TT 28: Correlated Electrons: Theory 1

Time: Thursday 9:30–13:00 Location: H23

TT 28.1 Thu 9:30 H23

General super-exchange Hamiltonians for magnetic and orbital physics in e_g and t_{2g} systems — •Xuejing Zhang[1], Erik Koch[1,2], and Eva Pavarini[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]JARA High-Performance Computing, 52062, Aachen, Germany

In strongly-correlated transition-metal oxides, spin- and orbital-ordering or spin- and orbital-liquid phenomena are often studied with low-energy super-exchange Hamiltonians, derived from multi-band Hubbard models in highly symmetric cases and in the basis of pseudo-spin operators. This captures the essence of the Kugel-Khomskii[1] super-exchange mechanism. Recently, via an irreducible-tensor operator representation, we derived the orbital super-exchange Hamiltonian for t^1_{2g} perovskites and successfully used it, in combination with many-body calculations based on dynamical mean-field theory, to explain the orbital physics in these systems. Then, we generalize our method to e^n_g and t^n_{2g} systems at arbitrary integer filling n, including both spin and orbital interactions[2,3]. Here, we identified the t^2_{2g} perovskite $LaVO_3$ as a rare case in which orbital-ordering is indeed controlled by the KK super-exchange interaction[4].

[1] K. I. Kugel' and D. I. Khomskii, Zh. Eksp. Teor. Fiz. **64**, 1429 (1973) [Sov. Phys. JETP **37**, 725 (1973)]
[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 **105**, 115104 (2022)
[3] X. J. Zhang, E. Koch, and E. Pavarini, Submitted to Phys. Rev. Lett.

TT 28.2 Thu 9:45 H23

Fluctuations analysis of the spin susceptibility: Néel ordering revisited in dynamical mean field theory — •Georg Rohringer[1] and Lorenzo Del Re[2] — [1]Institute of Theoretical Physic, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Georgetown University, 37th and O Sts., NW, Washington, DC 20057, USA

We revisit the antiferromagnetic (AF) phase diagram of the single-band three-dimensional Hubbard model on a simple cubic lattice studied within the dynamical mean field theory. Although this problem has been investigated extensively in the literature, a comprehensive understanding of the impact of the different one- and, in particular, two-particle local correlation functions of DMFT on the AF transition temperature is still missing. We have, hence, performed a fluctuation analysis of T_N with respect to different local bosonic fluctuations (charge, spin, particle-particle) contained in the two-particle vertex of DMFT. Our results indicate that, beyond weak coupling, the screening of the DMFT vertex by local fluctuations leads to an enhancement of T_N with respect to a random phase approximation (RPA) like calculation where this vertex is replaced by the bare interaction. The overall suppression of T_N in DMFT with respect to RPA is then solely due to the incoherence introduced by the DMFT self-energy in the one-particle Green's functions. This illustrates the Janus-faced role of the local moment formation in the DMFT solution of the Hubbard model, which leads to completely opposite effects in the one- and two-particle correlation functions.

TT 28.3 Thu 10:00 H23

Phase diagram of SU(N) antiferromagnet on a square lattice — •Jonas Schwab, Francesco Parisen Toldin, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

We investigate the ground state phase diagram of an antiferromagnetic, SU(N)-symmetric spin model on a square lattice, where the chosen irreducible representation of the $\mathfrak{su}(N)$ algebra is described by a square Young tableaux with $N/2$ rows and $2S$ columns. Using approximation-free fermionic quantum Monte Carlo simulations for $S \in \{1/2, 1, 3/2\}$ and even values of N in the range $N \in [2, 20]$, we present a phase diagram for this model. Our results are in line with the seminal work of Read and Sachdev. For any value S, we find Néel order at small values of N, and disordered valence-bond solid (VBS) states at large N. The degeneracy of the VBS state, 4 for $S = 1/2$ and $3/2$ and 2 for $S = 1$, close to the Néel state follows the lower bound obtained by analyzing monopole singularities in the large-S limit. In contrast in the large-N limit, the VBS ground state shows a four fold degeneracy for all values of S. In order to best image the dimerization patterns, so as to confirm the above, we use a pinning field approach.

TT 28.4 Thu 10:15 H23

Field-tunable Berezinskii-Kosterlitz-Thouless correlations in a quasi-2d spin-1/2 Heisenberg lattice — D. Opherden[1], M.S.J. Tepaske[2,3], F. Bärtl[1,4], M. Weber[3], M.M. Turnbull[5], T. Lancaster[6], S.J. Blundell[7], M. Baenitz[8], J. Wosnitza[1,4], C.P. Landee[9], R. Moessner[3], D.J. Luitz[2,3], and •H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden, HZDR — [2]Physikalisches Institut, Univ. Bonn — [3]MPI PKS, Dresden — [4]IFMP, TU Dresden — [5]Carlson School of Chemistry, Clark Univ. — [6]Durham Univ., Centre for Materials Physics — [7]Clarendon Laboratory, Univ. of Oxford — [8]MPI CPfS, Dresden — [9]Department of Physics, Clark Univ.

We discuss the manifestation of field-induced Berezinskii-Kosterlitz-Thouless (BKT) correlations in the weakly-coupled spin-1/2 Heisenberg layers of the material $[Cu(pz)_2(2\text{-}HOpy)_2](PF_6)_2$ (CuPOF). Due to the moderate intralayer exchange coupling of $J/k_B = 6.8$ K, laboratory magnetic fields induce a substantial XY anisotropy of the spin correlations. This provides a significant BKT regime, as the tiny interlayer exchange $J'/k_B \approx 1$ mK only induces 3d correlations upon close approach to the BKT transition. We employed NMR and μ^+SR measurements to probe the spin correlations that determine the critical temperatures of the long-range order and the BKT transition. Further, we performed stochastic series expansion QMC simulations based on the experimentally determined model parameters. Finite-size scaling of the spin stiffness yields an excellent agreement of the critical temperatures between theory and experiment.

Invited Talk TT 28.5 Thu 10:30 H23

Towards an *ab-initio* theory of Anderson localization for correlated electrons — •Liviu Chioncel — University of Augsburg, Augsburg, Germany

Great progress has been made in recent years towards understanding the properties of disordered electronic systems. This is made possible by recent advances in quantum effective medium methods which include Dynamical Mean-Field Theory and the Coherent Potential Approximation, and their cluster extension, the Dynamical Cluster Approximation. The recently developed typical medium dynamical cluster approximation captures disorder-induced localization and provides an order parameter for the Anderson localized states. We present an overview of various recent applications of the typical medium single-site and dynamical cluster approximation to the Hubbard model, and its combination to realistic systems in the framework of Density Functional Theory.

15 min. break

TT 28.6 Thu 11:15 H23

The crucial influence of side groups on magnetic superexchange - a modification of the Goodenough-Kanamori-rules — Dijana Milosavljevic[1], Oleg Janson[2], Stefan-Ludwig Drechsler[2], and •Helge Rosner[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

According to the famous Goodenough-Kanamori-Anderson rules, the key structural feature that determines the magnetic exchange coupling constant for superexchange in magnetic insulators is the magnetic ion-ligand-magnetic ion bond angle. Here, we demonstrate that this angle is not the only factor. An at least equally important influence on the exchange coupling has the presence of the side groups attached to the ligands. Applying density functional calculations and subsequently derived realistic parameters for a multiband model tight-binding model, we provide a quantitative analysis for the example case of edge-sharing Cu-O chains with bond angles near 90 degrees. We find that a single parameter, the difference in onsite energies of the ligand orbitals parallel and perpendicular to the Cu-O chain, is at least as important as the bond angle for sign and size of the superexchange. This parameter strongly depends on the position of side groups outside the

superexchange pathway. For a fixed bond angle, changes of a side group position, only, can cause changes in the superexchange of several hundred Kelvin and thus dramatic changes in the magnetic ground state.

TT 28.7 Thu 11:30 H23

The shared universality of charged black holes and the many many-body SYK model — •Jan Louw — Institute for Theoretical Physics, Georg-August-Universität Goettingen, Friedrich-Hund-Platz 1, 37077 Goettingen, Germany

We investigate the charged q/2-body interacting Sachdev-Ye-Kitaev (SYK) model in the grand-canonical ensemble. By treating q as a large parameter, we are able to analytically study its phase diagram. By varying the chemical potential or temperature, we find that the system undergoes a phase transition between low and high entropies, in the maximally chaotic regime. A similar transition in entropy is seen in charged AdS black holes transitioning between a large and small event horizon. Approaching zero temperature, we find a first-order chaotic-to-integrable quantum phase transition, where the finite extensive entropy drops to zero. This again has a gravitational analogue–the Hawking-Page (HP) transition between a large black hole and thermal radiation. An analytical study of the critical phenomena associated with the continuous phase transition provides us with two sets of critical exponents. These sets define two separate universality classes, both of which include several charged AdS black hole phase-transitions. Together, these findings indicate a connection between the charged large q SYK model and black holes.

TT 28.8 Thu 11:45 H23

Scrambling and Many-Body Localization in the XXZ-Chain — •Niklas Bölter and Stefan Kehrein — Institut für Theoretische Physik, Universität Göttingen

The tripartite information is an observable-independent measure for scrambling and delocalization of information. Therefore one can expect that the tripartite information is a good observable-independent indicator for distinguishing between many-body localized and delocalized regimes, which we confirm for the XXZ-chain in a random field. Specifically, we find that the tripartite information signal spreads inside a lightcone that only grows logarithmically in time in the many-body localized regime similar to the entanglement entropy. We also find that the tripartite information eventually reaches a plateau with an asymptotic value that is suppressed by strong disorder.
[1] N. Bölter and S. Kehrein, Phys. Rev. B 105, 104202

TT 28.9 Thu 12:00 H23

Nonlinear response theory and three-particle diagrams in strongly correlated systems — •Patrick Kappl, Friedrich Krien, Clemens Watzenböck, and Karsten Held — Institute of Solid State Physics, TU Wien, Austria

We study three-particle correlation functions of the Anderson impurity model by means of quantum Monte Carlo simulations in the hybridization expansion. We analyze the parameter regime in which vertex corrections beyond the bare bubble term become relevant for the three-particle correlator. Such three-particle correlators are hitherto by-and-large terra incognita and become relevant for the next level of diagrammatic extensions of dynamical mean-field theory. We here restrict ourselves to correlators consisting of three densities n and spins $S_{x,y,z}$. These are related to nonlinear response theory and its zero-frequency component to the density-dependence of the electronic compressibility.

TT 28.10 Thu 12:15 H23

Superconductivity in 2D and 3D lattice models of correlated fermions - combining matrix-product states with mean-field theory — Gunnar Bollmark[1], Svenja Marten[2], •Thomas Köhler[1], Lorenzo Pizzino[3], Yiqi Yang[4], Johannes-Stephan Hofmann[5], Hao Shi[6], Shiwei Zhang[7], Salvatore R. Manmana[2], Thierry Giamarchi[3], and Adrian Kantian[1,8] — [1]Uppsala University, Sweden — [2]Georg-August-Universität Göttingen, Germany — [3]University of Geneva, Switzerland — [4]College of William and Mary, Williamsburg, Virginia, USA — [5]Weizmann Institute of Science, Rehovot, Israel — [6]University of Delaware, Newark, USA — [7]Flatiron Institute, New York, USA — [8]Heriot-Watt University, Edinburgh, United Kingdom

Correlated electron states are at the root of many important phenomena including unconventional superconductivity (USC), where electron-pairing arises from repulsive interactions. Computing the properties of correlated electrons, such as the critical temperature Tc for the onset of USC, efficiently and unbiased remains a major challenge. Here, we combine matrix-product states (MPS) with static mean field (MF) to provide a solution to this challenge for 2D/3D materials comprised of weakly coupled correlated chains. This framework of Q1D fermions is developed and validated for attractive Hubbard systems and further enhanced via analytical field theory. Finally, we investigate the formation of transient non-equilibrum SC by a real-time evolution of a 3D extended Hubbard system out-of-equilibrium.

TT 28.11 Thu 12:30 H23

Non-local correlations and criticality in the triangular lattice Hubbard model — •Mario Malcolms de Oliveira[1], Julian Stobbe[2], Henry Menke[3], Marcel Klett[1], Georg Rohringer[2], and Thomas Schäfer[1] — [1]Max Planck Institute for Solid State Research — [2]University of Hamburg — [3]University of Erlangen-Nuremberg

We investigate the role of non-local electronic correlations at finite temperatures in the half-filled triangular lattice Hubbard model using the dynamical vertex approximation (DΓA), a diagrammatic extension [1] of the dynamical mean-field theory (DMFT). We analyze the impact of (quantum) phase transitions on finite temperature properties at the one- and two-particle level. We discuss the absence of magnetic ordering at finite temperatures due to the fulfilment of the Mermin-Wagner theorem and the (Mott) metal-insulator crossover. In addition we compare the results of this method to the ones obtained by other cutting-edge techniques like DMFT, its real-space cluster extension cellular dynamical mean-field theory (CDMFT) and diagrammatic Monte Carlo (DiagMC) [2].
[1] G. Rohringer, H. Hafermann, A. Toschi, A.A. Katanin, A.E. Antipov, M.I. Katsnelson, A.I. Lichtenstein, A.N. Rubtsov, K. Held, Rev. Mod. Phys. 90, 025003 (2018)
[2] A. Wietek, R. Rossi, F. Šimkovic IV, M. Klett, P. Hansmann, M. Ferrero, E.M. Stoudenmire, T. Schäfer, A. Georges, Phys. Rev. X 11, 041013 (2021)

TT 28.12 Thu 12:45 H23

Non-local correlation and entanglement of ultracold bosons in the two-dimensional Bose-Hubbard lattice at finite temperature — Ulli Pohl, •Sayak Ray, and Johann Kroha — Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, Nußallee 12, 53115, Bonn, Germany

The temperature-dependent behavior emerging in the vicinity of the superfluid (SF) to Mott-insulator (MI) transition of interacting bosons in a 2D optical lattice, described by the Bose-Hubbard model is investigated. The equilibrium phase diagram at finite temperature is computed using the cluster mean-field (CMF) theory including a finite-cluster-size-scaling. The SF, MI, and normal fluid (NF) phases are characterized as well as the transition or crossover temperatures between them are estimated by computing physical quantities such as the superfluid fraction, compressibility and sound velocity using the CMF method. It is found that the nonlocal correlations included in a finite cluster, when extrapolated to infinite size, leads to quantitative agreement of the phase boundaries with quantum Monte Carlo results as well as with experiments. Moreover, it is shown that the von Neumann entanglement entropy within a cluster corresponds to the system's entropy density and that it is enhanced near the SF-MI quantum critical point (QCP) and at the SF-NF boundary. The behavior of the transition lines near this QCP, at and away from the particle-hole symmetric point located at the Mott-tip, is also discussed.
[1] U. Pohl, S. Ray, J. Kroha, Ann. Phys. (Berlin) 2100581 (2022)