field. Our data reveal the presence of at least 3 magnetic phases below a temperature of about 1.5 K for the magnetic field along the [1 1 1] direction and even 4 magnetic phases for fields applied along the [1 1 0] or [0 0 1] directions.

This work is supported through CRC1238 (projects A02 and B01).

[1] J. Hopkinson, Phys. Rev. B, **74**, 224441 (2006);
[2] M. G. Gonzalez et al., Nat. Commun. **15**, 7191 (2024);
[3] I. Živković et al., Phys Rev. Lett. **127**, 157204 (2021).

TT 37.23 Wed 15:00 P4

Magnetic Order in the Low-Dimensional Quantum Magnet $Cu_2(OH)_3Br$ — •S. Luther[1], Z. Wang[2], A. Reinold[2], Z. Zhao[3], J. Wosnitza[1,4], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]Fakultät Physik, TU Dortmund — [3]Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences — [4]Institut für Festkörper- und Materialphysik, TU Dresden

Low-dimensional quantum magnets, such as the quasi-two-dimensional spin system $Cu_2(OH)_3Br$, can host exotic phenomena and ground states. We will present results of high-field magnetization and nuclear magnetic resonance (NMR) spectroscopy that probe the microscopic details of the magnetic structure at finite magnetic fields. In $Cu_2(OH)_3Br$, the Cu^{2+} ions in the distorted crystal structure form alternating ferromagnetic and antiferromagnetic spin-1/2 chains with finite interchain coupling, leading to a Néel temperature of 9.3 K at zero field. Here, we investigate the phase diagram for $H||b$, where a splitting of the NMR spectral lines below T_N and elevated fields reveals a commensurate long-range antiferromagnetic order. Maxima in the temperature-dependent spin-lattice relaxation rate $1/T_1$ at different magnetic fields indicate the transition temperature to the ordered phase. An anomaly in the high-field magnetization at low temperatures and around 16 T suggests the suppression of the magnetically ordered phase.

TT 37.24 Wed 15:00 P4

ESR Investigations of $AgCrSe_2$, $AgCrS_2$ and Cr_3Se_4 — •Jörg Sichelschmidt, Pierre Chailloleau, Michael Baenitz, Seo-Jin Kim, Helge Rosner, Vicky Hasse, and Marcus Schmidt — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We investigated the Electron Spin Resonance (ESR) of Cr in the layered triangular lattice systems $AgCrSe_2$, $AgCrS_2$ and the structurally related Cr_3Se_4. These materials display a variety of interesting physical properties such as unconventional magnetic ordering [1], a spin-polarized surface state [2], an unconventional anomalous Hall effect [3] in $AgCrSe_2$ or multiferroic behavior in $AgCrS_2$, or directional Kondo transport [4]. At low temperatures, all these materials show a divergent ESR spin relaxation, which is typical for low-dimensional spin systems and indicates an increasing importance of Cr^{3+} spin correlations. This also leads to the formation of internal fields, as evidenced by the marked decrease in the resonance field. The relatively narrow Cr^{3+} ESR spectra allow to determine an ESR intensity which reflects the static susceptibility probed locally at the site of the Cr spins.

[1] M. Baenitz *et al.*, Phys. Rev. B **104**, 134410 (2021);
[2] G.-R. Siemann *et al.*, npj Quantum Mater. **8**, 61 (2023);
[3] S.-J. Kim *et al.*, Adv. Sci. **11**, 2307306 (2024);
[4] J. Guimaraes *et al.*, Commun. Phys. **7**, 176 (2024).

TT 37.25 Wed 15:00 P4

Electronic Structures of $AgCrS_2$, $AgCrSe_2$, and Cr_3Se_4 — •Seo-Jin Kim, Jörg Sichelschmidt, Michael Baenitz, Marcus Schmidt, and Helge Rosner — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We study the electronic structures of triangular lattice systems $AgCrS_2$, $AgCrSe_2$, and the related compound Cr_3Se_4 using density functional theory (DFT). Although $AgCrSe_2$ and $AgCrS_2$ are isostructural, they exhibit different physical properties. $AgCrSe_2$ is a self-doped p-type semiconductor characterized by spin-polarized surface states[1], the cycloidal magnetic ordering[2], and the unconventional anomalous Hall effect[3] and directional Kondo transport[4]. In contrast, $AgCrS_2$ is an insulator that undergoes symmetry lowering to a monoclinic phase and exhibits a collinear double-stripe antiferromagnetic ground state below $T_N = 42$ K. This study aims to present a comprehensive analysis of the electronic structures of these compounds. Additionally, we extend our investigation to the structurally related compound Cr_3Se_4.

[1] M. Baenitz et al., Phys. Rev. B 104, 134410 (2021);
[2] G.-R. Siemann et al., npj Quantum Mater. 8, 61 (2023);
[3] S.-J. Kim et al., Adv. Sci. 11, 2307306 (2024);
[4] J. Guimaraes et al., Commun. Phys. 7, 176 (2024).

TT 37.26 Wed 15:00 P4

Synthesis and Physical Properties of 2D van der Waals Magnets $Fe_{1-x}TM_xPX_3$ (TM: Transition Metals) — •Masoumeh Rahimkhani, Saicharan Aswartham, Andreas Kreyssig, and Anna Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

Transition-metal phosphochalcogenides ($TMPX_3$) belong to the family of layered van-der-Waals materials in which TM is a transition-metal and X is a chalcogenide. These materials exhibit various electric, optical, and magnetic properties. $FePSe_3$ belongs to this family of $TMPX_3$ with interesting magnetic and electronic properties. Here, we describe the preparation of $FePSe_3$ and its substitution series with different transition metals through solid-state synthesis and CVT. The samples are characterized by X-ray diffraction and scanning electron microscope for structural and phase analysis. Further on, the magnetic and electronic properties will be investigated.

TT 37.27 Wed 15:00 P4

Single-Crystal Study of Kagome Magnets CrRhAs and CrNiAs — •Franziska Breitner, Bin Shen, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

CrRhAs and CrNiAs are metals with distorted kagome lattice of magnetic Cr atoms [1]. While CrRhAs is an antiferromagnet with a reported Néel temperature of 165 K for polycristalline samples, CrNiAs is ferromagnetic with T_C=170 K. More recently, interesting properties such as anomalous Hall effect were predicted for CrRhAs [2].

We report the first growth of CrRhAs and CrNiAs single crystals utilizing the flux method and present their specific heat, magnetic susceptibility and electrical transport. Magnetoresistance and Hall effect for CrRhAs indicate no anomalous behaviors. For CrNiAs we also investigate the influences of hydrostatic pressure as well as partial substitution of As with P on the ferromagnetic transition.

Supported by DFG-TRR 360*492547816 and the Alexander von Humboldt Foundation.

[1] S. Ohta et al., J. Mag. Mag. Mater. 90, 171 (1990).
[2] Y. N. Huang et al., npj Quantum Mater. 8, 32 (2023).

TT 37.28 Wed 15:00 P4

Inelastic Scattering in Anisotropic Heisenberg Models on Square and Honeycomb Lattice Via Continuous Similarity Transformations — •Vanessa Sulaiman[1], Dag-Björn Hering[1], Matthias R. Walther[2], Kai P. Schmidt[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany

We apply a continuous similarity transformation (CST) [1,2] with a magnon-conserving generator to the antiferromagnetic anisotropic XXZ model. For the square lattice, the resulting effective Hamiltonian has already been analyzed [3]. We extend the approach by applying the CST to observables as well. Using the continuous fraction representation, we calculate spectral densities for these observables on the square and honeycomb lattice. These are then compared to experimental data from RIXS measurements [4], for example with single-layered $Ca_2CuO_2Cl_2$.

[1] M. Powalski et al., Phys. Rev. Lett. **115**, 207202 (2015);
[2] M. Powalski et al., SciPost Phys. **4**, 001 (2018);
[3] M. R. Walther et al., Phys. Rev. Res. **5**, 013132 (2023);
[4] K.-J. Zhou et al., J. Synchrotron Rad. **29**, 563 (2022).

TT 37.29 Wed 15:00 P4

Stochastic Simulation of Spin Transport — •Franz Pöschl[1,4], Xin Zhang[1,2,3], Aristo Kevin Ardyaneira P[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [4]Ludwig-Maximilians Universität München, Fakultät für Physik, Geschwister-Scholl-Platz 1, 80539 München

Simulating out of equilibrium steady states of large systems is a hard task. It is therefore necessary to develop novel approaches permitting to simulate the dynamics of those systems efficiently. In our work, we use the Discrete Truncated Wigner Approximation which is a semiclassical approach mapping hamiltonians and dissipative processes into a classical phase space. This mapping allows to compute stochastic trajectories and to evaluate the evolution of the system. In this poster I will present this method and show how it can be employed to study the out-of-equilibrium phases of the XXZ spin model and to derive its transport properties.

TT 37.30 Wed 15:00 P4

Anisotropic Magnetoresistance and Hall Effect of $Sr_4Ru_3O_{10}$ — •Simone Seipel[1], Lara Pätzold[1], Zahra Ghazinezhad[1], Augustus A. Nugroho[2], Markus Braden[1], and Thomas Lorenz[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Bandung Institute of Technology, Indonesia

The layered transition-metal oxide $Sr_4Ru_3O_{10}$ is a member of the Ruddlesden-Popper series with a layered orthorhombic crystal structure. It is a ferromagnetic metal with $T \simeq 105\,\mathrm{K}$ and shows an additional metamagnetic transition below 50 K, of which a deeper understanding is still missing. Here, we present a single-crystal study of the anisotropic magnetization and electrical transport properties. For in-plane electric currents ($j||ab$) and $B||c$, we present normal and anomalous Hall effect data. The latter shows a non-monotonic temperature dependence and a characteristic sign change at low temperature which similarly occurs in the magnetoresistance $\rho_{xx}(B||c)$. Such a behavior is known from the sister compound $SrRuO_3$ and associated with Weyl points in the band structure [1]. In addition, we studied the out-of-plane resistivity that is highly anisotropic ($\rho_c >> \rho_{ab}$) due to the layered crystal structure and strongly changes at the metamagnetic transition. Based on magnetoresistance data $\rho_c(B||ab)$ we derive the magnetic-field induced metamagnetic transition at low temperatures and discuss the angular dependence of the transition fields and the magnetoresistance for in-plane magnetic fields.

Funded by the DFG via CRC 1238 Projects A02, B01 and B04

[1] K. Takiguchi et al., Nat. Commun. **11**, 4969 (2020).

TT 37.31 Wed 15:00 P4

Thermal Transport in Swedenborgite $CaBaCo_4O_7$ — •Reza Firouzmandi[1], Matthias Gillig[1], Yasujiro Taguchi[2], Yoshinori Tokura[2], Yusuke Tokunaga[2], Vilmos Kocsis[1], and Bernd Büchner[1] — [1]IFW-Dresden, Dresden, Germany — [2]RIKEN-CEMS, Wako, Japan

The interplay between electronic, magnetic, and lattice degrees of freedom in multiferroic materials gives rise to novel transport phenomena, including the thermal Hall effect (THE), thermal analog of the Hall effect, where heat flow is deflected under an external magnetic field. Here, we investigate the thermal transport properties of the multiferroic Swedenborgite $CaBaCo_4O_7$, a compound featuring alternating Kagome and triangular layers of edge-sharing CoO_4 tetrahedra in a mixed valence state. The longitudinal thermal conductivity exhibits anomalies associated with magnetic ordering, while the transverse thermal conductivity (κ_{xy}) reveals an anomalous thermal Hall effect that vanishes at low temperatures, resembling the magnon thermal Hall effect. These results provide insight into the role of spin-lattice coupling in the thermal transport of frustrated magnetic systems.

TT 37.32 Wed 15:00 P4

Strain dependance of the antiferromagnetic transition of $Ca_{1-x}Sr_xCo_2As_2$ with a substitution induced structural collapse — •Michael Paul, Maik Golombiewski, Teslin R. Thomas, N.S. Sangeetha, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

The tetragonal structure of $SrCo_2As_2$ undergoes a gradual collapse with the substitution of Sr by Ca atoms. This collapse is accompanied by the emergence of antiferromagnetic order with a transition temperature T_N of up to 55 K [1]. It has been shown that T_N can be tuned with biaxial strain that is created by cooling a thin $Ca_{1-x}Sr_xCo_2As_2$ sample that is glued to a quartz substrate [2].

A more controlled application of uniaxial force to the sample can be achieved with the use of the cryogenic stress cell Razorbill FC100. The modification of the antiferromagnetic transition of $Ca_{1-x}Sr_xCo_2As_2$ is investigated by applying uniaxial stress to the sample with this device.

We acknowledge the support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] N. S. Sangeetha et al., Phys. Rev. Lett. 119, 257203 (2017);
[2] T. R. Thomas et al., in preparation

TT 37.33 Wed 15:00 P4

Single crystal synthesis of $FeSb_2$ and investigation of its electronic transport properties — •Maximilian van de Loo, Maik Golombiewski, Andreas Kreyssig, and Anna E. Böhmer — Experimentalphysik IV, Ruhr-Universität Bochum, 44801 Bochum, Germany

$FeSb_2$ is a diamagnetic narrow band gap semiconductor with interesting electronic transport properties [1]. Huge thermoelectric power factor and a paramagnetic crossover have been reported at low temperatures [1, 2] and attempts to influence and understand these properties by doping have been made [3]. A metal-semiconductor crossover along the b axis can be observed under certain growth conditions. We have synthesized single crystals of $FeSb_2$ via self-flux growth and successfully realized substitutions $(Fe_{1-x}TM_x)Sb_2$ with different transition metals (TM). The samples were characterized with electron microscopy, energy-dispersive x-ray spectroscopy, powder x-ray diffraction and Laue diffraction measurements, as well as electrical resistivity measurement. The appearance of the metal-semiconductor crossover has been investigated by varying the growth conditions.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] C. Petrovic, J. W. Kim, S. L. Bud'ko, A. I. Goldman, P. C. Canfield, W. Choe, and G. J. Miller, Phys. Rev. B 67, (2003).
[2] C. Homes, Q. Du, C. Petrovic, W. H. Brito, S. Choi, and G. Kotliar, Sci. Rep. 8, (2018).
[3] Y. Cao, S. Yuan, M. Liu, B. Kang, B. Lu, J. Zhang, and S. Cao, J. Cryst. Growth 363, (2013).

TT 37.34 Wed 15:00 P4

Feshbach resonance in a strongly repulsive ladder of mixed dimensionality: a possible scenario for bilayer nickelate superconductors — •Hannah Lange[1,2,3], Lukas Homeier[1,3], Eugene Demler[4], Fabian Grusdt[1,3], and Annabelle Bohrdt[3,5] — [1]LMU Munich — [2]Max-Planck-Institute for Quantum Optics, Garching — [3]Munich Center for QST, Munich — [4]ETH Zurich — [5]University of Regensburg

Since the discovery of superconductivity in cuprate materials, the minimal ingredients for high-Tc superconductivity have been an outstanding puzzle. Motivated by the recently discovered nickelate bilayer superconductor LNO under pressure, we study a minimal bilayer model,

in which, as in LNO, inter- and intralayer magnetic interactions but no interlayer hopping are present: a mixed-dimensional (mixD) t-J model. The single and coupled mixD ladders we study feature a crossover from tightly bound pairs of holes (closed channel) at small repulsion, to more spatially extended, correlated pairs of individual holes (open channel) at large repulsion. We derive an effective model for the latter, in which the attraction is mediated by the closed channel, in analogy to atomic Feshbach resonances. Using density matrix renormalization group (DMRG) simulations we reveal a dome of large binding energies at around 30% doping, accompanied by a change of the Fermi surface volume. Our work provides a microscopic theory of pairing in the doped mixD system with dominant repulsion and our predictions can be tested in state-of-the-art quantum simulators.

TT 37.35 Wed 15:00 P4

Fluctuation Spectroscopy on $La_2NiO_{4+\delta}$ RRAM devices — •Demian Ranftl[1], Yingxin Li[2], Tristan Stadler[1], Eszter Piros[2], Aleksandra Koroleva[3], Lambert Alff[2], Mónica Burriel[3], and Jens Müller[1] — [1]Institute of Physics, Goethe University, Frankfurt am Main, Germany — [2]Institute of Materials Science, TU Darmstadt, Darmstadt, Germany — [3]Laboratory in Materials Science and Physical Engineering, Université Grenoble Alpes, Grenoble, France

Memristive devices, whose resistance is programmable and retainable, are considered to be most promising for the next generation of nonvolatile memory. Low-frequency current noise spectroscopy is a noninvasive investigative tool for probing the effect of defects on resistive switching [1, 2]. Annealing $La_2NiO_{4+\delta}$ films under inert (Ar) or oxidising (O_2) atmospheres results in devices with filamentary and interfacial-type resistive switching respectively [3]. In this work we explore the effect of the switching mechanism, readout voltage and area dependency on the noise characteristics of LNO-based RRAM.

[1] E. Piros, M. Lonsky *et al.* Phys. Rev. Appl. **14** (2020)
[2] T. Thyzel, M. Kopp *et al.* Meas. Sci. Technol. **36** (2025)
[3] A. Koroleva *et al.* Adv. Electron. Mater. 2400096 (2024)

TT 37.36 Wed 15:00 P4

Resistance Fluctuation (Noise) Spectroscopy in EuS and $LiCu_3O_3$ — •Philipp Swoboda[1], Demian Ranftl[1], Nazia Kaya[1], Katharina Zoch[1], Kristin Kliemt[1], Simon Moser[2], Cornelius Krellner[1], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]Institute of Physics, University Würzburg, Würzburg, Germany

Noise spectroscopy gives insights into the low-frequency dynamics of charge carriers in condensed-matter systems, which is energy-resolved information that can't be obtained from mean values alone. Here the interest lies in $1/f^{\alpha}$-noise, which can be described as a superposition of independent two-level processes. For instance it has been used to identify energy scales of thermally-activated switching processes like fluctuating polar nanoregions (PNR) in the past [1, 2]. In general the processes observed by resistance fluctuation are sensitive to slow dynamics. Examples are the slowing down of charge carriers in the vicinity of a metal insulator transition and the freezing of PNR at the onset of glassy dynamics. This work aims to use noise spectroscopy as a function of temperature and magnetic field in order to investigate how magnetic polarons influence the colossal magnetoresistance in the ferromagnetic semiconductor EuS, as well as to investigate the exotic electron glass phase in $LiCu_3O_3$.

[1] npj Spintronics 2, 24 (2024).
[2] Meas. Sci. Technol. 36 (2025) 015501.

TT 37.37 Wed 15:00 P4

Single spin-flip dynamics in the Ising model — •Luca Cervellera and Björn Sothmann — Faculty of Physics and CENIDE, University Duisburg- Essen, 47057 Duisburg

The surface of Si(001) consists of buckled Si dimers with alternating orientation in the ground state. At around 190 K, the system undergoes an order-disorder phase transition which can be described in terms of an antiferromagnetic 2D Ising model with anisotropic couplings [1]. Here, we aim at understanding the switching dynamics of a single Ising spin by means of Monte Carlo simulations of the temperature-dependent dynamics using different algorithms which allow us to analyze the waiting-time distribution and full counting statistics of spin flips.

[1] C. Brand et al., Phys. Rev. Lett. 130, 126203 (2023).

TT 37.38 Wed 15:00 P4

Quantum Monte-Carlo study of the bond- and site-diluted transverse-field Ising model — •Calvin Krämer, Max Hörmann, and Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik V, Staudtstraße 7, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We study the transverse-field Ising model on a square lattice with bond- and site-dilution at $T = 0$ by quantum Monte Carlo simulations. By tuning the transverse field h and the dilution p, the phase diagram of both models is explored. Finite-size scaling of the order parameter and averaged Binder ratios is employed to determine the positions of critical points and the critical exponents β and ν along the critical lines and at the multi-critical point. Dynamical properties in the vicinity of the quantum critical point are analyzed through the local susceptibility. We complement these findings by stochastic analytical continuation [1] of imaginary-time Green's functions, providing momentum-resolved insights into the behavior of excitations.

[1] Anders W. Sandvik, Phys. Rev. B 57, 10287

TT 37.39 Wed 15:00 P4

Typical medium theory for disordered electronic systems on simple lattices with Cauchy distribution of on-site potentials — Andreas Ostlin[1], Hanna Terletska[2], Dylan Jones[1], and •Liviu Chioncel[1,3] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Middle Tennessee State University, Murfreesboro, Tennessee, USA — [3]ACIT, University of Augsburg, Augsburg, Germany

Effective medium approaches using single-site averaging procedures of various kinds contributed substantially in understanding the density of states of electronically disordered systems in models and materials. The nature and the conditions for appearance of single-particle (Anderson) localization seems to be qualitatively understood, yet discussions concerning special applied methods and quantitative results for the critical conditions are still ongoing. Here we present results using the typical medium theory for the one-particle and two-particle Green's function (conductivities) for the special case of Cauchy-distribution.

TT 37.40 Wed 15:00 P4

Excitations and Their Decay: Calculating the Non-Lorentzian Line Shape of Excited States at the Ti $L_{2,3}$ edge in $SrTiO_3$ — •Sarah L. Görlitz[1], Sina Shokri[1], Widad Louafi[2], Martin Brass[1,3], Marc Merstorf[1], Jonas Hoecht[1], Michelangelo Tagliavini[1], Kevin Ackermann[1], and Maurits W. Haverkort[1] — [1]Institut for Theoretical Physics, Heidelberg University, 69120 Heidelberg — [2]Laboratory of Theoretical Physics, Faculty of Exact Sciences, University of Bejaia, 06000 Bejaia, Algeria — [3]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

Understanding electron dynamics in real materials following photon excitations is a challenging task. Ultrafast pump-probe and multi-color experiments require precise control, while strong electron correlations in excited states complicate the theoretical description. Accurate calculations must reproduce absorption line shapes for single-photon absorption, often non-Lorentzian due to multi-channel decay processes.

In this work, we calculate the line shape of Ti 2p $\rightarrow$ 3d core excitations in $SrTiO_3$. While crystal-field models predict seven delta-function peaks, the real spectrum reveals distinct line widths and non-Lorentzian line shapes. Incorporating Auger-Meitner decay, fluorescence decay, and coupling to the valence-conduction bath continuum, we establish a framework to explain these broadenings. This approach is critical for predicting higher-order response functions, essential for modeling resonant inelastic X-ray scattering (RIXS) and ultrafast spectroscopies, providing insights into the interplay of decay processes and electron dynamics.

TT 37.41 Wed 15:00 P4

Role of interlayer coupling and anisotropy in 1T-TaS_2 studied by ellipsometry — •Achyut Tiwari[1], Renjith M. Roy[1], Christian Prange[1], Yuan Yan[2], Bruno Gompf[1], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]School of Physics, Nankai University, Tianjin, 300071 China

The layered transition metal dichalcogenide 1T-TaS_2 has attracted considerable attention due to its rich electronic phase diagram, characterized by multiple charge density wave (CDW) phases. With decreasing temperature, the material transitions from a metallic incommensurate phase to a metallic nearly commensurate phase and finally to an insulating commensurate phase featuring the star-of-David lattice

distortion. The metal-insulator transition (MIT) is a first-order phase transition that exhibits hysteresis during cooling and heating, with an additional intermediate phase in the 215 K-280 K range upon heating. Here, temperature-dependent ellipsometry revealed pronounced anisotropy between in-plane and out-of-plane responses, attributable to significant interlayer interactions. The temperature-dependent out-of-plane dielectric constant exhibited marked changes across the MIT, highlighting the role of interlayer coupling. Furthermore, the effective medium approximation confirmed the existence of the intermediate phase during heating, providing a microscopic description. These findings underscore the importance of interlayer coupling in layered materials and elucidate on the previously unexplored intermediate phase of 1T-TaS_2.

TT 37.42 Wed 15:00 P4

The Interplay Between Diagonal and Off-Diagonal Electron-Phonon Coupling in two-dimensional systems — •Jadson Lucas Portela e Silva[1,2], Gabriel Rein[2], Sebastião A. S. Júnior[1], Willdauany C. F. da Silva[1], Fakher F. Assaad[2], and Natanael C. Costa[1] — [1]instituto de física universidade federal do rio de janeiro, rio de janeiro, brasil — [2]institut für theoretische physik und astrophysik, universität würzburg, würzburg, germany

The interplay between diagonal and off-diagonal electron-phonon coupling in two-dimensional systems is explored using the Holstein-Su-Schrieffer-Heeger (HSSH) model through non-perturbative Monte Carlo simulations on a square lattice at half-filling. Electron-phonon coupling is crucial in determining exotic phases like charge-density waves (CDW), valence bond solids (VBS), and superconductivity. The HSSH model uniquely combines features of the Holstein and SSH models, where the former modulates the on-site potential energy, and the latter modifies the electron's kinetic energy through lattice displacements. The study constructs phase diagrams by analyzing charge-charge, bond-bond, and pairing correlation functions. Key findings include a competition between CDW and VBS phases, similar to one-dimensional systems. However, unlike the 1D case, no metallic phase is observed between these states, likely due to perfect nesting and van Hove singularities in the density of states, which destabilize the Fermi liquid state. Further exploration beyond half-filling shows that melting of CDW and VBS phases leads to superconductivity.

TT 37.43 Wed 15:00 P4

Picosecond periodic oscillation modulated by Higgs amplitude mode in a superconductor-metal hybrid metasurface — •Siyu Duan[1,2], Jingbo Wu[1], Caihong Zhang[1], Kebin Fan[1], Biaobing Jin[1], and Zhe Wang[2] — [1]School of Electronic Science and Engineering, Nanjing University, Nanjing, China — [2]Department of Physics, TU Dortmund University, Dortmund, Germany

We report on a time-resolved terahertz spectroscopic study of a superconductor-metal hybrid metasurface that is fabricated by introducing superconducting microbridges into metallic resonators. By exploiting the nonlinear response of the superconducting NbN microbridges to a multicycle narrowband terahertz excitation pulse, we observe a picosecond periodic oscillation of terahertz transmission spectra. This oscillation contains components of the fundamental frequency of the narrowband excitation pulse and its second harmonic, which we ascribe tentatively to an excited Higgs mode oscillation. Furthermore, we can modulate the amplitude and duration of periodic oscillations by changing the field strength of the terahertz excitation pulse and the sample temperature.

TT 37.44 Wed 15:00 P4

Density Functional Theory-based Multiplet Ligand Field Theory Calculations of Ultrafast Pump-Probe Electron Dynamics in Correlated Materials — •Ruth Kaiser, Sina Shokri, and Maurits W. Haverkort — Heidelberg University, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Ultrafast pump-probe spectroscopy allows one to study and steer quantum materials on their fundamental time-scales. In correlated molecules and solids a theoretical understanding is challenging and quantitative predictions how coherently driven excitations decohere is highly non-trivial. We have developed a recipe for quantitatively predicting pump-probe spectra, starting with a Hamiltonian on a basis of local Wannier orbitals derived from density-functional calculations, describing the charge-transfer in the system and, on top of that, we include the full local Coulomb repulsion [1]. Using non-linear response theory, we then calculate the time-resolved spectra, such as photo-emission spectroscopy, x-ray absorption spectroscopy and resonant inelastic x-ray scattering, which captures the pump-probe dynamics. Our routine can be used for different types of correlated materials, such as Mott-Hubbard and Charge-Transfer insulators as well as molecules [2, 3]. Furthermore, we show examples where we implemented our method for real materials like NiO and SF_6 and compare our results with experiments.

[1] PRB 85, 165113 (2012);
[2] PRL 128, 153001 (2022);
[3] PRA 108, 032816 (2023).

TT 37.45 Wed 15:00 P4

Understanding Resonant Inelastic X-ray Spectroscopy Using Dynamical Mean-Field Theory and Model Hamiltonians — •Lukas Hellmann, Aleksandrs Zacinskis, Sina Shokri, Michelangelo Tagliavini, Kevin Ackermann, and Maurits W. Haverkort — Universität Heidelberg, Institut für Theoretische Physik, Philosophenweg 19, Heidelberg 69120 Germany

Using model Hamiltonians with local Coulomb interactions, we demonstrate how resonant inelastic X-ray scattering spectra (RIXS) can be interpreted within the framework of the dynamical mean-field approximation. Our approach incorporates both valence correlations and core-valence Coulomb repulsion, enabling a detailed examination of spectral features across the metal-insulator transition. The calculated RIXS spectra reveal two distinct types of excitations: (1) locally excited excitons exhibiting a resonant enhancement at constant energy loss, and (2) a fluorescence regime characterized by resonant intensity enhancement at constant emitted energy. We analyze the transition in intensity between these two excitation regimes and discuss its implications for understanding electronic dynamics. All calculations are performed directly on the real frequency axis using the software package Quanty (www.quanty.org). This methodology not only provides accurate predictions for RIXS spectra but also offers a versatile framework for studying the dynamics of other correlated systems.

TT 37.46 Wed 15:00 P4

Material Specific Real Frequency LDA+DMFT Calculations of Transition Metals — •Johann Collard, Michelangelo Tagliavini, Kevin Ackermann, Sina Shokri, Aleksanders Zacinskis, Lukas Hellmann, and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120, Heidelberg, Germany

3d transition metals exhibit a wide range of intriguing properties. At the same time their accurate theoretical description is challenging task due to the presence of correlated electrons in their open d-shells. Ab-initio approaches, such as LDA+DMFT (Local Density Approximation + Dynamical Mean-Field Theory), have proven successful in capturing many material-specific properties and electron correlation effects. Most existing DMFT algorithms rely on Quantum Monte Carlo simulations, which operate on imaginary frequencies. While effective for static property calculations, these methods require analytical continuation to compute spectral functions, a process that is ill-posed and thus computationally challenging. In this work, we demonstrate how real-frequency DMFT, as implemented in Quanty, can directly compute spectral functions within the LDA+DMFT framework for real materials. This approach avoids the complications of analytical continuation, providing a more straightforward and reliable means of exploring the spectral properties of 3d transition metals.

TT 37.47 Wed 15:00 P4

An Accessible Implementation and Detailed Test of Real-Frequency Dynamical Mean-Field Theory — •Aleksandrs Zacinskis, Sina Shokri, Kevin Ackermann, Michelangelo Tagliavini, and Maurits W. Haverkort — Heidelberg University, Institute for Theoretical Physics, Philosophenweg 19, 69120 Heidelberg, Germany

Dynamical Mean-Field Theory (DMFT) has become a powerful tool for studying materials with correlated electrons. However, most DMFT solvers operate on imaginary Matsubara frequencies, making the extraction of accurate spectral functions challenging due to the need for analytical continuation.

Here, we perform DMFT calculations using a real-frequency solver implemented in Quanty [1]. This implementation utilizes a one-particle basis of natural impurity orbitals [2] to investigate several correlated model systems with local interactions. We systematically examine critical metal-insulator transition interaction strengths and the chemical potential as a function of filling, comparing different bath discretization schemes and numerical cut-offs to manage Hilbert space size.

Our results demonstrate robust and satisfactory convergence at moderate computational costs, validating the reliability of this approach. All calculations were performed using the open-source quantum many-body code *Quanty* (www.quanty.org), emphasizing its accessibility for broader applications in correlated electron systems.
[1] Phys. Rev. B 85, 165113 (2012);
[2] Phys. Rev. B 90, 085102 (2014).

TT 37.48 Wed 15:00 P4

Engineering Correlated Electrons in Adatom Lattices on Semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project we explore other promising material candidates on SiC and other substrates that might realize (one-, two-, and three-band) Hubbard models at different fillings and a potential impact of spin-orbit coupling. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field.
[1] H.Menke, N.Enderlein *et al.*, arXiv:2410.17165.

TT 37.49 Wed 15:00 P4

Calculating Moments for Many-Electrons Systems — •Elaheh Adibi and Erik Koch — Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a combinatorial approach to calculate the M^{th} moment of an N-electron system, defined as $\langle E^M \rangle = \mathrm{Tr}\, H^M$. Working in the basis of Slater determinants $|\boldsymbol{\alpha}\rangle = \prod c^\dagger_{\alpha_i}|0\rangle$, matrix elements $\langle \boldsymbol{\alpha}|H^M|\boldsymbol{\alpha}\rangle$ may only be non-zero for terms where the orbital indices of the creation operators in H^M are permutations of the orbital indices of the annihilators. The trace for a given permutation can then be evaluated combinatorially, without having to deal with the many-body Hilbert space explicitly. Since all permutations related by cyclic rotations give the same contribution, we classify them into groups and evaluate the trace only for a single group member. For the special case of all orbitals in the permutation being different, the calculation simplifies further, as in this irreducible case all permutations written in terms of cycles with a given number of descents give the same contribution to the moment. Relating the groups of permutations for the irreducible and the reducible terms allows us to efficiently evaluate the moments.

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Exact t^1_{2g} Superexchange Hamiltonians for Complex Orbital Ordering — •Amit Chauhan, Xue-Jing Zhang, and Eva Pavarini — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

We derive exact superexchange interactions for t^1_{2g} systems with spin-orbit coupling. To this end we extend the formalism developed in [1], which we have successfully used in [2,3] to study the origin of orbital ordering. As first application we consider the case of cubic and tetragonal lattices and study the stability of complex orbital ordering in the presence of spin-orbit interaction and crystal-field splitting.
[1] X.-J.Zhang, E.Koch, E.Pavarini, Phys.Rev. B **105**, 115104 (2022);
[2] X.-J.Zhang, E.Koch, E.Pavarini, Phys.Rev. B **102**, 035113 (2020);
[3] X.-J.Zhang, E. Koch, E.Pavarini, Phys.Rev. B **106**, 115110 (2022).

TT 37.51 Wed 15:00 P4

Scaling and convergence behaviour of linked-cluster expansions — •Harald Leiser, Max Hörmann, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, Friedrich-Alexander Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

We derive effective block-diagonal Hamiltonians $H_{\text{eff}} = T^\dagger H T$ using the projective-cluster additive transformation (PCAT) [1]. Numerical linked-cluster expansions (NLCEs) are employed to study the (anti)ferromagnetic transverse-field Ising model (TFIM) on diverse lattice geometries such as chains and various ladders. By calculating energy gaps, we compare the scaling behavior with other methods such as deepCUT [2]. A key challenge arises from the presence of avoided-level crossings (ALCs) [3] which complicates convergence. To probe this issue, we analyze ALCs in the simplified setting of the XXZ model on a chain. A key property of PCAT is the cluster additivity of both H_{eff} and the generator $S = \log(T)$. This allows transforming larger systems via a cluster expansion in S. Using S from clusters up to size N, we compute $\exp(-S)H\exp(S)$ in the thermodynamic limit and compare it with standard NLCE and CUT methods [4]. Notably, S for local clusters generates higher-order terms, mitigating some scaling challenges in traditional cluster expansions.
[1] M. Hörmann et al., SciPost Phys. 15 (2023) 097.
[2] H. Krull et al., Phys. Rev. B 86.
[3] K. Coester et al., EPL, 110(2):20006.
[4] C. Knetter et al., EPJ B 13:209.

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Computing Excited States in Quantum Many-Body Clusters with Neural Network Support — •Max Kroesbergen[1], Louis Thirion[1], Gianluca Levi[3], Pavlo Bilous[2], Paul Fadler[1], Yorick Schmerwitz[3,4], Elvar Ö. Jónsson[3], Hannes Jónsson[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]University of Iceland, Reykjavik — [4]Max Planck Institute for Coal Research, Mühlheim

In this study, we used SOLAX [1], our newly developed Python library for configuration interaction (CI) calculations of fermionic quantum systems, to compute the energies of ground and excited states for various quantum clusters. SOLAX can leverage the power of a neural network (NN) classifier to perform selective CI which mitigates the exponential growth of the many-body Hilbert space. Our benchmarks indicate a significant boost in computational efficiency while maintaining high accuracy. We validate our method for the (discrete) Single Impurity Anderson Model [2] as well as molecular systems, such as N_2 and H_2 [3]. For the latter, we study the dissociation curves of ground- and excited states and their dependence on the underlying single-particle basis, including Hartree-Fock orbitals optimized for excited states. Additionally, SOLAX enables us to simulate spectral functions defined by a transition operator, providing deeper insights into the excitation dynamics of these systems.
[1] L. Thirion, P. Hansmann, P. Bilous, arXiv:2408.16915v1.
[2] P. Bilous *et al.*, arXiv:2406.00151.
[3] Y. L. A. Schmerwitz *et al.*, arXiv:2406.08154.

TT 37.53 Wed 15:00 P4

Using the Anderson Impurity Model to Look for Particles Beyond the Standard Model — •Vera Butz and Maurits W. Haverkort — Universität Heidelberg, Institut für theoretische Physik, Philosophenweg 19, 69120 Heidelberg

High-precision comparisons between experimental measurements and numerical simulations [1] not only test the accuracy of computational methods but also offer deeper insights into fundamental physics. In this work, we investigate the interaction of charged ions with multiple electrons and continuum states, presenting a generalized Anderson impurity model. The continuum states considered include photons, free electrons, or as-yet-unobserved particles, such as axions. These interactions can be described through the self-energy or hybridization function [2]. The real part of the self-energy induces energy shifts in atomic multiplets, such as the Lamb shift, while the imaginary part results in finite lifetimes for excited states, leading to phenomena like fluorescence or Auger-Meitner decay. When applied to highly charged heavy ions, whether in laboratory settings or astrophysical environments such as the Sun, these enhanced electron-photon (or other particle) interactions provide a platform to probe the Standard Model. Additionally, they may reveal evidence of new physics, including the potential detection of axions, a leading dark matter candidate that could also address the strong CP problem.
[1] Nat. Phys. 20, 921 (2024).
[2] arXiv:2307.13812v1.

TT 37.54 Wed 15:00 P4

Properties of the Density Matrix for Metavalent Materials — •Niklas Penner[1,2], Lucia Reining[1], Matteo Gatti[1], and Matthias Wuttig[2] — [1]ETSF, LSI, CNRS, CEA/DRF/IRAMIS, Ecole Polytechnique, Institut Polytechnique de Paris, France — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

In the experimental investigation of phase change materials and their unique properties, peculiarities in the bonding character were determined. A corresponding classification of these metavalent materials has so far been carried out on the basis of shared and transferred electrons. The corresponding values were determined using density functional theory (DFT) calculations. Density functional theory has become one of the most universal methods in condensed matter physics and material science to determine and investigate properties of materials. The longer-term goal of the present work is to investigate to which extent the spatial extension of the density matrix is characteristic for metavalent materials, and whether numerical calculations based on the Kohn-Sham formulation of density functional theory can capture this aspect.

TT 37.55 Wed 15:00 P4

Traces of powers of many-body Hamiltonians — •Marcus Kollar — Theoretische Physik III, University of Augsburg

The high-temperature expansion of the partition function for a many-body system of fermions or bosons involves Fock space traces of powers of the Hamiltonian. Here we use algebraic means to evaluate such moments for a fixed number of non-interacting particles with arbitrary discrete spectrum and express them as polynomials of power sums of the single-particle energies. In the fermionic case our expressions agree with those obtained by combinatorial considerations [1]. We discuss possible applications and generalizations of our results.
[1] E. Adibi and E. Koch, Verhandl. DPG, Berlin TT 80.44 (2024).

TT 37.56 Wed 15:00 P4

Ising model on a sphere — •Grigorios Makris[1], Fabian Hassler[2], Stefan Wessel[1], and Ion Cosma Fulga[3,4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]Institute for Quantum Information, RWTH Aachen University, Germany — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany

The study of the Ising models is of primary interest in the theory of phase transitions. The models have been extensively studied in flat space and analytical solutions exist in two dimensions. Their scaling behavior is known to substantial precision and confirms the theory of finite-size scaling.

Here, we study Ising models on the surface of a sphere. As it is generally not possible to place a regular lattice on a sphere, for arbitrary number of points, we implement the Fibonacci lattice. The lattice is tested to have a reasonably uniform distribution of points. In order to establish the expected $SO(3)$ symmetry, we first solve the free-particle problem as a tight-binding model and then utilize the hopping coefficients as interaction terms on the Ising model. This is shown to yield better, approximate, $SO(3)$ degeneracies on the low energy levels of the transverse-field Ising model. Having set up the Hamiltonian, we further investigate the critical point of the expected phase transition.

TT 37.57 Wed 15:00 P4

Two site entanglement in the two dimensional Hubbard model — Anna Kauch[1], •Gergo Roosz[2], Frederic Bippus[1], Daniel Wieser[1], Fakher Assaad[3,4], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]HUN-REN Wigner RCP, Budapest — [3]Universitat Wurzburg, 97074 Wurzburg, Germany — [4]Wurzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Wurzburg, Germany

We calculate the reduced density matrix of two sites in the two-dimensional Hubbard model using the D Gamma A method. We calculate the density matrix by calculating the expectation value of a complete set of hermitian operators in the subspace of the two sites. We can express these eigenvalues with the one- and two-particle Greens functions, and the imaginary time derivatives of these functions. The derivatives are calculated in Matsubara representation. To test convergence we compare our results for the second Renyi entropy with quantum Monte Carlo data. To investigate the entanglement and correlations of the Hubbard model we calculate the mutual information and the entanglement negativity between the two sites.

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Thouless time in a spin-1/2 XX ladder — •Kadir Çeven[1], Lukas Peinemann[1], Rohit Patil[2], Marcos Rigol[2], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany — [2]Department of Physics, Pennsylvania State University, University Park, USA

The eigenstate thermalization hypothesis (ETH) offers a powerful framework for understanding many properties of thermalization dynamics in non-equilibrium quantum many-body systems. Here, determining the time scales associated with thermalization is a key focus in the research of nonequilibrium dynamics of such systems. In this study, we investigate a spin-1/2 XX ladder, an experimentally realizable model exhibiting diffusive dynamics, to explore the connections among ETH, transport properties, and measures purely based on its energy spectrum. Specifically, we analyze the spectral form factor and the smooth spectral function, each of which provides a characteristic relaxation time scale potentially linked to the Thouless time–the longest relaxation time defined in terms of the diffusion constant. Using various numerical methods, we compare the time scales obtained from these different measures to identify potential discrepancies and similarities.

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Nonequilibrium Phenomena in Strongly Correlated Systems under Structured Fields — •Sajad Mirmohammadi and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg Karl-Freiherr-von-Fritsch-Str. 3 06120 Halle/Saale

Strongly correlated systems provide a rich platform for exploring quantum phenomena and understanding nonequilibrium many-body dynamics. A central challenge lies in unraveling the interplay of various interactions that govern the emergence of exotic quantum states. Here, we investigate how phase- and polarization-structured electromagnetic fields interact with strongly correlated materials modeled by the extended Peierls Hubbard Hamiltonian. Using exact diagonalization with the Lanczos algorithm, we demonstrate how structured fields imprint their characteristics onto excitation dynamics, including charge and spin density waves.

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Application of the TraSPI Method to Aharonov-Bohm Interferometry with Interacting Quantum Dots — •Alexander Hahn, Jürgen König, and Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen and CENIDE, 47048 Duisburg, Germany

Utilizing the *Transfer-matrix Summation of Path Integrals* (TraSPI) approach, we extend the method's application to the study of quantum transport in an Aharonov-Bohm interferometer housing two parallel quantum dots. Here the usage of TraSPI allows the calculation of the current influenced by the enclosed magnetic flux, in presence of Coulomb interaction. The numerical accuracy and efficiency of the TraSPI method allow for a detailed exploration of the interplay between quantum coherence and dot interactions.

TT 37.61 Wed 15:00 P4

Metastability in Correlated Electron Systems — •Lara Bremer[1], Martin Eckstein[1], Hugo Strand[2], and Tim Wehling[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [2]School of Science and Technology, Örebro University, SE-701 82 Örebro, Sweden

The objective of this study is to describe metastable states in correlated electron systems, with a particular focus on numerically accessing unstable solutions within coexistence regions of first-order phase transitions. Our work is based on the well-established phenomenon observed in the Mott transition of the single-orbital Hubbard model, where a coexistence region between a metallic phase and an insulating phase, accompanied by a third unstable solution, has been demonstrated within the framework of Dynamical Mean Field Theory. A Phase Space Extension algorithm is employed to effectively identify and analyse these solutions. By accessing this unstable solution, the double occupancy on this branch can be calculated, thus enabling the Landau free energy to be calculated via a thermodynamic route, as opposed to fitting a Landau free energy functional.

TT 37.62 Wed 15:00 P4

Simulating nonequilibrium systems in the steady-state: GW+EDMFT — •Fabian Künzel — University of Hamburg, 20355 Hamburg, Germany

The Keldysh formalism for nonequilibrium Green's functions provides a versatile theoretical framework for analyzing the dynamics and structure of correlated many-body systems. To address the intrinsic cubic

scaling of computational time in the Kadanoff-Baym equations (KBE) for nonequilibrium Green's functions, a truncation of the underlying memory kernel can be incorporated into the time-stepping algorithm of the NESSi simulation package. This reduces the computational cost to linear scaling with respect to the maximum simulation time. For systems where long-time dynamics extend beyond the capabilities of state-of-the-art methods, the KBE can be formulated within the Keldysh steady-state formalism. The resulting equations are then solved using a Fourier transform, enabling the description of systems with exponentially separated timescales. We aim to introduce new methods that extend the reach of the existing NESSi package and present a steady-state study of a Mott insulator, incorporating nonlocal correlations through a steady-state GW+EDMFT formalism.