TT 15: Correlated Electrons: Metal-Insulator Transition 2

Time: Tuesday 9:30–13:00 Location: HSZ 301

TT 15.1 Tue 9:30 HSZ 301

Indications for a line of continuous phase transitions at finite temperatures connected with the apparent metal-insulator transition in two-dimensional disordered systems — •Arnulf Möbius — Leibniz Institute for Solid State and Materials Research IFW Dresden, PO Box 270116, D–01171 Dresden, Germany

In a recent experiment, Lai and coworkers studied the apparent metal-insulator transition of a Si quantum well structure tuning the charge carrier concentration n, see [1]. They observed linear temperature dependences of the conductivity $\sigma(T,n)$ around the Fermi temperature and found that the corresponding $T \to 0$ extrapolation $\sigma_0(n)$ exhibits a sharp bend just at the MIT.
Here, reconsidering data from [1], it is shown that this sharp bend is related to a peculiarity of $\sigma(T = \text{const}, n)$ clearly detectable in the whole T range up to 4 K, the highest measuring temperature in [1]. Since this peculiarity seems not to be smoothed out with increasing temperature, it may indicate a sharp continuous phase transition between the regions of apparent metallic and activated conduction to be present at finite temperature. Hints from other investigations of such a behavior are discussed. Finally, a scaling analysis illuminates similarities to previous experiments and provides understanding of the shape of the peculiarity and of sharp peaks found in $\mathrm{d}\log_{10}\sigma/\mathrm{d}n$ as function of n. Details of this study are given in [2].

[1] K. Lai, W. Pan, D.C. Tsui, S. Lyon, M. Mühlberger, and F. Schäffler, Phys. Rev. B **75**, 033314 (2007).
[2] A. Möbius, Phys. Rev. B **77**, 205317 (2008).

TT 15.2 Tue 9:45 HSZ 301

Scanning tunneling spectroscopy across the insulator-to-metal transition in $La_{0.67}Ca_{0.33}MnO_3$ thin films — •Silvia Seiro[1,2], Yanina Fasano[2,3], Ivan Maggio-Aprile[2], Edmond Koller[2], Rolf Lortz[2,4], and Øystein Fischer[2] — [1]MPI-CPfS, Nöthnitzer Str. 40, 01187 Dresden, Germany — [2]DPMC-University of Geneva, Quai Ernest-Ansermet 24, 1211 Geneva, Switzerland — [3]Centro Atómico Bariloche, Av. E. Bustillo 9500, 8400 S. C. de Bariloche, Argentina — [4]Department of Physics, The Hong Kong University of Science & Technology, Clear Water Bay, Kowloon, Hong Kong

We present the temperature evolution of scanning tunneling spectra of $La_{0.67}Ca_{0.33}MnO_3$ thin films across the insulator-to-metal transition. A depletion in normalized conductance is observed over an energy range of a few hundred meV around the Fermi level. This depletion globally narrows upon cooling but is still present in the metallic phase. The link to macroscopic transport behavior is provided by the tunnel conductance at zero bias, which decreases upon cooling in the insulating phase, reaches a minimum close to the insulator-to-metal transition temperature and increases on cooling in the metallic phase. These results are interpreted in terms of dynamical short-range antiferromagnetic/charge order correlations.

TT 15.3 Tue 10:00 HSZ 301

Realistic model Hamiltonians for correlated organics — •Erik Koch — Institut für Festkörperforschung und Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

For a description of strongly correlated materials we have to resort to model Hamiltonians. These generalized Hubbard models have to be simple enough that they can be treated by non-perturbative many-body approaches, yet complex enough to capture the specifics of real materials. We discuss how to derive such realistic model Hamiltonians for molecular crystals starting ab-initio. We focus in particular on the calculation of screened Coulomb matrix elements for which we use a two-step approach: treating intra-molecular screening with density-functional theory, while describing inter-molecular screening via a lattice of distributed polarizabilities. We discuss the surprising screening effects that appear in highly polarizable lattices and present model Hamiltonians for quasi one- and two-dimensional organics.

TT 15.4 Tue 10:15 HSZ 301

How frustrated is the charge transfer salt κ-(BEDT-TTF)$_2$Cu$_2$(CN)$_3$ at ambient and elevated pressures? A first principles investigation. — •Harald O. Jeschke, Hem C. Kandpal, and Roser Valenti — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

The charge transfer salt κ-(BEDT-TTF)$_2$Cu(CN)$_3$ has been intensely discussed as it possibly represents a realization of a 2D quantum spin liquid. We employ first principles calculations to shed light on the underlying Hamiltonian. We carefully prepare equilibrium structures at ambient and elevated pressure using constant pressure Car Parrinello ab initio molecular dynamics calculations on the basis of the projector augmented wave method. We determine the hopping parameters of the underlying Hubbard Hamiltonian using tight binding fits to the calculated band structures. We find that increasing pressure reduces the frustration of the model.

15 min. break

TT 15.5 Tue 10:45 HSZ 301

LDA+DMFT study of the Sn/Si(111)($\sqrt{3} \times \sqrt{3}$)R30° surface states — •Sergej Schuwalow, Lewin Boehnke, and Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany

Experimental studies [1] and LDA+U calculations [2] for the Sn/Si(111)($\sqrt{3} \times \sqrt{3}$)R30° surface suggest a Mott-insulating surface state originating dominantly from strongly correlated Sn (5p) orbitals below about 70K. Interestingly, the Sn atoms form a 1/3 monolayer on an effective triangular lattice. Hence the issue of spin liquid physics may arise due to possible frustration effects.

In the scope of this work, we have first obtained an effective Hamiltonian for the surface states of this system in terms of maximally localized Wannier functions from LDA calculations. From there, we performed DMFT calculations for both a 1-band and a 3-band effective Hamiltonian to map out the temperature-dependent behavior of the spectral function close to the suggested metal-insulator transition and to investigate the importance of the different surface bands. In the case of the 3-band Hamiltonian, the full U matrix was used for the calculations. Finally, we compared the results of our dynamical approach to those obtained within the static LDA+U formalism.

[1] S. Modesti *et al.*, PRL **98**, 126401 (2007)
[2] G. Profeta and E. Tosatti, PRL **98**, 086401 (2007)

TT 15.6 Tue 11:00 HSZ 301

Metal-insulator transition in polymer surfaces modified by low-energy ion irradiation — •Yuri Koval, Irina Lazareva, and Paul Müller — Department für Physik, Universität Erlangen-Nürnberg, Germany

The surface of several polymers like polyimide, PMMA, or PET was graphitized by low-energy (0.15-1.5 keV) ion irradiation at different temperatures (150-700 K). Due to the small penetration depth of ions the thickness of conducting layers is substantially less than 10 nm. Depending on the energy of ions and the temperature of irradiation the sheet conductance can be changed from 10^{-11} S to 10^{-4} S. We show that with increase of the sample conductance the electric transport changes from variable range hopping to semi-metallic type.

Semi-metallic behavior was observed for samples with sheet conductances higher than the quantum conductance g. For samples with lower sheet conductance an exponential law $\sigma=\sigma_0\exp(-(T_0/T)^x)$ typical for variable range hopping transport was found. For samples with a power x=0.5 we have found a correlation between σ_0 and T_0 in the form $\sigma_0=\sigma_{00}\exp(T_0/T^*)^{0.5}$ with σ_{00} equal to the quantum conductance g. Analyzing the low temperature current-voltage characteristics, a similar correlation between the pre-exponential factor and the numerator in the exponent $j=j_0\exp(-(E_0/E)^{0.5})$ was observed, where j is the current density and E is the electric field.

TT 15.7 Tue 11:15 HSZ 301

Mott transitions at variable spin/orbital degeneracy — •Nils Blümer and Elena Gorelik — Institut für Physik, Universität Mainz, Mainz, Germany

The Mott transition between a metal and a paramagnetic insulator is central to the field of strongly correlated electron systems. Much insight into this phenomenon has been gained in numerical studies of the 1-band Hubbard model within dynamical mean-field theory (DMFT). In particular, the phase diagram and the behavior of characteristic observables (such as the effective mass) have been established with high

precision - despite the lack of analytic solutions. The physics of multiorbital models is richer (including the possibility of orbital-selective Mott transitions), but also much more challenging.

However, exact analytical results have been derived for the SU(2M) symmetric Hubbard model (where all spins/orbitals are equivalent) in the limit of large band multiplicity $M \to \infty$ [1]. So far, these predictions have only been checked/complemented by self-energy functional calculations with one bath site per orbital [2]; this method has quite substantial errors in the 1- band case [3].

We present numerically exact multigrid Hirsch-Fye quantum Monte Carlo estimates of the phase boundaries at half filling and for up to $M = 8$ bands. We also derive scaling laws which predict the phase boundaries for arbitrary orbital degeneracy M with high accuracy.

[1] S. Florens et al., Phys. Rev. B **66**, 205102 (2002).
[2] K. Inaba et al., Phys. Rev. B **72**, 085112 (2005).
[3] K. Požgajčić, arXiv:cond-mat/0407172v1 (2004).

TT 15.8 Tue 11:30 HSZ 301

Mott transitions in the repulsive SU(3) invariant Hubbard model — •Elena Gorelik and Nils Blümer — Institut für Physik, Universität Mainz, Mainz, Germany

Ultracold fermions on optical lattices are nowadays one of the most exciting fields of both experimental and theoretical studies. They are often considered as model systems for simulating complex condensed matter phenomena. On the other hand, fermionic atoms have large hyperfine multiplets, out of which *several* states can be trapped simultaneously, leading to new degrees of freedom that are unavailable in solid state physics. This feature has attracted a lot of attention as an origin of possible exotic superfluid states in the case of an attractive on-site interaction [1,2].

Here we focus on another important phenomenon that has not yet been addressed within the multiflavor context - the Mott transition in the repulsive case, both as a function of the local interaction U and of the chemical potential. We present the results of a DMFT study, using the multigrid Hirsch-Fye quantum Monte-Carlo impurity solver [3], for the repulsive three flavor fermionic system. The peculiarities and experimentally accessible signatures of Mott transitions in such a multiflavor system are discussed in comparison with the two flavor/spin case.

[1] Á. Rapp et al., Phys. Rev. Lett. **98**, 160405 (2007).
[2] R. W. Cherng et al., Phys. Rev. Lett. **99**, 130406 (2007).
[3] N. Blümer, arXiv:0801.1222 (2008).

15 min. break.

TT 15.9 Tue 12:00 HSZ 301

Phase diagram of the SU(N) Hubbard-Heisenberg model on the honeycomb lattice — •Thomas C. Lang[1], Zi Yang Meng[2], Stefan Wessel[2], Fakher F. Assaad[1], and Alejandro Muramatsu[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institut für Theoretische Physik III, Universität Stuttgart, Germany

We investigate the phase diagram of the half-filled $SU(N)$ Hubbard-Heisenberg model on the honeycomb lattice in the self-adjoint totally antisymmetric representation. By means of the projective ($T = 0$) quantum Monte Carlo method we simulate the model on lattices ranging up to $L = 15$. For $U = 0$ and in the quantum limit, $N = 2$, decreasing t/J triggers a quantum phase transition from semi-metal to an antiferromagnetic-insulator with no apparent intermediate phase. With increasing symmetry N the Hubbard-Heisenberg model exhibits purely paramagnetic phases. Our aim is to study in detail the phase diagram as a function of N from the quantum limit to the saddle point $N \to \infty$.

TT 15.10 Tue 12:15 HSZ 301

Quantum Monte Carlo study of the half-filled Hubbard model on the honeycomb lattice — •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

Using projective ($T = 0$) quantum Monte Carlo we investigate the ground-state properties of the half-filled Hubbard model on a honeycomb lattice. Our results confirm previous numerical findings[1] that antiferromagnetic long-range order sets in above a value of $U/t \approx 4.5$. However, examining the quasiparticle gap and the spin gap, we obtain preliminary indications, that the Mott-transition from the semimetal to an insulator occurs at a value of $U/t \approx 3.5$. A separation of two phase transitions allows for the possibility of an intermediate phase between the semi-metal and the antiferromagnetic insulator – a scenario, that has been discussed in recent theoretical studies[2,3]. Further numerical work, aiming at testing such propoals is in progress.

[1] S. Sorella and E. Tosatti, Europhys. Lett. **19**, 699 (1992).
[2] M. Hermele, Phys. Rev. B **76**, 035125 (2007).
[3] B. Uchoa and A. H. C. Neto, Phys. Rev. Lett. **98**, 146801 (2007).

TT 15.11 Tue 12:30 HSZ 301

Magnetic field induced semimetal-to-canted-antiferromagnet transition on the honeycomb lattice — •Martin Bercx and Fakher Assaad — TP1, Universität Würzburg

It is shown that the semi-metallic state with point like Fermi surface of the two-dimensional honeycomb lattice is unstable towards a canted anti-ferromagnetic insulator upon application of an in-plane magnetic field. This instability is already present at the mean-field level; the magnetic field shifts in opposite directions the up and down spin cones thereby generating a finite density of states at the Fermi surface and perfect nesting between the up and down Fermi sheets. This prefect nesting triggers a canted anti-ferromagnetic insulating state. Those conclusions, based on mean-field arguments, are confirmed with projective Quantum Monte Carlo methods on lattices up to 12×12 unit cells.

TT 15.12 Tue 12:45 HSZ 301

First order Mott transition at zero temperature in two dimensions: Variational plaquette study — •Matthias Balzer[1], Michael Potthoff[1], Bumsoo Kyung[2], David Senechal[2], and A.-M.S. Tremblay[2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]Département de physique and RQMP, Université de Sherbrooke, Québec, Canada

The nature of the metal-insulator Mott transition at zero temperature has been discussed for a number of years. Whether it occurs through a quantum critical point or through a first order transition is expected to profoundly influence the nature of the finite temperature phase diagram. We study the zero temperature Mott transition in the two-dimensional Hubbard model on the square lattice. Here we use the variational cluster approximation to embed a plaquette of four correlated sites and four or eight uncorrelated bath sites in the lattice. This takes into account the influence of antiferromagnetic short-range correlations. As the method is thermodynamically consistent and focuses on the optimization of a thermodynamical potential, it is ideally suited to distinguish between different phase diagram topologies. By contrast to single-site dynamical mean-field theory, the transition turns out to be first order even at zero temperature.