TT 34: Correlated Electrons: Theory 2

Time: Thursday 15:00–18:45 Location: H23

TT 34.1 Thu 15:00 H23

The fate of the spin polaron in the 1D t-J model — •Piotr Wrzosek — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland

We study the intrinsic origin of the well-established differences in the motion of a single hole in the 1D and 2D antiferromagnet. To this end, we consider a 1D t-J model, perform the slave fermion transformation to the holon-magnon basis, and solve the obtained model in a numerically exact manner. We explicitly show that the spin polaron quasiparticle, which is well-known from the studies of a single hole in the 2D antiferromagnet, is destroyed in the 1D t-J model by the magnon-magnon interactions. Nevertheless, we observe surprising similarities between the spectra obtained with and without magnon-magnon interactions, indicating that some of the key features of the spin polaron physics are still preserved in 1D.

TT 34.2 Thu 15:15 H23

Huge enhancement of the thermal conductivity in the Tomonaga-Luttinger-liquid region of $YbAlO_3$ — •Parisa Mokhtari[1,2], Ulrike Stockert[1], and Elena Hassinger[1,2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Physics Department, Technical University of Munich, Garching, Germany

In 2019, Wu et al. found the typical excitation spectrum of the spinons in the Q-1D material $YbAlO_3$ via neutron scattering at 1 K. $YbAlO_3$ exhibit AFM (J_c=2.3 K) and FM (J_ab=0.8 K) exchange interaction along and perpendicular to the chain direction, respectively [1, 2]. In zero field, a 3D AFM order is established at 0.88 K. For fields along a, perpendicular to the chain, this order is suppressed and replaced by an IC-AFM state, until the FI-FM state occurs for B >1.5 T.

It is an open question, if magnetic excitations in this material carry heat, and how they interact with phonons. Hence, we investigate the low-T κ of $YbAlO_3$ down to 30 mK in fields up to 4 T. The phase diagram is successfully reproduced with pronounced anomalies in both T and B sweeps. A clear additional anomaly in the field dependence at low T confirms a crossover within the IC phase, which was suggested before based only on a tiny plateau appearing in the magnetisation. We find a large variation of the κ throughout the phase diagram indicating strong magneto-elastic coupling. In addition, a substantial enhancement of kappa is observed in the proposed TLL region.

[1] L. S. Wu et al., Nat. Commun. 10, 698 (2019)
[2] L. S. Wu et al., Phys. Rev. B 99, 195117 (2019)

TT 34.3 Thu 15:30 H23

Counting statistics in interacting one-dimensional conductors — •Oleksiy Kashuba[1], Roman Riwar[1], Fabian Hassler[2], and Thomas Schmidt[3] — [1]Forschungszentrum Jülich — [2]RWTH Aachen — [3]Luxemburg Uni

The calculation of the cumulant generating function of a given observable, such as the charge, is nontrivial even for the non-interacting systems. This problem is closely connected to the problem of Toeplitz eigenvalues and the Szego-Kac theorem [1]. The application of the latter leads to a violation of the moment generating function's periodicity along the counting field. This periodicity can be restored using the Fisher-Hartwig conjecture, as was shown for non-interacting one-dimensional electrons [2]. Here, we aim to go beyond and include interactions. For weak interactions, a modification of the Matsubara diagrammatic approach was developed, allowing us explicit calculation of the interaction corrections to the cumulant generating function. All obtained terms preserve the periodic constraint of the moment generating function. The obtained result is in a good agreement at low filling with the noise suppression in Luttinger liquid for K<1. We also found a surprising counterpart of the charge-density wave effect in the cumulant generating function.

[1] Basor, Morrison, Linear Algebra and its Appl. 202 (1994), 129
[2] Aristov, Phys. Rev. B 57 (1998), 12825

TT 34.4 Thu 15:45 H23

Enhancement of pair correlations in the asymmetric Hubbard ladder — •Anas Abdelwahab and Eric Jeckelmann — Leibniz Universität Hannover, Hannover, Germany

We investigated an extension of the asymmetric two-leg Hubbard ladder model [1,2] that consists of different on-site interaction U_y and intra-hopping t_y on each leg y using the density matrix renormalization group method. We calculated pair binding energy, charge, spin and single particle gaps as well as pairing correlation functions for several sets of model parameters. It is possible to adjust the asymmetry of model parameters to retain finite pair binding energy and enhanced pairing correlation functions similar to those appearing in symmetric two-leg Hubbard ladders. Such adjustment represents an interpolation between doped Mott insulator and doped charge transfer insulator.

[1] A. Abdelwahab, E. Jeckelmann, M. Hohenadler, Phys. Rev. B 91, 155119 (2015)
[2] A. Abdelwahab and E. Jeckelmann, Eur. Phys. J. B 91, 207 (2018).

TT 34.5 Thu 16:00 H23

Magnetic properties of a quantum spin ladder material in proximity to the isotropic limit — •Sergei Zvyagin — Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

We report on the synthesis, crystal structure, magnetic, thermodynamic, and electron-spin-resonance properties of the coordination complex $[Cu_2(pz)_3(4\text{-HOpy})_4](ClO_4)_4$ [pz = pyrazine; 4-HOpy = 4-hydroxypyridine] [1]. This material is identified as a spin-1/2 Heisenberg ladder system with exchange-coupling parameters $J_{\rm rung}/k_B$ = 12.1(1) K and $J_{\rm leg}/k_B$ = 10.5(3) K [$J_{\rm rung}/J_{\rm leg}$ = 1.15(4)]. For single crystals our measurements revealed two critical fields, $\mu_0 H_{c1}$ = 4.63(5) T and $\mu_0 H_{c2}$ = 22.78(5) T (for $H \parallel a^*$), separating the gapped spin-liquid, gapless Tomonaga-Luttinger-liquid, and fully spin-polarized phase. No signature of a field-induced transition into a magnetically ordered phase was found at temperatures down to 450 mK. The material bridges an important gap by providing an excellent physical realization of an almost isotropic spin-1/2 strong-rung Heisenberg ladder system with modest exchange-coupling energy and critical-field scales.

[1] S. A. Zvyagin, A. N. Ponomaryov, M. Ozerov, E. Schulze, Y. Skourski, R. Beyer, T. Reimann, L. I. Zviagina, E. L. Green, J. Wosnitza, I. Sheikin, P. Bouillot, T. Giamarchi, J. L. Wikara, M. M. Turnbull, and C. P. Landee, Phys. Rev. B **103**, 205131 (2021)

TT 34.6 Thu 16:15 H23

Finite-temperature optical conductivity with density-matrix renormalization group methods for the Holstein polaron and bipolaron with dispersive phonons — •David Jansen[1], Janez Bonča[2,3], and Fabian Heidrich-Meisner[1] — [1]Institute for Theoretical Physics, University of Göttingen — [2]J. Stefan Institute, Ljubljana — [3]Faculty of Mathematics and Physics, University of Ljubljana

We compute the optical conductivity for the Holstein polaron and bipolaron with dispersive phonons at finite temperature using a matrix-product state based method. We combine purification [1], to obtain the finite-temperature states, together with the parallel time-dependent variational principle (pTDVP) [2] algorithm to compute the real time current-current correlation functions. The pTDVP algorithm utilizes local basis optimization [3] to efficiently treat the phononic degrees of freedom. For the polaron, we find that the phonon dispersion alters the optical conductivity at several temperatures in the weak, intermediate, and strong coupling regime. In the two first cases, we see that the spectrum goes from being continues to discrete when going from a downwards to a upwards phonon dispersion. In the strong coupling regime, the dispersion leads to a shift of the center of the spectrum. For the bipolaron, we study the effect of dispersion in both the weak and strong electron-phonon coupling regime, and thus see its influence on both a delocalized and a localized bipolaron.

This research was supported by the DFG via SFB 1073.

[1] Verstraete et al., Phys. Rev. Lett. 93, 207204 (2004)
[2] Secular et al., Phys. Rev. B 101, 235123 (2020)
[3] Zhang et al., Phys. Rev. Lett. 80, 2661 (1998)

TT 34.7 Thu 16:30 H23

Cavity-induced long-range interactions in strongly correlated systems — •Paul Fadler[1], Jiajun Li[2], Kai Phillip Schmidt[1], and Martin Eckstein[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Paul Scherrer Institut

In recent years, the coupling of optical cavity modes to solid states systems has emerged as a possible way to control material proper-

ties. Here we investigate cavity-induced long-range interactions between spins in a Mott insulator, which are a new feature of the coupling to the quantized cavity field, and are absent in a control of magnetism by classical light. In detail, for the Fermi-Hubbard model at half filling we show that the cavity coupling leads to long-range four-spin terms in the effective low spin model at large onsite interaction U, in addition to the conventional antiferromagnetic Heisenberg exchange interaction.

To obtain these long-range interactions, we compare exact diagonalization, a perturbative approach based on the effective spin-photon Hamiltonian description of the system, and fourth-order perturbation theory in the Hubbard model. We show that the phenomenologically motivated spin-photon Hamiltonian fails to describe the interactions properly close to resonances of the cavity and charge excitations. It is therefore not possible to perturbatively treat cavity coupled correlated systems in an effective spin basis.

15 min. break

TT 34.8 Thu 17:00 H23

Magnetism and Mottness in the anisotropic triangular lattice Hubbard model: a cellular dynamical mean-field study — •Marcel Klett[1], Henri Menke[2], Michel Ferrero[3], Antoine Georges[3], and Thomas Schäfer[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Erlangen-Nuremberg, Erlangen, Germany — [3]College de France, Paris, France

We investigate the phase diagram of the anisotropic triangular lattice Hubbard model in a center-focused cellular dynamical mean-field theory (CDMFT) approach using an impurity with 7 sites. We investigate the Mott metal-to-insulator transition and crossover region as well as the superconducting phase. Using a spin symmetry-broken approach of the CDMFT, allowing for a rotations of spins on the Bloch sphere, we are able to investigate the magnetic ordering of the different cluster schemes.

TT 34.9 Thu 17:15 H23

Competing orders in a two-dimensional Su-Schrieffer-Heeger model — •Anika Götz[1], Martin Hohenadler[1,2], and Fakher Assaad[1,3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Independent Researcher, Josef-Retzer-Str. 7, 81241 Munich, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany

We study a two-dimensional Su-Schrieffer-Heeger model of electrons coupled to Einstein phonons with auxiliary-field quantum Monte Carlo simulations. By adding a symmetry-allowed interaction, the phonons can be integrated out at the expense of imaginary-time correlations of the discrete Hubbard-Stratonovich fields. Using single spin-flip updates, we investigate the phase diagram at the O(4)-symmetric point as a function of hopping t and phonon frequency ω_0. For low phonon frequencies, the C_4 lattice symmetry is broken by valence bond order. Depending on t, the ordering wavevector is either (π,π) or $(\pi,0)$, the latter value being accompanied by a dynamically generated π-flux in each plaquette. At larger ω_0, the O(4) symmetry is spontaneously broken by long-range antiferromagnetic (AFM) order. In the limit $t\to 0$, the model maps onto an unconstrained Z_2 gauge theory coupled to fermions which is in its confined phase for the parameters considered. Whereas the $(\pi,0)$-VBS to AFM transition is a candidate for a deconfined quantum critical point, the details of the $(\pi,0)$-VBS to (π,π)-VBS and (π,π)-VBS to AFM transitions are still under investigation.

TT 34.10 Thu 17:30 H23

Splitting of topological charge pumping in an interacting two-component fermionic Rice-Mele Hubbard model — •Eric Bertok[1], Fabian Heidrich-Meisner[1], and Armando A. Aligia[2] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen — [2]Centro Atómico Bariloche and Instituto Balseiro, Bariloche, Argentina

A Thouless pump transports an integer amount of charge when pumping adiabatically around a singularity. We study the splitting of such a critical point into two separate critical points by adding a Hubbard interaction. Furthermore, we consider extensions to a spinful Rice-Mele model, namely a staggered magnetic field or an Ising-type spin coupling, further reducing the spin symmetry. The resulting models additionally allow for the transport of a single charge in a two-component system of spinful fermions, whereas in the absence of interactions, zero or two charges are pumped. In the SU(2)-symmetric case, the ionic Hubbard model is visited once along pump cycles that enclose a single singularity. Adding a staggered magnetic field additionally transports an integer amount of spin while the Ising term realizes a pure charge pump. We employ real-time simulations in finite and infinite systems to calculate the adiabatic charge and spin transport, complemented by the analysis of gaps and the many-body polarization to confirm the adiabatic nature of the pump. The resulting charge pumps are expected to be measurable in finite-pumping speed experiments in ultra-cold atomic gases. We discuss the implications of our results for a related quantum-gas experiment by Walter et al. [arXiv:2204.06561].

TT 34.11 Thu 17:45 H23

Thermodynamics of the metal-insulator transition in the extended Hubbard model from determinantal quantum Monte Carlo — •Alexander Sushchyev and Stefan Wessel — RWTH Aachen University

We use finite-temperature determinantal quantum Monte Carlo simulations to study the thermodynamic properties of the extended Hubbard model on the square lattice at half-filling. In particular, we consider the effect of a nearest-neighbor and a long-range Coulomb repulsion on the thermal metal-insulator transition in the Slater regime at intermediate coupling. Within the parameter regime accessible to sign-free quantum Monte Carlo simulations we explore in detail the temperature dependence of the double occupancy and entropy. Notably, we probe for signatures of a first-order metal-insulator transition driven by the suppression of correlation effects by the non-local interactions, as proposed in [1].

[1] M.Schueler et al., Sci. Post. Phys. 6, 067 (2019)

TT 34.12 Thu 18:00 H23

Surrogate models for quantum spin systems based on reduced order modelling — •Stefan Wessel[1], Michael Herbst[1], Benjamin Stamm[1], and Matteo Rizzi[2] — [1]RWTH Aachen University — [2]University of Cologne and FZ Jülich

We present a methodology to investigate phase-diagrams of quantum spin models based on the principle of the reduced basis method. It is based on constructing a low-dimensional basis built from solutions of snapshots, i.e., ground states corresponding to particular and well-chosen parameter values. We propose to use a greedy-strategy to assemble the reduced basis and thus to select the parameter points where the full model is solved. Once the reduced basis is computed, observables required for the computation of phase-diagrams can be computed with a computational complexity independent of the underlying Hilbert space for any parameter value. We illustrate the accuracy of this approach for a geometrically frustrated antiferromagnetic two-dimensional lattice model and quantum spin model that describes a chain of excited Rydberg atoms.

TT 34.13 Thu 18:15 H23

Bound by three-body interactions — •Gary Ferkinghoff[1], Leanna Müller[1], Umesh Kumar[2], Götz S. Uhrig[1], and Benedikt Fauseweh[3] — [1]Condensed Matter Theory, Technische Universitat Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [3]Institute for Software Technology, German Aerospace Center (DLR), Linder Hohe, 51147 Cologne, Germany

Stable bound quantum states are ubiquitous in nature. Mostly, they result from the interaction of only pairs of particles, so called two-body interactions, even when complex many-particle structures are formed. We show that three-quasi-particle bound states occur in a generic, experimentally accessible solid state system: antiferromagnetic spin ladders, related to high-temperature superconductors. Strikingly, this binding is induced by genuine three-quasi-particle interactions; without them there is no bound state. We compute the dynamic exchange structure factor required for the experimental detection of the predicted state by resonant inelastic x-ray scattering for realistic material parameters. Our work enables us to quantify these elusive interactions and unambiguously establishes their effect on the dynamics of the quantum many-particle state. In this talk we will present the main results of our study, briefly explain the theoretical tools that we used and present an experimental setting for verifying our theoretical results.

TT 34.14 Thu 18:30 H23

Non-linear response functions and disorder: The case of the photo galvanic effect — •Konstantinos Ladovrechis and Tobias

Meng — Institute for Theoretical Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

The circular photogalvanic effect (CPGE) is a non-linear photocurrent which is generated in materials with broken inversion symmetry when they are shed with circularly polarised light. In Weyl semi-metals, the CPGE is quantized in terms of fundamental constants and the Chern numbers associated with the Weyl nodes. In this work, we investigate the effect of pointlike disorder onto the quantization of CPGE. Implementing 1st-order and self-consistent Born approximations, we identify that the quantization of CPGE is broken and perturbative corrections in the scattering strength emerge, which we further classify in terms of self-energy and vertex corrections.