TT 48: CE: Metal-Insulator Transition 2

Time: Thursday 10:30–13:00 Location: HSZ 105

TT 48.1 Thu 10:30 HSZ 105

The x-ray induced Mott-Anderson scenario in organic charge-transfer salts studied by noise spectroscopy — •Robert Rommel[1], Takahiko Sasaki[2], and Jens Müller[1] — [1]Goethe-Universität Frankfurt, SFB/TR49, Frankfurt am Main — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

The organic molecular conductors $(BEDT\text{-}TTF)_2X$ are model systems for low-dimensional metals exhibiting both strong electronic correlations and electron-phonon interactions. With respect to the amount of disorder, different types of metal-to-insulator transitions (MIT) can occur. We will focus on the bandwidth-controlled Mott transition due to external pressure or chemical substitution and disorder-induced carrier localization caused by x-ray irradiation. We will discuss comparative studies of the clean correlation-driven Mott MIT and the Anderson scenario originating from the randomness in the lattice potential. To extract information about the influence of disorder on the electron dynamics we employ noise/fluctuation spectroscopy. The technique was systematically applied after subsequent doses of x-ray iradation of the pristine superconductor κ-$(ET)_2$-Cu$[N(CN)_2]$Br. We find that the increase of insulating behavior in the resistance is accompanied by the emergence of new energy scales pointing to distinct changes in the dynamic properties of the correlated charge carriers.

TT 48.2 Thu 10:45 HSZ 105

Localization-delocalization transition in the κ-(ET)$_2$X salts: Evidence from fluctuation spectroscopy — •Jens Brandenburg[1], Jens Müller[1], and John A. Schlueter[2] — [1]Johann Wolfgang Goethe-Universität, Frankfurt am Main — [2]Argonne National Laboratory, Argonne, IL, USA

Quasi-2D organic conductors κ-$(ET)_2X$ with X = Cu$[N(CN)_2]$Cl, Cu$[N(CN)_2]$Br and Cu$(NCS)_2$ are model systems for low-dimensional metals exhibiting both strong electron-electron and electron-phonon interactions. The interplay of charge, spin, and lattice degrees of freedom lead to a variety of different magnetic-insulating, metallic, and superconducting ground states. The normal-conducting state shows anomalous behavior at a temperature scale $T^* \sim 35 - 50\,\mathrm{K}$ interpreted, e.g., as a crossover from coherent to incoherent transport.
Fluctuation spectroscopy is a new powerful tool to study the intrinsic charge-carrier dynamics in these materials [1,2]. Systematic investigations of four compounds, situated at different positions in the generalized phase diagram, show clear signatures in the temperature dependence of the relative noise amplitude $a_R = S_R \cdot f/R^2$ at T^* depending on the correlation strength characterized by the ratio of bandwidth to on-site Coulomb interaction W/U_{eff}. This indicates a localization-delocalization transition in the interlayer transport on the metallic side of the phase diagram as a function of temperature or electronic correlation strength. Funded by SFB/TR 49
[1] PRB 79 (2009), 214521
[2] PRL 102 (2009), 047004

TT 48.3 Thu 11:00 HSZ 105

Scaling Theory of the Mott Transition and Breakdown of the Grüneisen Scaling Near a Finite-Temperature Critical End Point — •Lorenz Bartosch[1], Mariano de Souza[2], and Michael Lang[2] — [1]Institut für Theoretische Physik, Goethe-Universität, 60438 Frankfurt am Main, Germany — [2]Physikalisches Institut, Goethe-Universitat, 60438 Frankfurt am Main, Germany

We discuss a scaling theory of the lattice response in the vicinity of a finite-temperature critical end point. The thermal expansivity is shown to be more singular than the specific heat such that the Grüneisen ratio diverges as the critical point is approached, except for its immediate vicinity. More generally, we express the thermal expansivity in terms of a scaling function which we explicitly evaluate for the two-dimensional Ising universality class. Recent thermal expansivity measurements on the layered organic conductor κ-$(BEDT\text{-}TTF)_2X$ close to the Mott transition are well described by our theory.

TT 48.4 Thu 11:15 HSZ 105

Interacting electrons in a random potential: Absence of thermodynamic signatures of a metal-insulator transition in two dimensions — •Prabuddha Chakraborty[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135, Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, ul. Hoza 69, 00-681, Warszawa, Poland

The properties of a quantum phase transition where a two-dimensional metallic phase arises out of an Anderson insulator as a consequence of short-range electronic interactions are investigated using quantum Monte Carlo simulations. We present results for the compressibility and the antiferromagnetic and uniform susceptibilities. We demonstrate that, in contrast to predictions made using perturbative Renormalization Group calculations, the susceptibilities show no signature of the metal-insulator transition. To explore the nature of the metallic state itself the behaviour of thermodynamic quantities deep in the metallic phase is also explored.

TT 48.5 Thu 11:30 HSZ 105

Metal-insulator transition in 2D disordered bipartite systems — •Elio König[1], Pavel Ostrovsky[2], Ivan Protopopov[2], and Alexander Mirlin[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

We predict the novel type of metal-insulator transition in 2D disordered systems with a bipartite structure. This in particular applies to graphene with vacancies and/or ripples and to topological insulators of unconventional symmetry. We use the σ-model description of these disordered systems and identify specific vortex-like excitations giving rise to the Berezinsky-Kosterlitz-Thouless-type transition. This results in appearence of the minimal metallic conductivity and insulating phase at sufficiently strong disorder. Our results are in agreement with available numerical simulations and motivate further theoretical and experimental studies of exotic disordered systems.

15 min. break

TT 48.6 Thu 12:00 HSZ 105

Effective spin Hamiltonian for the spin liquid of the Hubbard model on the honeycomb lattice — •Hong-Yu Yang[1], Andreas Läuchli[2], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany — [2]MPI PKS, Nöthnitzerstr. 38, 01187 Dresden, Germany

Motivated by the spin liquid phase unveiled by quantum Monte Carlo simulations of the Hubbard model on the honeycomb lattice at intermediate values of U, we derive the effective spin-only model from the strong-coupling limit using continuous unitary transformations (CUTs). It turns out that the spin liquid phase is located in the non-perturbative regime. We therefore apply a recently developped non-perturbative extension of CUTs named graph-based CUT (gCUTs) in order to obtain a pure spin model as effective Hamiltonian for the intermediate U regime. We use exact diagonalizations to check the validity of the effective spin model by comparing its low-energy properties to the one of the Hubbard model on small clusters. Surprisingly, we find that besides a frustrating next-nearest neighbor two-spin exchange a family of six-spin interactions are the dominant corrections to the nearest-neighbor Heisenberg model.

TT 48.7 Thu 12:15 HSZ 105

Orbital selective phase transitions observed in dynamical cluster approximation calculations — Hunpyo Lee[1], Yu-Zhong Zhang[2], •Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Department of Physics, Tongji University, Shanghai 200092, PR China

We study a two-orbital Hubbard model with unequal bandwidths on the square lattice using the dynamical cluster approximation (DCA) based on the hybridization expansion continuous-time quantum Monte Carlo method. In the case of four site clusters, the competition between Slater and Mott physics leads to orbital selective phases for intermediate values of the interaction strength. We also investigate a two-orbital Hubbard model with equal bandwidths where we allow one orbital to have an antiferromagnetic solution (AF orbital) while we constrain the other orbital to be paramagnetic (PM orbital). We find an interesting phase diagram with orbital selective phases that are caused by the different magnetic states in the two orbitals: As function of the interaction strength, the PM orbital undergoes a transition from a Fermi liquid to a Mott insulator through an intermediate non-Fermi liquid phase while the AF orbital shows a transition from a Fermi liquid to an antiferromagnetic insulator through an intermediate antiferromagnetic metallic phase.

TT 48.8 Thu 12:30 HSZ 105

Giant Chemical Shifts of the Sulphur 2*s*-Line Close to the Glass-Like Transition of CT Salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Br- a Hard X-ray Photoemission Study — •G. Schönhense[1], M. de Souza[2], K. Medjanik[1], A. Gloskovskii[3], H.J. Elmers[1], J. Müller[2], and M. Lang[2] — [1]Institut für Physik, J. Gutenberg Univ. Mainz — [2]Institut für Physik, J. Wolfgang von Goethe Universität Frankfurt — [3]Institut für Anorganische und Analytische Chemie, J. Gutenberg Univ. Mainz

The organic (super-)conductors of the κ-(ET)$_2$-X family are characterized by a strongly-correlated π - electron system with close proximity of superconductivity and antiferromagnetic insulating states and a half-filled quasi-2D metallic conduction band. HAXPES was performed at beamline P09 of PETRA III [1]. In the regions of $T^* \sim 45$ K (anomalous metallic state) and $T_g \sim$77K (thermal glass-like transition), the S 2s core level spectrum changes dramatically in warming-up series: around T^*, the main-line intensity drops to 80 % of its initial value and a high-binding-energy shoulder arises. When approaching T_g, it further drops to 40 % and several new peaks appear, being strongly shifted by up to more than 10eV. Above the glass-transition, all satellites disappear instantaneously and the main line intensity jumps back to its initial value. This gives further evidence for changes in the electronic degrees of freedom at the T^* transition and indicates that the latter may be involved in the glass-like transition, as was already speculated in literature.

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[1] A.Gloskovskii et al., this conference;

TT 48.9 Thu 12:45 HSZ 105

Long range order effects in the Mott-Hubbard transition and the variational lattice approach — •Aljoscha Wilhelm[1], Christoph Jung[1], Hartmut Hafermann[2], and Alexander Lichtenstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9 — [2]Centre de Physique Théorique (CPHT), École Polytechnique, 91128 Palaiseau Cedex, France

We introduce an efficient strategy to treat long ranged correlations in fermionic lattices, the so called variational lattice approach (VLA). The VLA combines the recently developed dual fermion approach for k-dependent problems and the exact diagonalization technique. We present first benchmark results. The phase diagram of the half-filled paramagnetic Mott-Hubbard transition is discussed and compared results to CDMFT and DCA calculations.