TT 28: Correlated Electrons: Metal-Insulator Transition 1

Time: Thursday 9:30–12:45 Location: H 2053

TT 28.1 Thu 9:30 H 2053

Surface Effects on Oxide Heterostructures — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Perovskite heterostructures have attracted recent interest due to the discovery of metallic interlayers in an otherwise insulating structure. The physical properties of such a multilayer structure hence are not present in either of its constituents. For example, at the contact between the two band insulators $LaAlO_3$ and $SrTiO_3$ a quasi 2D electron gas with very high carrier density is formed. However, it was shown that the $LaAlO_3$ surface layer must reach a critical thickness of 4 unit cells for the interface to be conducting.

We report on surface effects on the electronic properties of interfaces in epitaxial $LaAlO_3/SrTiO_3$ heterostructures. Our results are based on DFT calculations for well-relaxed multilayer configurations, terminated by a thin $LaAlO_3$ surface layer. On varying the thickness of this layer, we find that the interface conduction states are subject to almost rigid band shifts due to a modified Fermi energy. Confirming experimental data, the electronic properties of heterointerfaces therefore can be tuned systematically by alterating the surface-interface distance.

TT 28.2 Thu 9:45 H 2053

Hubbard Model on the Bethe lattice with next-nearest neighbor hopping — •Robert Peters and Thomas Pruschke — Friedrich-Hund-Platz 1, 37077 Göttingen

We investigated the Bethe lattice with nearest-neighbor and next-nearest neighbor hopping t_1 and t_2 within dynamical mean-field theory using Wilson's numerical renormalization group as impurity solver. We study this model for various values of t_2 including $t_2 = t_1$ and $t_2 < 0$. We especially discuss the interplay between antiferromagnetism and the paramagnetic metal-insulator-transition at half-filling. For the doped model the existence of ferromagnetism depending on the value of U is analyzed.

TT 28.3 Thu 10:00 H 2053

Optical conductivity and specific heat anomalies in the proximity of the Mott-Hubbard transition — •Alessandro Toschi[1], Massimo Capone[2,3], Claudio Castellani[3], and Karsten Held[1] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]ISC-CNR, Via dei Taurini 19, I-00185 Roma, Italy — [3]SMC, CNR-INFM and Dipartimento di Fisica, Università di Roma 'La Sapienza', Piazzale Aldo Moro 2, I-00185 Roma, Italy

A landmark of electronic correlations is the strong renormalization of the quasiparticle peak in the spectral function, and, as it has been recently demonstrated [1], the appearance of kinks in the self-energy at low frequency. As a consequence, strong renormalization of the Drude peak, of the temperature dependence of the optical sum rules and of the specific heat can be expected in the vicinity of the Mott-Hubbard transition. Indeed similar features have been observed in cuprates and, more generally, in transition metal oxides. DMFT calculations, using exact Diagonalization as an impurity solver and a large number of sites in the electronic bath, allow us to perform a detailed comparison with experiments. Our calculations unveil the existence of an anomalous deviation from Fermi-liquid-behavior at temperatures much lower than expected. Taking this deviation into account is important for a correct interpretation of the experimental data.

[1] K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I.A. Nekrasov, Th. Pruschke, and D. Vollhardt, Nature Physics **3**, 168 (2007).

[2] A. Toschi and M. Capone, cond-mat/0708.3475.

[3] A. Toschi, M. Capone, C. Castellani, and K. Held in preparation.

TT 28.4 Thu 10:15 H 2053

Mott-Hubbard transition in a two-band model: From three to two dimensions — •Philipp Hansmann, Xiaoping Yang, Alessandro Toschi, Giniyat Khaliullin, Ole Krogh Andersen, and Karsten Held — Max Planck Institute for Solid State Research, Stuttgart

The influence of dimensionality on the Mott-Hubbard transition in a two-band model is studied. More specifically we consider a two e_g-band Hubbard model at quarter filling which is analyzed within dynamical mean field theory. Nearest neighbor hopping and hybridization are taken into account as well as a small crystal-field splitting of the two e_g-bands. Starting from the three dimensional cubic symmetry the hopping in the crystallographic z-direction is tuned to zero where results for the two dimensional system are recovered. Although electronic correlations on surfaces and in two dimensions are expected to be stronger than in the three dimensional case, our results show that this effect is weakened as a result of the hybridization between the two e_g-orbitals.

TT 28.5 Thu 10:30 H 2053

Orbital-selective Mott transitions in a doped two-band Hubbard model — •Eberhard Jakobi, Nils Blümer, and Peter van Dongen — Institute of Physics, KOMET 337, Johannes Gutenberg University Mainz

Within the last few years, it has been established within dynamical mean-field theory (DMFT) that orbital-selective Mott transitions occur in half-filled degenerate two-band Hubbard with different bandwidths under quite general circumstances. We extend extend these studies to the general doped case, using a high-precision quantum Monte Carlo DMFT solver. For sufficiently strong interactions, orbital-selective Mott transitions as a function of total band filling are clearly visible in the band-specific fillings, quasi-particle weights and double occupancies.

TT 28.6 Thu 10:45 H 2053

Quantum phase transition in the two-band Hubbard model — •Theodoulos Costi and Ansgar Liebsch — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The interaction between itinerant and Mott localized electronic states in strongly correlated transition metal oxide materials with anisotropic Hund's exchange is studied within dynamical mean field theory in combination with the numerical renormalization group method . For values of the Hund's exchange and Coulomb interactions typical of many transition metal oxides, a novel nonmagnetic zero temperature quantum phase transition is found in the bad-metallic orbital-selective Mott phase of the two-band Hubbard model [1]. We describe the critical properties of this quantum phase transition and relate the critical exponents to those of an exactly solvable model.

[1] T. A. Costi and A. Liebsch, Phys. Rev. Lett. (2007); arXiv:0707.4535

15 min. break

TT 28.7 Thu 11:15 H 2053

Static Screening and Delocalization Effects in the Hubbard-Anderson Model — •Peter Henseler[1], Johann Kroha[1], and Boris Shapiro[2] — [1]Physikalisches Institut, Universität Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Department of Physics, Technion-Israel Institute of Technology, Haifa 32000, Israel

We study the suppression of electron localization due to the screening of the disorder potential in a Hubbard-Anderson model within a static picture, where interactions are absorbed into the redefinition of the random on-site energies, leading to an interaction-induced renormalization of the random distribution of onsite energies.

First the one-dimensional case is discussed, where we focus on the change of the electron localization length at the Fermi level. Two different approximations are presented, either one yielding a non-monotonic dependence of the localization length on the interaction strength, with a pronounced maximum at an intermediate interaction strength. We then investigate the higher-dimensional case, applying the selfconsistent theory of Anderson localization to the present problem, and a comparison with recent numerical results is presented.

TT 28.8 Thu 11:30 H 2053

Real-space DMFT for inhomogeneous strongly correlated fermionic systems — •Michiel Snoek[1], Csaba Toke[1], Irakli Titvinidze[1], Krzysztof Byczuk[2], and Walter Hofstetter[1] — [1]J. W. Goethe-Universität, Frankfurt am Main, Deutschland — [2]Universität Augsburg, Augsburg, Deutschland

We introduce the real-space dynamical mean-field theory (R-DMFT) method to describe strongly interacting lattice fermions in the presence of an external, space dependent potential. This method relies only on the assumption that the self-energy is a local quantity and is exact

in infinite dimensions. The power of the method is demonstrated by calculating Friedel oscillations in an ultracold Fermi gas in an optical lattice. Using the numerical renormalization group (NRG) and exact diagonalization as impurity solvers, we study the Mott transition in a harmonically confined Fermi gas in an optical lattice. In particular, the emergence of antiferromagnetic structures in the Fermi gas is analyzed in detail.

TT 28.9 Thu 11:45 H 2053

Micro-domain formation near the first-order Mott-Hubbard transition — •Qinyong Liu and Johann Kroha — Physikalisches Institut, Universität Bonn, Germany

Near the first order Mott-Hubbard transition of the Hubbard model there is a region where metallic and insulating states can coexist in a finite range of temperatures. We study the formation of insulating or metallic micro-domains embedded in the metallic or insulating phase, respectively, within this coexistence region. In order to calculate the behavior of the density of states across a domain wall, the dynamical mean field theory (DMFT) is generalized to a layer-DMFT, where the selfenergy remains local, but the effective impurity is coupled to different dynamical baths, depending on its distance from the domain wall. We use the non-crossing approximation (NCA) as the impurity solver. Our results allow to compute the free energy of a micro-domain in dependence on its size and, hence, the thermal distribution of domain sizes in depencence of temperature. These results may be relevant for understanding the anomalous temperature dependence of the conductivity near the Mott-Hubbard transition.

TT 28.10 Thu 12:00 H 2053

Crossover behavior in the metallic state of the one-dimensional Holstein model — •Steffen Sykora, Arnd Hübsch, and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden, Germany

The Holstein model is perhaps the simplest realization of a coupled electron-phonon system with a local interaction between dispersionless phonons of frequency ω_0 and electrons with hopping matrix element t. By applying the projective renormalization method (PRM), the physical properties of the one-dimensional model in the metallic state are investigated for the adiabatic case ($\omega_0/t \ll 1$), for the antiadiabatic case ($\omega_0/t \gg 1$), as well as for the intermediate case ($\omega_0/t \approx 1$). As a result we find that in the adiabatic case a phonon softening is observed at the Brillouin zone boundary whereas for the opposite case a hardening is found.

TT 28.11 Thu 12:15 H 2053

Spectral properties of locally correlated electrons in a BCS superconductor — •Johannes Bauer[1], Alex Hewson[1], and Akira Oguri[2] — [1]Department of Mathematics, Imperial College, London SW7 2AZ, UK — [2]Department of Material Science, Osaka City University, Sumiyoshi-ku, Osaka

We present a detailed study of the spectral properties of a locally correlated site embedded in a BCS superconducting medium. To this end the Anderson impurity model with superconducting bath is analysed by numerical renormalisation group (NRG) calculations. We calculate one and two-particle dynamic response function to elucidate the spectral excitation and the nature of the ground state for different parameter regimes with and without particle-hole symmetry. The position and weight of the Andreev bound states is given for all relevant parameters. We also present phase diagrams for the different ground state parameter regimes. This work is also relevant for dynamical mean field theory extensions with superconducting symmetry breaking.

TT 28.12 Thu 12:30 H 2053

Quantum critical scaling behavior of deconfined spinons — •Flavio Nogueira —

The talk has been moved to TT 19.16.