TT 12: CE: Metal-Insulator Transition 1

Time: Tuesday 9:30–13:00 Location: H19

TT 12.1 Tue 9:30 H19

Nonequilibrium Mott-Hubbard Systems Driven by External Laser Fields — •Andreas Lubatsch and Johann Kroha — Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany

Mott-Hubbard insulating materials have the potential for use as ultrafast electric switches, driven by an external laser field, due to the short relaxation times characteristic for strongly correlated systems. We consider the Hubbard model at half filling, driven out of equilibrium by an external, time-periodic laser field. The vector nature of the external field and a gauge where the electric field couples to the dipole monent of the charge distribution, different from the "Peierls substitution" of previous authors' work, is essential for obtaining the correct infrared behavior. We generalize the dynamical mean-field theory (DMFT) to nonequilibrium in a time-periodic driving field, using a Floquet mode representation and the Keldysh formalism. We calculate the nonequilibrium electron distribution function, the spectral density, nonequilibrium relaxation times and the DC conductivity in the presence of the external laser field for the metallic and for the insulating phase of the Hubbard model. In the metallic pseudo-gap phase, enhanced quantum coherence due to a polariton-like coupling of electronic excitations to the discrete electromagnetic mode is predicted. This leads to a revival of the many-particle resonance at the Fermi energy at resonant laser frequencies. In the Mott insulating (equilibrium) phase, an insulator-metal transition occurs as a function of the laser frequency, while the Mott-Hubbard gap remains rubust. This corresponds to nonequilibrium pumping into the upper Hubbard band.

TT 12.2 Tue 9:45 H19

Efficient treatment of frequency dependent interactions in DMFT — •Philipp Werner[1] and Andrew Millis[2] — [1]Theoretische Physik, ETH Zurich, 8093 Zurich — [2]Department of Physics, Columbia University, New York 10027

First principles calculations of screened Coulomb interaction parameters lead in some materials to a strongly frequency dependent $U(\omega)$ [1]. The recently developed diagrammatic impurity solvers [2,3] enable a very efficient treatment of the resulting retarded interactions within the framework of dynamical mean field theory (DMFT). I will explain the main algorithmic ideas in the context of a DMFT simulation of the Holstein-Hubbard model [4] and show how this method can be adapted to models with arbitrary $U(\omega)$.

[1] F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. Biermann, and A. I. Lichtenstein, Phys. Rev. B **70**, 195104 (2004).

[2] A. N. Rubtsov, V. V. Savkin, A. I. Lichtenstein, Phys. Rev. B **72** 035122 (2005).

[3] P. Werner, A. Comanac, L. De Medici, M. Troyer, and A. J. Millis, Phys. Rev. Lett. **97**, 076405 (2006).

[4] P. Werner and A. J. Millis, Phys. Rev. Lett. **99**, 146404 (2007).

TT 12.3 Tue 10:00 H19

Electronic correlations in vanadium chalcogenides: $BaVS_3$ vs $BaVSe_3$ — •Daniel Grieger, Lewin Boehnke, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

As opposed to its structurally and electronically very similar selenide counterpart $BaVSe_3$, the vanadium sulfide $BaVS_3$ shows a metal-to-insulator transition at $T\sim$70K, which can be attributed to the correlation-induced formation of a charge-density wave [1]. The underlying subtle electronical differences cannot be resolved by pure density functional theory (DFT) in local density approximation (LDA), but require its combination with an explicit many-particle method such as dynamical mean-field theory (DMFT). In this presentation, we will discuss the correlated electronic structure of the named vanadium chalcogenides in view of the apparently different physics at low temperature. Thereby, special methodological attention is addressed to the interface between LDA and DMFT through a comparision of different interfacing techniques, namely maximally-localized Wannier functions and projected local orbitals.

[1] F. Lechermann, S. Biermann, and A. Georges, Phys. Rev. B **76**, 085101 (2007).

TT 12.4 Tue 10:15 H19

Inequivalent routes across the metal-to-insulator transition in V_2O_3 — •Alessandro Toschi[1], Philipp Hansmann[1,2], Giorgio Sangiovanni[1], Maurits Haverkort[2], Tanusri Saha-Dasgupta[3], Ole K. Andersen[2], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]S.N. Bose Centre for Basic Sciences, Kolkata (India)

The equivalence between the doping-driven and the pressure-driven metal-to-insulator transition, which was hitherto assumed in studies on Cr-doped V_2O_3, has been recently questioned by the results of novel optical and X-ray absorption spectroscopy experiments. Theoretical calculations, combining full multiplet cluster calculations and the merger of the local density approximation with the dynamical mean field theory (LDA+DMFT), shed light on the differences in the ground states of the two metallic phases obtained by reducing the Cr-doping or by applying pressure, and how these differences reflect in the results of different spectroscopic techniques[1].

[1] F. Rodolakis, P. Hansmann, J.-P. Rueff, A. Toschi, *et al.*, submitted.

TT 12.5 Tue 10:30 H19

Insulator-to-Insulator Transition in TiOCl upon Doping — •Yu-Zhong Zhang[1], Kateryna Foyevtsova[1], Harald Jeschke[1], Martin Schmidt[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt am Main, Germany

By applying Car-Parrinello molecular dynamics with a projector augmented-wave basis, we investigate the effect of sodium doping in the layered Mott insulator TiOCl and predict the lattice structure under doping. We find that the system remains insulating at all doping concentrations in agreement with recent photoemission spectroscopy experiments and propose that the behavior of Na-doped TiOCl can be understood on the basis of a multi-orbital ionic extended Hubbard model. We extend our study to alternative doping routes like substitutions of Cl, O, and Ti by S, F, V/Sc, respectively and discuss the possibility to metallize TiOCl.

TT 12.6 Tue 10:45 H19

Disorder enhanced fluctuations in κ-$(D_8$-ET$)_2$Cu[N(CN)$_2$]Br — •Jens Brandenburg[1], Jens Müller[2], Steffen Wirth[1], and John A. Schlueter[3] — [1]Max-Planck-Insitut für Chemische Physik fester Stoffe, Dresden — [2]Goethe-Universität Frankfurt am Main — [3]Argonne National Laboratory, Argonne, IL, USA

The way in which disorder influences the electronic properties in strongly correlated systems is an intriguing question in modern condensed matter physics. Here, we report on fluctuation spectroscopy studies of the organic charge transfer salt κ-$(D_8$-ET$)_2$Cu[N(CN)$_2$]Br. The degree of intrinsic disorder in this quasi-2D conductor can be tuned by varying the cooling rate at the structural glass-like transition around $T_g \simeq 75\,\mathrm{K}$ [1]. We compare data taken after slow ($0.05\,\mathrm{K/min}$) and fast ($5\,\mathrm{K/min}$) cooling. Larger cooling rates increase the amount of disorder and therefore enhance the resistance fluctuations. The total noise power originating from the vibrational degrees of freedom of the ET molecules [2] is about 25% higher for the faster cooling rate. In addition, our experiments reveal another contribution to the resistance noise. Since κ-$(D_8$-ET$)_2$Cu[N(CN)$_2$]Br is very close to a Mott metal-to-insulator transition the coexistence of electronic correlations and disorder may result in the formation of a so-called soft Hubbard gap in the DOS due to localization effects.

[1] N. Toyota, M. Lang, and J. Müller, Low-Dimensional Molecular Metals, Springer (2007)

[2] J. Müller et al., Phys. Rev. B 79, 214521 (2009)

15 min. break

TT 12.7 Tue 11:15 H19

Universal critical conductivity at the metal-insulator transition in the two-dimensional Anderson-Hubbard model — •Prabuddha Chakraborty[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretical Physics III, Center for Electronic Corre-

lations and Magnetism, University of Augsburg, D-86135, Augsburg, Germany — [2]Institute of Theoretical Physics, University of Warsaw, Warszawa, Poland

We demonstrate, through extensive quantum Monte-Carlo simulations, the existence of a universal critical conductivity at an Anderson insulator-metal transition in two dimensions.The universality of the critical conductivity across various models of disorder is presented, thus pointing to the existence of a quantum critical point with universal properties. We also present results for the compressibility and magnetic susceptibilities across the phase transition and compare them to experimental data and analytical renormalization group predictions. This research is supported through SFB 484 of the Deutsche Forschungsgemeinschaft.

TT 12.8 Tue 11:30 H19

Real-Space Renormalization Group for Anderson Localization of Interacting Electrons in the Hubbard-Anderson Model — •Roman Katzer, Peter Henseler, and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Anderson localization of interacting fermions remains a controversial issue even for short-range interaction. We construct a real-space renormalization group (RG) approach for the disordered Hubbard model with random onsite single-particle energies ε_i. The Hubbard interaction U leads to a non-trivial random distribution of many-body energy levels. In the atomic limit (hopping $t \to 0$ adiabatically, while keeping the chemical potential equal on all sites) this distribution can be calculated exactly, depending on ε_i, U and the filling fraction, and can be expressed in terms of a modified ("screened") single-particle level distribution [1]. Switching on hopping ($t \neq 0$), successively increasing the real-space cluster size and mapping a cluster onto a single site generates an RG flow in the space of disordered many-body Hamiltonians. Restricting the flow to low energies and observing the spin structure, the Fock space may be decimated in each RG step to keep only three Fock-space sectors with consecutive cluster occupation numbers and in each sector the lowest energy state. This leads to an RG flow of disordered Hubbard models, where the flow of the random distribution of energy levels serves as indicator for localization or delocalization. The evaluation of this scheme in $d = 1$ agrees with previous results.
[1] P. Henseler, J. Kroha and B. Shapiro, Phys. Rev. B **77**, 075101 (2008); **78**, 235116 (2008).

TT 12.9 Tue 11:45 H19

Microdomain Formation near the First-Order Metal-Insulator Transition of the Hubbard Model — •Qinyong Liu and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Since the metal-insulator transition (MIT) in Mott-Hubbard systems at finite temperature is of first order, there must be a region in the vicinity of the transition where metallic and insulating phases coexist. Thus, in this region insulating microdomains are thermally excited within the thermodynamically stable metallic phase or vice versa. The existence of such microdomains has recently been demonstrated experimentally in VO_2. We calculate the size distribution of microdomains as a function of temperature and Hubbard repulsion U. The electronic spectra and the free energy per site are calculated in metallic and in insulating regions as well as across a metal-insulator domain wall, using the generalization of dynamical mean field theory (DMFT) for inhomogeneous systems, with the non-crossing approximation (NCA) as impurity solver. The domain-size distribution is obtained from the resulting free energy difference, including volume and domain wall energies, and exhibits non-trivial, non-monotonic behavior. The first-order MIT of Mott-Hubbard systems may, hence, be viewed as a percolation problem with an anomalous resistivity due to self-generated domain disorder.

TT 12.10 Tue 12:00 H19

Interplay of thermal and quantum spin fluctuations on the Kagome lattice — •Dirk Wulferding[1,2], Patric Scheib[1], Peter Lemmens[1,2], Jens Röder[3], Philippe Mendels[4], Young Lee[5], Wing-Ho Ko[5], and Mark de Vries[6] — [1]IPKM, TU-BS, Braunschweig — [2]IGSM, TU-BS, Braunschweig — [3]IPTC, TU-BS, Braunschweig — [4]Univ. Paris Sud, France — [5]MIT, Cambridge, MA, USA — [6]CSEC and SC, Univ. Edinburgh, UK

Raman scattering in the Herbertsmithite $ZnCu_3(OH)_6Cl_2$, the first realization of a Heisenberg spin 1/2 AF on a kagome lattice, shows two components, a high temperature quasi elastic signal and a low temperature, broad maximum, extending to high energy. We have investigated the temperature dependence and symmetry properties of both signals in this highly frustrated material. Work supported by ESF-HFM and DFG.

TT 12.11 Tue 12:15 H19

Quantum magnetism of the Hubbard model on the Triangular Lattice — •Hong-Yu Yang[1], Andreas Läuchli[2], Frederic Mila[3], and Kai Phillip Schmidt[1] — [1]Lehrstuhl für Theoretische Physik I, Otto-Hahn-Strasse 4, TU Dortmund, 44221 Dortmund, Germany — [2]Max Planck Institut für Physik komplexer Systeme, Nöthnitzerstrasse 38, 01187 Dresden, Germany — [3]Institute for Theoretical Physics, EPF Lausanne, 1015 Lausanne, Switzerland

The organic compound κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ exhibits strong evidence for a spin liquid phase at low temperatures. To study this possible spin liquid phase we investigate the quantum magnetism of the Hubbard model on the isotropic and anisotropic triangular lattice at half filling. First, we quantitatively derive effective quantum spin models using perturbative continuous unitary transformations. The accuracy of this spin model is determined by comparing it with exact diagonalizations (ED) on the original Hubbard model. In the second step we use ED to analyze the properties of the spin model on larger clusters. We find clear evidence for the existence of a spin liquid phase located between the long-range ordered antiferromagnet and the metallic phase. Finally, the anisotropic case is tackled which is expected to give further insights into the quantum magnetism of the organic compound.

TT 12.12 Tue 12:30 H19

Quantum spin-liquid state emerging in two-dimensional correlated Dirac fermions — Zi Yang Meng[1], •Thomas C. Lang[2], Stefan Wessel[1], Fakher F. Assaad[2], and Alejandro Muramatsu[1] — [1]Institut für Theoretische Physik III, Universität Stuttgart, Germany — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany

We analyze the ground-state of the Hubbard model of spin-$\frac{1}{2}$ Dirac fermions on the honeycomb lattice at half-filling, using large-scale quantum Monte Carlo simulations. We find that the weak coupling semimetal and the antiferromagnetic Mott insulator at strong interactions are separated by an extended gapped phase in an intermediate coupling regime. Exploring excitation gaps, correlation functions as well as probing for flux quantization, we conclude that a spin liquid, lacking any conventional order (i.e. symmetry breaking), emerges in the vicinity of the Mott transition with local correlations best described by resonating valence bonds.

TT 12.13 Tue 12:45 H19

Competing interactions and symmetry breaking in the Hubbard-Holstein model — •Johannes Bauer — Max-Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

This contribution has been withdrawn.