TT 28 Correlated Electrons: General Theory

Time: Thursday 10:00–13:00 Room: HSZ 301

TT 28.1 Thu 10:00 HSZ 301

Transport and optical properties of the Kondo lattice model — •Theo Costi — Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

Dynamical mean field theory is used to investigate transport and optical properties of the Kondo lattice model as a function of increasing hole doping around the Kondo insulating state. The two low energy scales of the model [1,2,3], the lattice coherence scale or single-ion Kondo scale, and the Fermi liquid coherence scale, are identified in spectral, transport, and optical properties. The gaps in transport and optics for Kondo insulators are identified and compared with those found by other approaches. The temperature dependence of the resistivity and frequency dependent optical conductivity is described. Close to the Kondo insulating state we find an incoherent metallic behaviour. Dynamical mean field theory is shown to provide a straightforward interpretation of the resistivity of such prototypical paramagnetic heavy fermion systems as $CeAl_3$.

[1] Pruschke, Th., R. Bulla, and M. Jarrell, 2000, Phys. Rev. B **61**, 12799.
[2] S. Burdin, A. Georges, D. R. Grempel, Phys. Rev. Lett. **85**, 1048-1051 (2000).
[3] T. A. Costi and N. Manini, J. Low Temp. Phys. **126**, 835 (2002).

TT 28.2 Thu 10:15 HSZ 301

Symmetry projection schemes for Gaussian Monte Carlo methods. — •F. F. Assaad[1], P. Werner[2], P. Corboz[2], E. Gull[2], and M. Troyer[2] — [1]Universität Würzburg — [2]ETH-Zürich

A novel sign-free Monte Carlo method for the Hubbard model has recently been proposed by Corney and Drummond. High precision measurements on small clusters show that ground state correlation functions are not correctly reproduced. We argue that the origin of this mismatch lies in the fact that the low temperature density matrix does not have the symmetries of the Hamiltonian. Here we show that supplementing the algorithm with symmetry projection schemes provides reliable and accurate estimates of ground state properties.

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TT 28.3 Thu 10:30 HSZ 301

Single hole dynamics in the bilayer Heisenberg model — •Christian Brünger and Fakher Assaad — Universität Würzburg

We consider a bilayer Heisenberg model exhibiting a quantum phase transition between ordered and disordered magnetic phases as a function of the interplanar coupling. Our aim is to study the following points: i) The evolution of the single particle spectral function from the disordered to ordered phase. ii) The coupling of the hole to critical magnetic fluctuations and the related fate of the quasiparticle residue in the vicinity of the critical point. As a function of decreasing interplanar coupling, the spectral function deforms continuously from its strong coupling behavior with band maximum at $\vec{k} = (\pi, \pi)$ to that of the planar t-J model with maximum at $\vec{k} = (\pi/2, \pi/2)$. Surprisingly, and on lattices up to 20×20, both for static and dynamic holes, the quasiparticle residue does not seem to be affected by critical magnetic fluctuations.

TT 28.4 Thu 10:45 HSZ 301

Static and dynamic properties of the spinless Falicov-Kimball model — •Steffen Sykora[1], Klaus W. Becker[1], and Veliko Zlatic[2] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Institute of Physics, Bijenika c. 46, P.O.B 304, 10000 Zagreb, Croatia

The spinless Falicov-Kimball model in one dimension is studied by use of a recently developed projector-based renormalization method (PRM) for many-particle Hamiltonians. The method is used to evaluate static and dynamic quantities of the system at half-filling. To these belong the quasiparticle excitation energy $\tilde{\varepsilon}_{\mathbf{k}}$ and the momentum distribution $n_{\mathbf{k}}$ of the conduction electrons and spatial correlation functions of the localized electrons. One of the most remarkable results is the appearance of a gap in $\tilde{\varepsilon}_{\mathbf{k}}$ at the Fermi level of the order of the Coulomb repulsion U which is accompanied by a smooth behavior for $n_{\mathbf{k}}$. The density of states for the conduction electrons and the one-particle spectral functions for the localized electrons are also discussed. In both quantities a gap opens with increasing U.

TT 28.5 Thu 11:00 HSZ 301

Correlated hybridization in transition metal complexes — •Arnd Hübsch[1], Jong-Chin Lin[2], Jianping Pan[2], and Daniel L. Cox[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden — [2]Department of Physics, University of California, Davis, CA 95616, USA

We apply local orbital basis density functional theory (using SIESTA) coupled with a mapping to the Anderson impurity model to estimate the Coulomb assisted or correlated hybridization between transition metal d-orbitals and ligand sp-orbitals for a number of molecular complexes. We find remarkably high values which can have several physical implications including: (i) renormalization of effective single band or multiband Hubbard model parameters for the cuprates and, potentially, elemental iron, and (ii) spin polarizing molecular transistors.

TT 28.6 Thu 11:15 HSZ 301

Momentum-resolved spectral functions of $SrVO_3$ calculated by LDA+DMFT — •M. Kollar[1], I. A. Nekrasov[2,1], K. Held[3], G. Keller[1], D. E. Kondakov[4], Th. Pruschke[5], O. K. Andersen[3], V. I. Anisimov[4], and D. Vollhardt[1] — [1]Theoretical Physics III, University of Augsburg — [2]Institute for Electrophysics, Ekaterinburg, Russia — [3]MPI for Solid State Research, Stuttgart — [4]Institute of Metal Physics, Ekaterinburg, Russia — [5]Institute for Theoretical Physics, University of Göttingen

We have calculated momentum-resolved spectral functions of $SrVO_3$ using LDA+DMFT [1]. To this end, we have employed Nth order muffin-tin (NMTO) downfolding to set up an effective low-energy Hamiltonian with three t_{2g} orbitals. This effective Hamiltonian was solved by DMFT. Our results for momentum-dependent spectra show renormalized quasiparticle bands over a broad energy range from -0.7 eV to +0.9 eV with small "kinks" discernible in the dispersion below the Fermi energy. A similar feature was also found recently in angle-resolved photoemission experiments [2].

[1] I. A. Nekrasov *et al.*, cond-mat/0508313.
[2] T. Yoshida *et al.*, cond-mat/0504075.

— 15 min. break —

TT 28.7 Thu 11:45 HSZ 301

Self-energy-functional approach (SFA) as a scheme for reduction of finite size effects — •Krunoslav Požgajčić — Institut für Physik, KOMET 337, Universität Mainz, 55099 Mainz, Germany

Self-energy-functional approach (Michael Potthoff, Eur. Phys. J. B 32, 429(2003)) and its extensions (Ning-Hua Tong, Phys. Rev. B 72, 115104(2005)) have been proposed as a general framework for embedded cluster methods. We will use SFA for different models in regimes which are characterized by strong finite size effects, like is the case with metallic states. It will be demonstrated that SFA can be regarded as a prescription for reduction of those effects. Other schemes devised for reduction of finite size effects will also be discussed.

TT 28.8 Thu 12:00 HSZ 301

Static vs. Dynamical Mean Field Theory of Mott Antiferromagnets — •Giorgio Sangiovanni[1], Alessandro Toschi[1], Erik Koch[2], Karsten Held[1], Massimo Capone[3,4], Claudio Castellani[4], and Olle Gunnarsson[1] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart — [2]Institut für Festkörperforschung, Forschungszentrum, Jülich — [3]Istituto dei Sistemi Complessi del CNR, Rom — [4]Dipartimento di Fisica Università di Roma "La Sapienza", Rom

In recent years, our ability to calculate strongly correlated materials has substantially improved. For instance, local density approximation supplemented by a local Coulomb interaction U treated in the static Hartree-Fock (HF) mean field theory (LDA+U), gives extremely accurate results for ground-state properties at large U, especially in the presence of magnetic or orbital ordering. On the other hand, dynamic properties are not well described by LDA+U, due to the too poor treatment of excited states given by HF. To go beyond this approximation, the more sophisticated LDA+DMFT has been recently developed. Considering the antiferromagnetic phase of a simple model, the single-band Hubbard

model, we explicitely analyze the differences between static and dynamical mean field theory. In DMFT the HF band is strongly renormalized and spectral weight is trasferred to spin-polaron side bands. Already for intermediate U the overall bandwidth is larger than in HF and the gap is considerably smaller. Such differences survive any renormalization of U. We compare our results with photoemission experiments for Cr-doped V_2O_3 obtaining extremely good qualitative agreement.

TT 28.9 Thu 12:15 HSZ 301

Non-local corrections to DMFT: magnetic correlation effects on the spectral function — •Alessandro Toschi, Andrey Katanin, and Karsten Held — Max-Planck Institut für Festkörperforschung, Heisenbergstr. 1,*D-70569 Stuttgart, Germany

We consider non-local corrections to the dynamical mean-field theory (DMFT) self-energy and spectral functions in the presence of strong magnetic fluctuations. Specifically, we evaluate the momentum-dependent self-energy starting from the one- and two-particle DMFT Green functions. Contrary to previous studies (e.g., the GW+DMFT approach) the local three-frequency vertex corrections are taken into account. Unlike the dynamical cluster approximation or the cellular DMFT approach, our method allows to study the effect of magnetic fluctuations with large correlation length. The effect of antiferromagnetic fluctuations is studied for the single-band Hubbard model at half filling. Going beyond DMFT we find precursor effects of the antiferromagnetic order already in the paramagnetic phase: the momentum dependence of the self-energy becomes particularly strong in the vicinity of the antiferromagnetic transition.

TT 28.10 Thu 12:30 HSZ 301

Thermodynamics of a Fermi liquid in a magnetic field. — •Dmitri Efremov[1], Joseph Betouras[2], and Andrey Chubukov[3] — [1]Technical University of Dresden — [2]University of Leiden — [3]University of Wisconsin

We present calculations of the non-analytic terms in the spin susceptibility $\chi_s(T)$ and the specific heat $C(T)$ to systems in a magnetic field. Without a field, $\chi_s(T)$ and $C(T)/T$ are linear in T in 2D, while in 3D, $\chi_s(T)$ is proportional to T^2 and $C(T)/T$ proportional to $T^2 \log T$. We show that in a magnetic field, the linear in T terms in 2D become scaling functions of $\mu_B H/T$. We present explicit expressions for these functions and show that at high fields, $\mu_B H \gg T$, $\chi_s(T,H)$ scales as $|H|$. We also show that in 3D, $\chi_s(T,H)$ becomes non-analytic in a field and at high fields scales as $H^2 \log |H|$

TT 28.11 Thu 12:45 HSZ 301

Exotic excitations with fractional charges on frustrated lattices — •Frank Pollmann[1], Peter Fulde[1], and Erich Runge[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Technische Universität Ilmenau, Weimarer Str. 25, 98693 Ilmenau, Germany

Geometrical frustration of lattices can lead to a macroscopic degeneracy in the classical limit and thus to many interesting physical effects. In spin systems these are e.g. translational invariant spin liquid ground states and deconfined spinons. In contrast to magnetic properties, one began only recently to explore the charge degrees of freedom on frustrated lattices.

For the systematic study of charge degrees of freedom, we consider a model of spinless fermions with nearest-neighbor hopping t and Coulomb repulsion V. Quantum fluctuations reduce the classical ($t = 0$) macroscopic degeneracy. For the strongly correlated limit $V \gg |t|$, it has been predicted that an added electron can decay into two mobile quasiparticles, leading to fractional charges of $e/2$ in 2D and 3D systems.

For a deeper understanding of these charge degrees of freedom we calculated numerically the properties of static and dynamic charges on the 2D checkerboard lattice. Evidence for a weak mutual confinement of two fractional charges is found, leading to excitations with very large spatial extend. We argue that the fractional charges should be deconfined on the 3D pyrochlore lattice.