TT 34: Correlated Electrons: Metal-Insulator Transition 1

Time: Wednesday 16:30–18:00 Location: H 3010

TT 34.1 Wed 16:30 H 3010

Periodized Matsubara Green's functions — •Andro Sabashvili, Mats Granath, and Stellan Östlund — Department of Physics, University of Gothenburg, Gothenburg, Sweden

A new formalism for Fermionic thermal Green's functions that are periodized in imaginary (Matsubara) frequency space is developed. The periodization requires a generalisation of the Dyson equation and Luttinger-Ward-Baym-Kadanoff functional. Due to the Matsubara Green's function periodicity imaginary frequency space is relatively small which allows calculations at the extremely high precision which is necessary to perform a reliable analytic continuation. The formalism was tested on dynamical mean field theory calculations using iterated perturbation theory for the paramagnetic Hubbard model [1]. Currently the method together with the DRPA (dressed random phase approximation) is being used to study particular 2D models.
[1] arXiv:1103.3516v2

TT 34.2 Wed 16:45 H 3010

Emergence of a joint low-energy scale close to the orbital-selective Mott transition — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretical Physics III, Electronic Correlations and Magnetism, Universität Augsburg

We investigate the microscopic precondition for the appearance of kinks in the self-energy [1] and their relation to low-energy spin-excitations [2] within the framework of Dynamical Mean Field Theory. To this end we investigate the two-band Hubbard model with unhybridized, differently correlated orbitals close to the orbital selective Mott transition [3]. We find the emergence of one common energy-scale which is shared by the self-energy kinks and the diagonal spin-susceptibilities. A physical explanation of this energy-scale is obtained from a minimal Kondo-type model.
[1] K. Byczuk *et al.*, Nat. Phys. **3**, 168 (2007).
[2] C. Raas, P. Grete, and G. Uhrig, Phys. Rev. Lett. **102**, 076406 (2009).
[3] C. Knecht, N. Blümer, and P. G. J. van Dongen, Phys. Rev. Lett. **72**, 081103 (2005).

TT 34.3 Wed 17:00 H 3010

Correlated multiorbital systems, a Gutzwiller study — Nicola Lanata'[1], •Hugo U. R. Strand[1], Xi Dai[2], and Bo Hellsing[1] — [1]University of Gothenburg, SE-412 96 Gothenburg, Sweden — [2]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

We present a numerical method for the minimization of general multi-orbital Gutzwiller variational wavefunctions in the Gutzwiller approximation [1]. The method is general in the sense that it can treat any type of local interaction, in particular spin-flip and pair-hopping interactions. To construct the variational wavefunction, we apply the ϕ-matrix formalism [2], and present a general approach for how to reduce the variational space by imposing lattice point group symmetries.

Using our numerical method we study the multiorbital Hubbard model for d-electron systems with rotational invariant Kanamori-interaction. The variational wavefunction is restricted to cubic symmetry and the properties of the model is studied with respect to; total electron filling, e_g-t_{2g} crystal field splitting and interaction strength.

This work is an extension of the Gutzwiller solver, used in the first principles LDA+Gutzwiller method [3], to general local interactions.
[1] N. Lanatà, H. U. R. Strand, X. Dai, B. Hellsing, (arXiv:1108.0180)
[2] N. Lanatà, P. Barone, M. Fabrizio, Phys. Rev. B **78**, 155127 (2008)
[3] X. Y. Deng, L. Wang, X. Dai, Z. Fang, Phys. Rev. B **79**, 075114 (2009)

TT 34.4 Wed 17:15 H 3010

The role of rotational symmetry in the magnetism of multiorbital Hubbard model — •Andrey Antipov[1,2] and Alexey Rubtsov[2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Moscow State University, Department of Physics, 1-2 Leninskiye Gory, 119991 Moscow, Russia

The effects associated with orbital fluctuations play an important role in the physics of strongly correlated electron systems. Examples worth noting are the orbital ordering effects and the orbital-selective Mott transition. A full quantitative description of these systems require taking into account the complete Coulomb interaction between the valence band electrons, a difficult task for quantum impurity solvers. This complexity often leads to taking into account only the density-density part of the Coulomb interaction which is diagonal in the orbital space. As it was shown in [1] this reduction can lead to a breakdown of a Kondo-peak in the metallic density of states of a multiorbital Hubbard model due to the change in the degree of the degeneracy of the ground state.

In order to access the finite-temperature regime the interaction-expansion quantum Monte Carlo impurity solver was employed. It is shown that taking into account the full rotationally invariant Coulomb interaction leads to double decrease of the metal-insulator transition temperature in a doubly-occupied three-band model and to a 20% change in a half-filled two-band and three-band models. The change in the density of states is compatible with the results of [1].
[1] Th. Pruschke and R. Bulla, Eur. Phys. J. B 44, 217 (2005)

TT 34.5 Wed 17:30 H 3010

Model study of the Dzyaloshinskii-Moriya interaction in strongly correlated itinerant systems — •Sergej Schuwalow, Christoph Piefke, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

In low symmetry systems, the combination of spin-orbit interaction and broken inversion symmetry may give rise to effective noncollinear magnetic interactions first described in [1,2]. With the recently increasing interest in the effects of spin-orbit coupling, it becomes important to assess the role of such effects in the scope of complex solid state systems with different competing interactions.

Within this work, we investigate the interplay between strong electronic correlations and noncollinear magnetism induced by the Dzyaloshinskii-Moriya interaction in an itinerant model system within the framework of the Rotationally-Invariant Slave-Boson formalism (RISB)[3,4]. It allows us to capture the low-energy physics of the interacting system while retaining full rotational degrees of freedom which are essential for the magnetic structure at hand. Our main focus lies on determining the magnetic properties of the system and their behaviour under the influence of a finite Hubbard U.
[1] Dzyaloshinskii, J. Phys. Chem. Solids **4**, 241 (1958).
[2] Moriya, Phys. Rev. **120**, 91 (1960).
[3] Lechermann, Georges, Kotliar, Parcollet, PRB **76**, 155102 (2007).
[4] Piefke, Boehnke, Georges, Lechermann, PRB **82**, 165118 (2010).

TT 34.6 Wed 17:45 H 3010

Heat transport in a disordered and interacting electron system — •Georg Schwiete[1] and Alexander Finkelstein[2,3] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, Germany — [2]Texas A&M University, Texas, USA — [3]The Weizmann Institute of Science, Rehovot, Israel

We study thermal conductivity in a disordered two dimensional electron gas at low temperatures. To this end we calculate the heat density correlation function. In comparison to the case of the well-studied charge density correlation function additional logarithmic corrections appear. Particular care is taken to confirm the compatibility of these corrections with the energy conservation law. The purpose of this study is to develop a renormalization group treatment for heat transport. This would allow to describe thermal transport near the metal-insulator transition.