TT 23: Correlated Electrons – Poster I

Time: Monday 18:00–20:00 Location: P1

TT 23.1 Mon 18:00 P1

High-field magnetization of clinoatacamite $Cu_2Cl(OH)_3$ — •David Röll[1], Leonie Stödter[2], Carolin Kastner[1], Sven Luther[3], Ralf Feyerherm[4], Dirk Menzel[1], Anja U. B. Wolter[5], Kirrily Rule[6], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig — [2]FZ Jülich, JCNS at MLZ, Garching, Germany — [3]HLD-EMFL, HZDR, Dresden-Rossendorf, Germany — [4]HZB, Berlin, Germany — [5]Leibniz IFW Dresden, Dresden, Germany — [6]ANSTO, Lucas Heights, Australia

The mineral clinoatacamite $Cu_2Cl(OH)_3$ is closely related to the Kagome material herbertsmithite $ZnCu_3Cl_2(OH)_6$ and has been discussed as a geometrically frustrated magnet. Its Kagome structure of Cu^{2+} ions features antiferromagnetic in-plane coupling and weaker ferromagnetic interlayer exchange, giving rise to exotic quantum states at low temperatures and in applied magnetic fields. In recent years, we have extensively characterized the magnetic phase diagram up to 14 T, revealing multiple distinct magnetic phases.

Here, we present high-field magnetization measurements on a single-crystalline sample up to 52 T. The magnetization at 2.2 K increases with field but begins to saturate at about 15 T, reaching only a fraction of full magnetization and indicating that the system is not fully magnetized. This stands in clear contrast to previously published results, where the mineral is reported to be fully magnetized at around 35 T. Consequently, we expect the magnetization to rise again at fields beyond our current range, implying the possible presence of a magnetization plateau.

TT 23.2 Mon 18:00 P1

Anisotropic spin models on frustrated lattices: from spin liquids to supersolids — •Martin Ulaga[1], Jure Kokalj[2,3], Takami Tohyama[4], and Peter Prelovšek[3] — [1]MPIPKS, Dresden, Germany — [2]University of Ljubljana, Faculty of civic and geotedic engineering, Ljubljana, Slovenia — [3]Institute "Jožef Stefan", Ljubljana, Slovenia — [4]Science universigy of Tokyo, Tokyo, Japan

Recent experiments on novel materials, best described by easy-axis spin models on a triangular lattice, stimulated renewed theoretical interest in basic properties of anisotropic spin models on frustrated planar lattices. While the thermodynamic properties of the model on the Kagome lattices are consistent with the spin-liquid scenario in the whole range of anisotropies, the case of the triangular lattice is more complex. Several numerical studies indicate that anisotropic systems should follow the supersolid scenario with broken translation symmetry in the ground state, as well as the transverse magnetic order, implying a gapless Goldstone mode. Confirming this scenario at finite magnetic fields, we find numerically that at zero field, the available evidence points instead to a solid with a finite gap.

TT 23.3 Mon 18:00 P1

Observation of spin-glass behavior in Nd — •Lorenz Pech[1], Lukas Bauer[1], Jiří Pospíšil[4], Christoph Franz[1], Leo Maximov[1], Andreas Bauer[1,3], Marc A. Wilde[1,3], and Christian Pfleiderer[1,2,3] — [1]Technical University of Munich (TUM) — [2]MCQST, Munich — [3]TUM Center for Quantum Engineering — [4]Charles University, Prague

Frustration and effective disorder in Nd are expected to produce frozen, disordered spins with slow, history-dependent dynamics [1]. We investigate the low-temperature magnetic and electronic properties of single-crystal neodymium to map its complex phase behavior and search for a spin-glass like state. To identify such phases, we combine temperature and field sweeps with ac magnetization (frequency-resolved), dc magnetization (ZFC/FC), and relaxation measurements. From anomalies in $\chi'(T)$, $\chi''(T)$, $M(H)$, and $\mathrm{d}M/\mathrm{d}H$ along principal crystallographic directions, we construct a T–B phase diagram. Established spin glass freezing criterias are the presence of a ZFC/FC bifurcation, a frequency-dependent shift of the χ' and χ'' peak, and slow non-exponential relaxation [2]. These benchmarks, together with more recent perspectives on complex low-temperature phases in correlated systems, provide the framework for interpreting our Nd data and distinguishing glassy behavior from conventional long-range magnetic order.

[1] Kamber, Umut et al. Science 368, eaay6757 (2020).
[2] K. Binder and A. P. Young, Rev. Mod. Phys. 58, 801 (1986).

TT 23.4 Mon 18:00 P1

Exploring Quantum Phases of Magnetic Skyrmions — •Marc Currle, Sopheak Sorn, and Markus Garst — Karlsruhe Institute of Technology, Karlsruhe, Germany

The topological skyrmion density in the continuum theory of two-dimensional magnets obeys both a dipole conservation law and the Girvin-MacDonald-Platzman algebra, suggesting a close correspondence with the quantum Hall problem [1]. Motivated by this observation, we explore quantum phases of skyrmions using analogies with integer and fractional quantum Hall states. Employing an effective description in terms of collective coordinates for skyrmions, we demonstrate that quantum states of the skyrmion many-body system can be represented as holomorphic wavefunctions similar to the states within the lowest Landau level. We highlight the consequences of this correspondence, in particular, the possibility of systematically applying methods from quantum Hall physics to identify skyrmion liquid states.
[1] S. Sorn, J. Schmalian, M. Garst, Phys. Rev. X 15, 041037 (2025)

TT 23.5 Mon 18:00 P1

Quantum Phase Transitions of Kitaev's Toric Code on a Honeycomb lattice — •Viktor Kott, Matthias Mühlhauser, Jan Alexander Koziol, and Kai Phillip Schmidt — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

We investigate the robustness of the topological phase of Kitaev's toric code in a uniform magnetic field on the honeycomb (and triangular) lattice using perturbative linked-cluster expansions (LCEs) based on a hypergraph decomposition, together with quantum Monte Carlo (QMC) simulations. The LCE approach allows us to correctly account for the nontrivial mutual exchange statistics of elementary anyonic excitations. By extracting the ground-state energy and excitation energies of the topological phase, we determine the quantum phase transitions out of the topologically ordered state. In addition, we use QMC to explore the full quantum phase diagram. In contrast to the conventional toric code on the square lattice, the ground-state phase diagram depends on the sign of the magnetic field, which distinguishes between unfrustrated and frustrated parameter regimes. This leads to distinct quantum-critical properties and a richer phase diagram.

TT 23.6 Mon 18:00 P1

The XY Toric Code on the Kagome lattice — •Constanze Kölbl, Maximilian Vieweg, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, 91058 Erlangen

This theoretical work investigates the XY toric tode on the Kagome lattice, constituting a generalisation of the 2024 introduced XY checkerboard toric code on the square lattice [1]. Main objectives are deriving ground state and low-excitation properties and further extracting the parameter-dependent quantum phase diagram of the model. Besides a four-spin z-flavour star operator, two kinds of plaquette operators are introduced, including both Pauli x and y interactions and realising a bipartition. Due to the geometry of the lattice, the plaquette operators connect three and six spins each. Star operators still act as symmetries of the Hamiltonian, whereas different plaquette operator types generally do not commute. The behaviour in the limit of isolated plaquettes is examined analytically using first-order perturbation theory, checking for topological order. Further intuition is gained from exact diagonalisation of the full Hamiltonian for a system comprising 24 spins. A duality mapping is performed, giving rise to a self-dual model built from four- and six-spin Ising interactions. Symmetries of the dual model are investigated, and high-order perturbation theory is performed. The general goal is to understand the influence of geometry on the physical properties of topological codes.
[1] M. Vieweg, K.P. Schmidt, Phys. Rev. Res., 7 (2025)

TT 23.7 Mon 18:00 P1

Stochastic series expansion quantum Monte Carlo for quantum lattice models beyond spin 1/2 — •Melanie A. R. Wolf, Anja Langheld, Calvin Krämer, Jan Alexander Koziol, and Kai Phillip Schmidt — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtdtr. 7, 91058 Erlangen, Germany

Stochastic series expansion quantum Monte Carlo is a well established

method for the quantitative investigation of quantum spin models with spin 1/2. Especially, the sampling of quantum Ising models with arbitrary interactions [1] without a sign problem, constitutes an important milestone in the development of the method. Therefore, it follows naturally to ask how to transfer this efficient sampling scheme to quantum systems with a larger local Hilbert space like spin-one or quantum Potts models. In our work we implement the stochastic series expansion quantum Monte Carlo scheme [2] and explore the quantum and thermal properties of quantum Potts models.
[1] A. Sandvik, Phys. Rev. E 68, 056701
[2] C. Ding et al., arXiv:1702.02675

TT 23.8 Mon 18:00 P1

Convergence behavior of non-perturbative linked-cluster expansions at criticality — •Harald Leiser, Max Hörmann, and Kai Phillip Schmidt — Chair for Theoretical Physics V, FAU Erlangen-Nürnberg, Germany

Non-perturbative linked-cluster expansions (NLCE) provide a systematic framework for computing properties of quantum lattice models directly in the thermodynamic limit. For applying it to excited states, we use a transformation T that block-diagonalizes cluster Hamiltonians, like the Schrieffer-Wolff transformation, while satisfying cluster-additivity. In perturbative linked-cluster expansions up to order N, certain classes of transformations all yield identical and exact results at order N. However, in non-perturbative LCE this equivalence breaks down entirely, as the hierarchical structure of contributions is absent. As a result, the non-perturbative effects introduced by different transformations can produce different convergence behavior, also depending on the observable under study. Our goal is to understand how different choices of T influence the convergence behavior and what these differences reveal about the transformations themselves. Furthermore, we aim to understand the role of the transformation T in extracting quantum-critical behavior from NLCEs. For that, we analyze the energy gap of the transverse-field Ising chain at its quantum critical point, since its exact solution reduces the computational complexity to polynomial, enabling comparison up to large system sizes.

TT 23.9 Mon 18:00 P1

Optimized Crystal Synthesis and Anistropic Magnetism of the 2D Layered Magnets $M\mathbf{PSe_3}$ (M = Fe, Ni, Mn) — •Masoumeh Rahimkhani[1], Saicharan Aswartham[2], Martin Kostka[1], Ashwini Balodhi[1], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]International Centre for Interfacing Magnetism and Superconductivity with Topological Matter, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland

Transition-metal phosphochalcogenides $M\mathrm{PSe_3}$ (M = Fe, Ni, Mn) are important layered van der Waals materials with rich magnetic and electronic behavior. Among them, $\mathrm{FePSe_3}$ is a much investigated layered antiferromagnet with strong potential for applications in two-dimensional spintronics and quantum devices.

Here, we use an additive-free chemical vapor transport technique for growth of single crystals of $\mathrm{FePSe_3}$. Single crystals reach up to 3 mm in length and show nearly ideal atomic ratio composition in energy-dispersive x-ray spectroscopy. Magnetic measurements reveal an antiferromagnetic transition around 120 K. We studied the effect of substitution at the Fe site on the anistropic magnetism. We will discuss how substituted $\mathrm{Fe_{1-x}}M_x\mathrm{PSe_3}$ single crystals can be prepared and how substitution at the Fe site affects the anisotropic magnetism.

TT 23.10 Mon 18:00 P1

Electronic and Magnetic Properties of $\mathbf{CaMn_2P_2}$ and $\mathbf{SrMn_2P_2}$ Single Crystals — •Jule Kirschke, Joscha Grunwald, T. R. Thomas, N. S. Sangeetha, Ashiwini Balodhi, Andreas Kreyssig, and Anna E. Böhmer — Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany

$\mathrm{CaMn_2P_2}$ and $\mathrm{SrMn_2P_2}$ are insulators that adopt the trigonal $\mathrm{CaAl_2Si_2}$-type structure containing corrugated Mn honeycomb layers. Here, we report a systematic study of single crystals grown from Sn flux, including attempts to synthesize $\mathrm{Sr_{1-x}K_xMn_2P_2}$, which revealed that K does not substitute in the $\mathrm{SrMn_2P_2}$ structure. In contrast, $\mathrm{CaMn_2P_2}$ exhibits an unexpected sensitivity to the Ca content used during growth. While powder x-ray diffraction confirms identical crystal structures for all batches, their transport properties differ drastically. Samples prepared with high Ca content during the growth anomalously show almost metallic temperature dependence of the resistivity, whereas others show the insulating behavior commonly reported in the literature. The electronic and magnetic properties of different samples were studied by heat capacity and magnetization measurements.
We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288.

TT 23.11 Mon 18:00 P1

Quantum effects in the magnon spectrum of 2D altermagnets on a square lattice and anisotropic honeycomb lattice via continuous similarity transformations. — •Dag-Björn Hering[1], Vanessa Sulaiman[1], Raymond Wiedmann[3], Matthias R. Walther[2], Götz S. Uhrig[1], and Kai P. Schmidt[2] — [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 — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569, Stuttgart, Germany

We investigate quantum effects on magnon excitations in a minimal spin-1/2 Heisenberg model for 2D altermagnets on the square lattice and for an anisotropic honeycomb lattice. For both, a continuous similarity transformation is applied in momentum space to derive an effective Hamiltonian that conserves the number of magnon excitations. This allows us to quantitatively calculate the one-magnon dispersion, the effects of magnon-magnon interactions, and the dynamic structure factor in a certain range of parameters. For the altermagnet, we focus on the altermagnetic spin splitting of the magnon bands and the size of the roton minimum. For the honeycomb, we additionally analyze the ground state energy and the staggered magnetization. We further analyze the stability of the assumed long-range order and the magnons by different generators.

TT 23.12 Mon 18:00 P1

Spectral densities for inelastic scattering in anisotropic Heisenberg models on mono- and bilayer square lattices and the 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] with a magnon-conserving generator to the antiferromagnetic anisotropic XXZ model. For the square lattice, the resulting effective Hamiltonian has already been analyzed [2]. 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, as well as the bilayer square lattice. These are compared to experimental data from RIXS measurements [3], for example with single-layered $\mathrm{Ca_2CuO_2Cl_2}$ and bilayer $\mathrm{Sr_3Ir_2O_7}$.
[1] M. Powalski et al., Phys. Rev. Lett. **115**, 207202 (2015) and SciPost Phys. **4**, 001 (2018)
[2] M. R. Walther et al., Phys. Rev. Research **5**, 013132 (2023)
[3] K.-J. Zhou et al., J. Synchrotron Rad. **29**, 563 (2022)

TT 23.13 Mon 18:00 P1

Hall Response, Angular Magnetoresistance, and Field-Induced Metamagnetism in $\mathbf{Sr_4Ru_3O_{10}}$ — •Ilke Masa[1], Simone Seipel[1], Lara Pätzold[1], Zahra Ghazinezhad[1], Agustinus Agung Nugroho[2], Markus Braden[1], and Thomas Lorenz[1] — [1]Institute of Physics II; University of Cologne, Germany — [2]Bandung Institute of Technology, Indonesia

$\mathrm{Sr_4Ru_3O_{10}}$ is a ferromagnetic metal with $T_C \approx 105$ K and exhibits an additional metamagnetic transition below 50 K, whose microscopic origin remains unclear. We investigate single crystals to characterize the anisotropy of magnetization and electrical transport. For in-plane currents, we measure both the normal and anomalous Hall effects, finding a non-monotonic temperature dependence and a low-temperature sign reversal of the anomalous Hall signal, similar to behavior known from $\mathrm{SrRuO_3}$ and associated with Weyl points in its band structure. Due to the layered crystal structure, the out-of-plane resistivity is highly anisotropic ($\rho_c \gg \rho_{ab}$) and shows pronounced changes across the metamagnetic transition. From magnetoresistance data, we extract the field-induced metamagnetic transition at low temperatures and analyse the angular dependence of both the transition fields and the in-plane magnetoresistance. We also identify a clear angular magnetoresistance response in $\mathrm{Sr_4Ru_3O_{10}}$. Possible low-temperature phases remain sub-

jects of ongoing research.

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TT 23.14 Mon 18:00 P1

Heat Transport and Thermodynamic Properties of the Quasi-Two-Dimensional Quantum Magnet $Cu_2(OH)_3Br$ — •Nainish Tickoo[1], Rohit Sharma[1], Lucas Berger[1], Zhiying Zhao[2], Zhe Wang[3], and Thomas Lorenz[1] — [1]Institute of Physics II, University of Cologne, D-50937 Cologne, Germany — [2]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China — [3]Department of Physics, TU Dortmund University, D-44227 Dortmund, Germany

$Cu_2(OH)_3Br$ is a quasi-two-dimensional quantum magnet that can be seen as a system of coupled antiferromagnetic spin-1/2 chains. Specific heat, magnetisation and magnetostriction measurements have shown pronounced anomalies at T_N = 9.3 K. These measurements, along with Monte Carlo simulations, have shown that below the T_N, the system undergoes a field-induced transition from a 3D ordered state to a partially decoupled state when a magnetic field (B_c = 16.3 T) is applied transverse to the ordered spins. This transition is interpreted as a dimensional reduction arising from the distinct responses of the AFM chains to an external magnetic field [1]. This study examines the thermal conductivity κ (T, B) of $Cu_2(OH)_3Br$ single crystals under magnetic fields applied along the crystallographic b axis. Strong anomalies in κ near T_N reveal a significant interplay between phonons and magnetic excitations in low-temperature heat transport

Funded by the DFG via CRC 1238 Projects A01, B01 and B04.

[1] A. Reinoldet al., Phys. Rev. B 111, L100405 (2025)

TT 23.15 Mon 18:00 P1

Magnetic and Electronic Transport Behavior in Cr-Based Quantum Materials — •Shitao Qu, Ran Tao, Mengmeng Long, Mads Fonager Hansen, and F. Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Unconventional superconductivity among transition metal compounds is seen in Cu-, Fe- and most recently Ni-based materials. What about other transition metal systems? There are a surprising number of **chromium**-based superconductors, often in conjunction with applied pressure: CrAs, $A_2Cr_3As_3$ (with A an alkaline metal), ACr_3As_3, and $CsCr_3Sb_5$. Moreover, CrSb is one of the best-studied metallic altermagnets. These findings motivate a wider study of Cr-based correlated electron materials.

We initially investigate (i) CrP – an isostructural and isoelectronic relative to CrAs, (ii) CrSe – an altermagnet candidate, and (iii) the Kagome lattice systems $CsCr_3Sb_5$ and $CsCr_6Sb_6$.

Single crystals are prepared via flux and vapour-transport techniques and characterised in standard X-ray, magnetometry and transport measurements. They enable studies of the electronic structure and magnetic/superconducting phase diagram, forming a promising basis for exploring correlated-electron behavior in Cr-based quantum systems more widely.

TT 23.16 Mon 18:00 P1

Correlated Electronic Structure of Layered Cathode Material LiMnO2 — •Owen Colire, Francesco Cassol, and Silke Biermann — Centre de Physique Théorique (CPHT), Ecole Polytechnique, Institut Polytechnique de Paris, CNRS, Palaiseau, France

Electronic Coulomb correlations are ubiquitous in transition metal compounds. Our work focuses on layered LiMnO2, a cathode material used in Li-ion batteries, which crystallizes in a monoclinic structure with alternating Lithium and MnO6 layers. The compound is a Mott insulator with a high-spin d4 configuration undergoing a transition to an antiferromagnetically ordered state below the Néel temperature of 250 K. We investigate the electronic structure using Density Functional Theory calculations and combined Density Functional - Dynamical Mean Field Theory, with an emphasis on the interplay of the intra-atomic Hund's exchange coupling and crystal field splittings.

TT 23.17 Mon 18:00 P1

Non-equilibrium Charge Dynamics at the metal-insulator transition in κ-$(BETS)_2Mn[N(CN)_2]_3$ — •Sangeeta Panwar[1], Tim Thyzel[1], Jens Müller[1], Mark Kartsovnik[2], and Natalia Kushch[3] — [1]Institute of Physics, Goethe-Universität Frankfurt, Frankfurt (Main), Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften,Garching, Germany — [3]private

Low-dimensional molecular conductors have been shown to host electronic ferroelectricity, where electronic degrees of freedom cause polar order, allowing for fast switching and phase control [1]. Using fluctuation spectroscopy, we recently investigated the nature of electronic ferroelectricity in the organic conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ [2], representative of a broader class of quasi two-dimensional correlated electron systems. Here, we explore how these phenomena evolve when tuning the bandwidth by applying hydrostatic pressure. We will investigate the slow dynamics of polar nanoregions (PNR) and the evolution of drastic changes in the dynamics as the system is tuned from the insulating to the superconducting phase. By employing fluctuation spectroscopy under pressure, we aim to study how superconductivity emerges from the ferroelectric/multiferroic insulating state and to examine how PNR formation and glassy dipolar freezing evolve [3].

[1] Lang et al., J. Electronic Materials 54, 5087 (2025)
[2] Thomas et al., npj Spintronics 2, 24 (2024)
[3] Zverev et al. PRB 82, 155123 (2010)

TT 23.18 Mon 18:00 P1

Ru L-edge RIXS on the dimer compound $Ba_3CeRu_2O_9$: a cluster Mott insulator? — •Lara Pätzold[1], Frederik Paech[1], Enrico Bergamasco[1], Henrik Schilling[2], Anna Sandberg[3], Hlynur Gretarsson[4], Petra Becker-Bohatý[2], Maria Hermanns[3], and Markus Grüninger[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Kristallographie, University of Cologne, Germany — [3]KOMKO, University of Stockholm, Sweden — [4]DESY, Hamburg, Germany

Cluster Mott insulators host charge carriers in quasi-molecular orbitals on, e.g., dimers or tetramers [1-2]. With strong spin-orbit coupling, this may yield unconventional quasi-molecular magnetic moments tunable via, e.g., intracluster hopping. Cluster Mott insulators emerge in 5d transition-metal compounds due to large hopping, whereas in 3d materials one expects conventional Mott behavior with carriers localized on individual sites. To clarify whether cluster Mott insulators are realized in 4d compounds, we address the electronic structure of $Ba_3CeRu_2O_9$ that hosts Ru_2O_9 dimers with 4 t_{2g} holes. Ru L-edge RIXS and exact diagonalization reveal a rich excitation spectrum on top of an intricate non-magnetic ground state in the intermediate regime. Compared to 5d cluster Mott insulators, $Ba_3CeRu_2O_9$ shows reduced intracluster hopping, smaller spin-orbit coupling, and larger electronic correlations, realizing an intriguing part of phase space.

[1] Revelli *et al.*, Sci. Adv. **5**, eaav4020 (2019).
[2] Magnaterra *et al.*, PRL **133**, 046501 (2024).

TT 23.19 Mon 18:00 P1

Sample-Based Quantum Diagonalization of Similarity-Transformed Hamiltonians for Strongly Correlated Systems — •Emanuele Ricci[1,2] and Werner Dobrautz[1,2,3,4] — [1]Technical University Dresden, 01069 Dresden, Germany — [2]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

One of the central challenges in electronic structure theory is the accurate description of strongly correlated systems. We address this using a hybrid quantum-classical scheme, sample-based quantum diagonalization, in which a quantum computer acts as a dedicated sampler to identify a compact, problem-adapted subspace of important Slater determinants. The corresponding reduced Hamiltonian is then diagonalized classically to obtain the ground state. To mitigate quantum errors, we apply a classical post-processing step that projects samples onto the correct particle-number sector.

Before sampling, we perform a similarity transformation of the Hamiltonian that concentrates the ground-state weight into a smaller set of determinants, reducing the relevant subspace and improving accuracy at the cost of a non-Hermitian effective Hamiltonian. While non-Hermiticity would ordinarily hinder quantum algorithms, we demonstrate that it can still be exploited within a sampling-based framework using the UCJ (unitary cluster Jastrow) ansatz initialized with single and double amplitudes from the transformed Hamiltonian.

TT 23.20 Mon 18:00 P1

A Local-Wave Basis for the Hubbard Model — •Leon Wastl[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069

Dresden, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

The Fermi-Hubbard model is the prototypical model for interacting electrons and can be employed to describe a wide variety of physical phenomena. Its 2D version is believed to contain the fundamental physics describing low-temperature superconductivity. We present a new basis for the two-dimensional Hubbard model which we call the local-wave basis as it is a hybrid between real space and momentum space. We numerically study the advantages of our newly found transformation using the density matrix renormalization group (DMRG). Since DMRG in its more recent form is a method that is inherently one-dimensional as it is built on top of the matrix product state (MPS) formalism, we combine our local-wave basis with a new way of ordering the sites in the MPS based on a modified version of simulated annealing (SA) using the two-site mutual information as its objective function. Combined with this approach to find the optimal ordering, we show that our method yields lower energies for the same maximal bond dimension than both the pure momentum space and the real space formulation in the low to intermediate U/t regime.

TT 23.21 Mon 18:00 P1

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

We describe an approach for computing the M^{th} moment of an N-electron system, defined as $\langle E^M \rangle = \mathrm{Tr}\, H^M$. Since the Hamiltonian H consists of pairs of creation-annihilation operators and the calculation is performed in the basis of Slater determinants $\{|\mathrm{I}\rangle\}$, the matrix element $\langle \mathrm{I}|H^M|\mathrm{I}\rangle$ contributes to the moment only when the orbital indices of the creation operators form a permutation of those of the annihilation operators. Writing the permutations in cycle notation, the simplest contributions arise from permutations creating a single cycle in which all orbitals are different. These permutations are classified by their number of descents. Permutations with the same number of descents contribute equally to $\sum_{\mathrm{I}} \langle \mathrm{I}|H^M|\mathrm{I}\rangle$. Since the number of permutations with the same number of descents is given by the Eulerian numbers, it suffices to compute the trace for one permutation and multiply the result by this number. In this way the trace can be evaluated combinatorially, without explicitly constructing the many-body Hilbert space. We are able to calculate the all other permutations with respect to these permutations. Finally, we present a recursive formula for the moment that is computationally efficient.

TT 23.22 Mon 18:00 P1

Polynomial Neural Networks in Quantum Many-Body Physics — •Ashish Yashwanth Kangen[1,2] and Werner Dobrautz[1,2,3,4] — [1]Technical University Dresden, 01069 Dresden, Germany — [2]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Polynomial neural networks were originally derived by applying tensor decompositions to high-order weight tensors. This derivation yields a model architecture that is inherently non-linear through Hadamard products, effectively eliminating the need for standard, tensor-unfriendly activation functions like ReLU.

In this work, we investigate the utility of this architecture within the context of quantum many-body physics and chemistry. We demonstrate that the algebraic properties of these polynomial expansions allow them to serve as robust, activation-free representations of complex quantum correlations. We explore two specific applications: (1) as a standalone wave function ansatz, which can be optimised via both deterministic Density Matrix Renormalization Group sweeps and Variational Monte Carlo, and (2) as a Jastrow correlation factor within the Transcorrelated approach for Quantum Chemistry, trainable via standard gradient-based machine learning optimisation. This framework suggests that the tensor structure underlying polynomial networks offers a flexible and numerically stable bridge between classical deep learning and quantum simulation.

TT 23.23 Mon 18:00 P1

Quantics tensor trains: Quantifying entanglement across length scales — Stefan Rohshap[1], Jheng-Wei Roshap[2], •Alena Lorenz[3], Serap Hasil[1], Karsten Held[1], Anna Kauch[1], and Markus Wallerberger[1] — [1]TU Wien — [2]Univ. Grenoble Alpes — [3]JMU Würzburg

Understanding entanglement remains one of the most intriguing problems in physics. In contrast to particle and site entanglement, length or energy scale entanglement, quantifying the information exchange between different length scales, has received far less attention. Here, we identify the quantics tensor train (QTT) technique, a matrix product state-inspired approach for overcoming computational bottlenecks in resource-intensive numerical calculations, as a renormalization group method by analytically expressing an exact cyclic reduction-based real-space renormalization scheme in QTT language. We precisely match the QTT bond dimension, a measure of length scale entanglement, to the number of rescaled couplings generated in each coarse-graining renormalization step and present our results for the one-dimensional tight-binding model with n-th-nearest-neighbor hopping. Furthermore, though analytically unfeasible, we numerically generate the bond-dimension of the two- and three-dimensional case of the interacting and non-interacting Green's function in momentum space and find, that for the interacting as well as for the one-dimensional non-interacting Green's function, the bond dimension saturates when lowering the temperature.

TT 23.24 Mon 18:00 P1

DMFT-Lanczos study of Alkali-Doped Fullerides: Superconductivity across the (U,J) plane — •Lara Bremer, Lorenzo Crippa, Igor Krivenko, and Tim O. Wehling — I. Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg

Alkali-doped fullerides (A_3C_{60}) provide a versatile platform for studying unconventional s-wave superconductivity in a strongly correlated setting, where superconducting phases emerge in close proximity to Mott insulating states. These molecular superconductors exhibit critical temperatures up to about 40 K. Theoretical descriptions of alkali-doped fullerides commonly employ a three-orbital Hubbard-Kanamori model whose defining feature is an effective negative Hund's coupling arising from the coupling of the electronic states to intramolecular Jahn-Teller phonon modes, thereby reversing the usual Hund's rules.

In this contribution we present calculations performed with the multi-orbital Lanczos impurity solver of the EDIpack library within a dynamical mean-field theory framework. We explore the (U, J) interaction space, focusing on the evolution from the regime of weak negative Hund's coupling to regimes with strongly negative Hund's coupling. We analyze how the interplay between the Mott insulating phase present for large Hubbard interaction U and the charge-disproportionated insulating phase present for large negative values of J influences the character of the superconducting states and ehances critical temperatures.

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Investigating Non-Hermitian Dynamics in Neural Quantum States — •Mohammed Boky[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [2]Technical University Dresden, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Both the Neural Quantum States (NQS) and the Transcorrelated (TC) method have proven to be impactful approaches in Ab Initio quantum chemistry and quantum many-body settings. The potential of combining these methods remains largely unexplored. In this work, the application and impact of the combination of these methods are explored with a focus on the computational cost.

The application of the similarity transform in the TC method yields non-Hermitian Hamiltonians. The optimization and impact of this non-Hermiticity on NQS dynamics pose both a great challenge and a source of unexplored possibilities to navigate physics with correlations that differ in magnitude.

In order to investigate both the impact and challenges of these methods, a study is done on a variety of different systems. These systems range from Ab Initio quantum chemistry problems such as hydrogen chains, to lattice models such as the non-Hermitian Transverse Field Ising and the Hubbard model.

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Non-equilibrium DMFT solved with the help of Tensor Cross Interpolation — •Bastian Schindler[1], Eva Paprotzki[1,2], and Martin Eckstein[1,2] — [1]I. Institute for Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

The non-perturbative solution of the quantum impurity problem provides the biggest computational challenge when DMFT is applied in non-equilibrium. Most applications of non-equilibrium DMFT are based on simplified perturbative solutions [1]. In diagrammatic approaches to the impurity model, the numerical integration of high-dimensional expressions poses the main computational bottleneck, limiting feasible expansion orders and the number of accessible time steps. Tensor Cross Interpolation (TCI) has recently emerged as a powerful technique to mitigate the exponential scaling of computational cost with dimensionality [2]. In this work, we apply TCI to diagrammatic expressions obtained from a pseudo-particle expansion of the hybridization around the atomic limit in the non-equilibrium steady state. We demonstrate that, with an appropriate parametrization and an FFT-based integration scheme [3], TCI yields a significant speed-up for higher-order contributions. Moreover, we employ TCI to efficiently evaluate the multidimensional integrals required for higher-order spectroscopy, in particular time-resolved resonant inelastic x-ray scattering.

[1] Murakami et al., Rev. Mod. Phys. 97.3 (2025)
[2] Núñez Fernández, et al., SciPost Physics 18.3 (2025)
[3] Eckstein, arXiv:2410.19707 (2024)

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Stochastic semiclassical electron-lattice dynamics with DMFT — •Tom Kahana, Francesco Valiera, and Martin Eckstein — I. Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany

The interplay between lattice motion and strongly correlated electronic phases poses a major challenge in nonequilibrium condensed-matter systems, especially near phase transitions where ionic distortions strongly affect the electronic state. We address this problem by solving the coupled electron-lattice dynamics using a quasi-equilibrium (adiabatic) Dynamical Mean-Field Theory on an inhomogeneous lattice defined by the instantaneous phonon configuration. Conservative forces, friction, and stochastic contributions to the lattice dynamics are obtained from the electronic correlation functions. Because each lattice site must be treated as an impurity embedded in a self-consistent bath, this approach is computationally demanding. To make it feasible, we replace the DMFT impurity solver with a trained neural-network emulator that reproduces high-order impurity solutions. This NN-accelerated DMFT loop enables computationally efficient simulations of the coupled electron-lattice dynamics on inhomogeneous lattices. We present benchmarks for the Hubbard-Holstein model. The method provides a path toward simulations of photo-induced transitions in correlated materials, such as Mott and charge-ordered states.

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Superradiance in Higher-Order Correlated Collective Emission — •Daniil Platonov[1,2], Xin H. H. Zhang[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

We investigate supercorrelated decay of an initially inverted ensemble of two-level emitters, where cooperative emission is governed by higher powers of the collective decay operator beyond conventional Dicke superradiance. We develop a qualitative theoretical framework that captures the essential mechanism of generalized supercorrelated decay and predicts the corresponding scaling laws. This framework clarifies the physical distinctions between conventional superradiance and higher-order supercorrelated emission. We further analyze the phenomenon in a waveguide quantum electrodynamics setting, where guided modes mediate strong collective interactions. By deriving an effective semiclassical theory, we obtain a computationally efficient description that enables large-scale simulations of the dynamics.

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Hierarchy of timescales in a disordered spin-1/2 XX ladder — •Kadir Çeven, Lukas Peinemann, and Fabian Heidrich-Meisner — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Understanding the timescales associated with relaxation to equilibrium in closed quantum many-body systems is one of the central focuses in the study of their non-equilibrium dynamics. At late times, these relaxation processes exhibit universal behavior, emerging from the inherent randomness of chaotic Hamiltonians. In our work [1], we investigate a disordered spin-1/2 XX ladder – an experimentally realizable model known for its diffusive dynamics – to explore the connection between transport properties and spectral measures derived solely from the system's energy levels via these relaxation timescales. We begin by analyzing the spectral form factor, which yields the time when the system begins to follow the random matrix theory (RMT) statistics, known as the RMT time. We then determine the Thouless times – the average times for a local excitation to diffuse across the entire finite system – through the linear-response theory for both spin and energy transport. Our numerical results confirm that the RMT time scales quadratically with system size and upper bounds the Thouless times. Interestingly, we also find that, unlike other non-integrable models, spin diffusion proceeds faster than energy diffusion.

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[1] K.Çeven,L.Peinemann,F.Heidrich-Meisner,arXiv:2509.20078(2025).

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Charge carrier relaxation dynamics in the one-dimensional Kondo lattice model — •Arturo Perez Romero, Mica Schwarm, and Fabian Heidrich-Meisner — Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

A generic question in the field of ultrafast dynamics is concerned with the relaxation dynamics and the subsequent thermalization of optically excited charge carriers. Among several possible relaxation channels available in a solid-state system, we focus on the coupling to magnetic excitations. In this paper, we study the real-time dynamics of a paradigmatic model, the Kondo lattice model in one dimension. We conduct a comprehensive study of the relaxation processes by evaluating the spin polarization of the conduction electron, the local spin-spin correlation between localized and conduction electrons, and the electronic momentum distribution. While in the well-studied cases of one or two charge carriers in a ferromagnetic background, no thermalization occurs, we demonstrate that the stationary state is compatible with thermalization if either the electronic filling is finite or the magnetic background is in the singlet sector. Our real-time simulations using the time-dependent Lanczos method are corroborated by a direct comparison with finite-temperature expectation values and an analysis of the spectrum in terms of the gap ratio.

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TT 23.31 Mon 18:00 P1

Collective dynamics in $SmNiC_2$ probed by time resolved spectroscopy — •Priyanka Yogi[1], Chandra V Kotyada[1], Bhageerath Swaraj[1], Amon. P Lanz[1], Amir.A Haghighirad[2], Sofia. M Souliou[2], Matthieu Le Tacon[2], and Jure Demsar[1] — [1]JGU Mainz — [2]KIT

Rare-earth transition-metal carbides $RNiC_2$ are a unique class of intermetallic compounds that crystallize in a non-centrosymmetric orthorhombic $CeNiC_2$-type structure. Except for $LaNiC_2$ and $CeNiC_2$, where exotic superconductivity has been reported, most members of this family exhibit quasi-1D charge-density-wave (CDW) order and competing magnetic order at low temperature. $SmNiC_2$ is unique, where an incommensurate CDW order appearing below $T_{CDW} \approx 148$ K gets fully suppressed below a first-order transition into a ferromagnetic (FM) phase at $T_M \approx 18$ K.

Here, we employ optical pump-probe spectroscopy to investigate the interplay between the FM and CDW phases by probing single-particle and collective dynamics as a function of temperature. The FM phase is characterized by rather slow (10 ps) demagnetization dynamics, while in the CDW phase, we observe characteristic CDW collective modes. The dominant amplitude mode is found at 1.45 THz, showing pronounced softening towards T_{CDW}. Excitation density-dependent studies provide additional information on the strength of the two phases.

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High precision physics in Anderson impurity models, from neutrino mass to axion production in the sun. — •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 not only test the accuracy of computational methods but also offer deeper insights into fundamental physics. In this work, we investigate how charged ions with multiple electrons interact with continuum states, such as photons, free electrons, or as-yet-unobserved particles. This is achieved by using a generalized Anderson impurity model, in which the interactions can be described via the

self-energy or hybridization function. 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. Using this method of high-precision calculations of decay rates, on highly charged heavy ions in laboratory or astrophysical settings, allows us to probe the Standard Model. Be that by measuring unknowns, like the neutrino mass [1] or discovering new potential particles like dark matter candidates [2].
[1] Nat. Phys. 20, 921 (2024)
[2] JCAP 09 (2021) 006

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Critical dynamics at isostructural instabilities — •Nick Sander — Karlsruhe Institute of Technology

At an elastic structural instability at least one of the elastic moduli vanishes. An acoustic phonon only softens at such an instability if it is accompanied with a change of crystal symmetry. At isostructural transitions with vanishing bulk modulus, however, no softening occurs and all microscopic phonon modes remain non-critical [1]. Nevertheless, we demonstrate that there exist four macroscopic critical elastic modes that will determine the critical dynamics at such an instability. These modes represent conformal symmetry transformations and the displacement vector satisfy a corresponding Killing equation, whose exact form depends on the crystal symmetry. We discuss implications for instabilities in correlated materials like the Mott metal-insulator transition, and realizations with mechanical metamaterials.
[1] R. A. Cowley, Phys. Rev. B 13, 4877 (1976)

TT 23.34 Mon 18:00 P1

Quantum geometry in the context of many-body perturbation theory — •Mario Geoffroy and Corentin Morice — Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, Orsay, France

Quantum geometry gives rise to some of the most topical physical phenomena in the past decades, but our current understanding of it remains based on single-particle topological band theory, and fails in the presence of electronic correlations [1]. This is particularly problematic given the overwhelming usage of density functional theory for the diagnosis of topological states in materials [2]. Many-body generalizations of the Chern number and other invariants have been put forward, but many-body quantum geometry remains elusive. We study the influence of electronic interactions on the Berry curvature in tractable systems, in view of developing formalisms adapted to accurate predictions in real materials.
[1] J. Vidal et al., PRB 84, 041109(R) (2011)
[2] B. Bradlyn et al., Nature 547, 298 (2017)

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Higher-harmonic generation in the driven Mott-Hubbard model — •Abdelrahman Azab, Friedemann Queisser, and Ralf Scheutzhold — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Motivated by recent experiments, we study the generation of higher harmonics in the Mott insulator state of the Fermi-Hubbard model under the influence of an oscillating external electromagnetic field, see also [1]. We find a strong dependence of the higher-harmonic intensity on the spin order (e.g., anti-ferromagnetic versus paramagnetic phase).

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[1] F. Queisser and R. Schützhold, Phys. Rev. B 109, 205110 (2024).