TT 6 Correlated Electrons - (General) Theory I

Zeit: Freitag 14:00–16:15 Raum: TU H2053

TT 6.1 Fr 14:00 TU H2053

Theory of optical spectral weights in Mott insulators with orbital degeneracy — •Peter Horsch[1], Giniyat Khaliullin[1], and Andrzej M. Oles[1,2] — [1]Max-Planck-Institut fuer Festkoerperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Marian Smoluchowski Institute of Physics, Jagellonian University, Reymonta 4, PL-30059 Krakau, Poland

Introducing partial sum rules for the optical multiplet transitions, we outline a unified approach to magnetic and optical properties of strongly correlated transition metal oxides. On the examples of $LaVO_3$ and $LaMnO_4$ we demonstrate how the temperature and polarization dependences of different components of the optical multiplet are determined by the underlying spin and orbital correlations dictated by the low-energy superexchange Hamiltonian.

G. Khaliullin, P. Horsch, and A.M. Oleś, Phys. Rev. B 70, 195103 (2004).

TT 6.2 Fr 14:15 TU H2053

Spectral functions of some frustrated lattice structures with charge degrees of freedom — •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, Fakultät für Mathematik und Naturwissenschaften, 98684 Ilmenau, Germany

Geometrical frustration of lattices leads to many interesting physical effects. While the magnetic properties of frustrated lattices have already received wide interest, one recently began to explore the charge degrees of freedom. In particular it has been proposed that excitations carrying charge e/2 should exist. However, it is not clear whether these excitations can separate from each other or are confined. For a deeper understanding of the dynamics of these charge degrees of freedom we calculated numerically the spectral functions of spinless fermions on finite checkerboard- and kagomé lattices. In both cases the spectral functions indicate a strong non-Fermi liquid behaviour. Furthermore we compare our results with analogous bosonic systems.

TT 6.3 Fr 14:30 TU H2053

Phase diagram of the half-filled two-dimensional SU(N) Hubbard-Heisenberg model. — •Fakher Assaad — Universität Würzburg

We investigate the phase diagram of the half-filled SU(N) Hubbard-Heisenberg model with hopping t, exchange J and Hubbard U, on a two-dimensional square lattice. In the large-N limit, and as a function of decreasing values of t/J, the model shows a transition from a d-density wave state to a spin dimerized insulator. A similar behavior is observed at N=6 whereas at N=2 a spin density wave insulating ground state is stabilized. The N=4 model, has a d-density wave ground state at large values of t/J which as a function of decreasing values of t/J becomes unstable to an insulating state with no apparent lattice and spin broken symmetries. In this state, the staggered spin-spin correlations decay as a power-law, resulting in gapless spin excitations at $\vec{q} = (\pi, \pi)$. Furthermore, low lying spin modes with small spectral weight are apparent around the wave vectors $\vec{q} = (0, \pi)$ and $\vec{q} = (\pi, 0)$. This gapless spin liquid state is equally found in the $SU(4)$ Heisenberg ($U/t \to \infty$) model in the self-adjoint antisymmetric representation. An interpretation of this state in terms of a π-flux phase is offered. Our results stem from projective ($T = 0$) quantum Monte-Carlo simulations on lattice sizes ranging up to 24×24.

TT 6.4 Fr 14:45 TU H2053

Electron-phonon interaction in strongly correlated materials — •Oliver Rösch and Olle Gunnarsson — Max-Planck-Institut für Festkörperforschung, Heisenbergstr.1, 70569 Stuttgart

We study the interplay of electron-phonon and eletron-electron interactions for a t-J model with electron-phonon coupling. Using exact sum rules, we find that the effect of the electron-phonon interaction on the phonon self-energy is strongly suppressed at low doping, while there is no corresponding suppression for the electron self-energy or the phonon-induced electron-electron interaction.[1]

Photoemission experiments suggest polaronic behavior in undoped cuprates due to coupling to bosons. Calculating the electron-phonon interaction in a shell model, we find sufficiently strong coupling to give polaronic behavior. Using an adiabatic approximation we explain why the broad peak from phonon sidebands shows a dispersion consistent with that of a quasi-particle in a purely electronic model without electron-phonon interaction.[2]

[1] O. Rösch and O. Gunnarsson, cond-mat/0407064, Phys. Rev. Lett. in press.
[2] O. Rösch and O. Gunnarsson, cond-mat/0410247.

TT 6.5 Fr 15:00 TU H2053

Kombination von Vielteilchen- und Ab-Initio-Methoden zur Berechnung der elektronischen Struktur von Metallen — •Olaf Peschel[1], Gerd Czycholl[1] und Ilan Schnell[2] — [1]Universität Bremen, Institut für Theoretische Physik — [2]Los Alamos National Laboratory, Theoretical Division

Wir gehen von den Bloch-Wellenfunktionen einer DFT-Hartree-Rechnung (ohne Austausch-Korrelationspotential) aus, mit denen wir die statische Suszeptibilität und dielektrische Funktion in Random Phase Approximation (RPA) berechnen. Die Bloch-Wellenfunktionen transformieren wir zu maximal lokalisierten Wannier-Funktionen, und berechnen bezüglich dieser Basis alle relevanten Hopping- und statisch abgeschirmten Coulomb-Matrixelemente. Wir haben damit den Hamilton-Operator in Zweiter Quantisierung unter Berücksichtigung statischer Abschirmung, mit ab-initio berechneten Parametern. Dies ermöglicht die Anwendung von Verfahren der Vielteilchentheorie.

Konkrete Rechnungen wurden für Li als denkbar einfachstes Metall durchgeführt. Es zeigt sich, daß nur on-site-Beiträge bei den abgeschirmten Coulomb-Matrixelemente relevant sind, so daß wir ein verallgemeinertes Vierband-Hubbard-Modell erhalten. Da die Größe der abgeschirmten Coulomb-Wechselwirkung deutlich geringer als die Bandbreite ist, kann die Selbstenergie in zweiter Ordnung Störungsrechnung (SOPT) berechnet werden. Dadurch wird dynamische Abschirmung mitberücksichtigt. Wir vergleichen die Ergebnisse der SOPT mit denen einer statisch abgeschirmten Hartree-Fock-Rechnung.

TT 6.6 Fr 15:15 TU H2053

Transportgrößen von Systemen schwerer Fermionen in DMFT/NRG — •Claas Grenzebach, Frithjof Anders und Gerd Czycholl — Institut für Theoretische Physik, Universität Bremen

Systeme schwerer Fermionen werden durch das periodische Andersonmodell (PAM) beschrieben, welches mittels der dynamischen Molekularfeldtheorie (DMFT) auf ein effektives Einzelstörstellenproblem (SIAM) abgebildet wird. Dieses behandeln wir mit numerischer Renormierungsgruppentheorie (NRG), einem nicht-störungstheoretischen Verfahren, das sich für Rechnungen mit kleinen, mittleren und großen Wechselwirkungen U eignet und die Kondoskala korrekt wiedergibt.

Damit werden in Abhängigkeit von der Temperatur statische und dynamische Leitfähigkeiten und die Thermokraft berechnet.

TT 6.7 Fr 15:30 TU H2053

Influence of Electron Correlations on Electron Transfer — •Sabine Tornow, Ning-Hua Tong, and Ralf Bulla — Theoretische Physik III, Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Electron transfer is a basic chemical process and is found, e.g. in corrosion of metals, enzymatic activities, cell metabolism or photosynthesis. The donor and acceptor sites may be transition metal ions (e.g., in some basic biological processes) and are strongly coupled to environmental modes (bath). To include electron correlations and multi electron transfer we propose a new model which extends the spin-boson model. We calculate static and dynamic properties using Wilsons Numerical Renormalization Group method. We discuss the thermal transition rate and discuss polaron, bipolaron and exciton formation.

TT 6.8 Fr 15:45 TU H2053

Arbitrary-range hopping on the Bethe lattice: Exact results for densities of states and dynamical mean-field theory — •Marcus Kollar[1], Martin Eckstein[1], Krzysztof Byczuk[2], and Dieter Vollhardt[1] — [1]Theoretische Physik III, Elektronische Korrelationen und Magnetismus, Institut für Physik, Universität Augsburg, 86135 Augsburg — [2]Institute of Theoretical Physics, Warsaw University, ul. Hoza 69, 00-681 Warszawa, Poland

We develop a new method which relates an arbitrary hopping Hamiltonian on the Bethe lattice to the Hamiltonian with nearest-neighbor hopping [1]. This provides an exact expression for the density of states for any hopping. We present analytic results for the DOS corresponding to hopping between nearest and next-nearest neighbors, and also for exponentially decreasing hopping amplitudes. Conversely it is possible to construct a hopping Hamiltonian on the Bethe lattice for any given DOS. We also derive the exact self-consistency equations arising in the context of dynamical mean-field theory, which lead to a new starting point for studies of the Hubbard-type models with frustration.

[1] M. Eckstein *et al.*, cond-mat/0409730.

TT 6.9 Fr 16:00 TU H2053

A Quantum Central Limit Theorem for Interacting Many Particle Systems and its Applications — •Michael Hartmann[1,2], Günter Mahler[2], and Ortwin Hess[3] — [1]DLR Stuttagrt, Pfaffenwaldring 38-40, 70569 Stuttgart — [2]Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart — [3]Advanced Techology Institute, University of Surrey, Guildford GU2 7XH, UK

We present a central limit theorem for the distribution of the total energy in a product state of a quantum many body system with nearest neighbor or next nearest neighbor interactions [1]. Using this result, one can draw estimates on quantities which are functions of the total energy without diagonalizing the Hamiltonian. Interesting examples are the density of states and the partition function [2]. On the other hand, information about the local (subsystem-) states can be obtained, too [3]. An advantage of our approach is its applicability to strongly interacting and frustrated systems.

[1] Hartmann, Mahler and Hess: Lett. Math. Phys. 68 (2004) 103
[2] Hartmann, Mahler and Hess: cond-mat/0406100
[3] Hartmann, Mahler and Hess: Phys. Rev. Lett. 93 (2004) 080402