TT 23: Correlated Electrons: (General) Theory

Time: Wednesday 14:00–18:45 Location: H 0104

TT 23.1 Wed 14:00 H 0104

Multigrid Hirsch-Fye quantum Monte Carlo solver for dynamical mean-field theory — •Nils Blümer — Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz

The dynamical mean-field theory (DMFT) is a nonperturbative approach to Hubbard-type models in which an impurity model has to be solved self-consistently. This is possible nonperturbatively using the Hirsch-Fye quantum Monte-Carlo (HF-QMC) algorithm which introduces an imaginary-time discretization $\Delta\tau$. The associated Trotter error impacts all "raw"HF-QMC results including phase boundaries, Green functions, spectra, and scalar observables such as energies and quasiparticle weights. Unbiased estimates of scalar observables can be derived from HF-QMC data by extrapolation $\Delta\tau \to 0$, with high precision and efficiency [1]. However, this *a posteriori* correction of the Trotter error is problematic close to phase boundaries and could so far not be applied to Green functions and spectra.

In this talk, I show how numerically exact Green functions can be extrapolated from HF-QMC estimates and construct a multigrid HF-QMC algorithm which eliminates the discretization error within the DMFT self-consistency cycle. In contrast to conventional HF-QMC, the multigrid algorithm converges to the numerically exact fixed point(s) and allows for the direct determination of phase boundaries without further extrapolation. It extends the useful range of $\Delta\tau$ values and yields unbiased estimates of observables with high precision and efficiency, even close to phase transitions.

[1] N. Blümer, to appear in Phys. Rev. B [arXiv:0708.1749v3].

TT 23.2 Wed 14:15 H 0104

Bath-symmetries and hybridization sum-rules for CDMFT and DCA — •Erik Koch[1], Giorgio Sangiovanni[2], and Olle Gunnarsson[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart

In the Hamiltonian formulation of CDMFT and DCA, the point symmetries of the cluster imply symmetries of the hybridization, which can substantially reduce the number of independent parameters to fit the bath Green function. We review these symmetries and derive general sum-rules for the hybridizations, which (i) allow to check the quality of a fit using a finite set of bath sites and (ii) imply what hybridizations vanish. As examples we discuss calculations for the Hubbard model in one-dimension and for 2×2 clusters.

TT 23.3 Wed 14:30 H 0104

Dual Fermion Approach to Susceptibility of Correlated Lattice Fermions — •Sergey Brener[1], Hartmut Hafermann[1], Alexey N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute of Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands

We show how the two-particle Green function can be obtained within the framework of the recently developed Dual Fermion approach. This facilitates the calculation of the susceptibility in strongly correlated systems where long-ranged non-local correlations cannot be neglected. We formulate the Bethe-Salpeter equations for the full vertex in the particle-particle and particle-hole channels and introduce an approximation for practical calculations. The scheme is applied to the two-dimensional Hubbard model at half filling. The spin-spin susceptibility is found to strongly increase for the wavevector $\mathbf{q} = (\pi, \pi)$, indicating the antiferromagnetic instability. Combining this approach with the cluster dual formalism and applying it to the Hubbard model at finite doping we get the possibility to capture all the essential physics of HTSC.

TT 23.4 Wed 14:45 H 0104

Cluster Dual Fermion Approach to Nonlocal Correlations — •Hartmut Hafermann[1], Sergey Brener[1], Alexey N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute of Molecules and Materials, Radboud University, 6525 ED Nijmegen, The Netherlands

We formulate a cluster generalization to the recently developed Dual Fermion approach to nonlocal correlations in crystals.

The scheme allows the treatment of long-range correlations beyond the cluster DMFT and nonlocal effects in realistic calculations of multiorbital systems. It is shown that in the simplest approximation one exactly recovers the free-cluster DMFT. Recent results are presented, among them the application to the one-dimensional Hubbard model. Already the first dual fermion correction to the free cluster leads to a drastic improvement of the calculated Green function.

TT 23.5 Wed 15:00 H 0104

Competing Instabilities in One Dimension - Functional Renormalization Group With Symmetry Breaking Terms — •Matthias Ossadnik[1,2] and Carsten Honerkamp[1] — [1]Universität Würzburg — [2]ETH Zürich

Fermionic renormalization group flows often lead to strong coupling, i.e. certain components of the interactions diverge at low energy scale and temperatures. By including appropriate types of symmetry-breaking via counterterms in the initial conditions of the flow, the divergence can however be avoided and properties of the low-temperature state can be computed. Here we show for a one-dimensional example that this approach allows us to describe competing order and quantum phase transitions between ground states with different symmetries, in qualitative agreement with bosonization analysis.

15 min. break

TT 23.6 Wed 15:30 H 0104

Understanding Supersolids — Andre Stoffel and •Miklos Gulacsi — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We model the newly discovered supersolid phase of 4He by a hard-core bosonic quantum lattice model in 3 dimension including nearest and next-nearest neighbor interactions. As hard-core Boson exhibit the same algebra as spin-1/2 operators there exists a one-to-one correspondence to the anisotropic Heisenberg model in an external field. To solve this Heisenberg model we used the Tyablikov Green's function technique and in order to obtain a closed set of equations we used a cumulant decoupling scheme. The obtained Green's functions have been used to study the properties of the system. Here, we are particularly interested in the normal-solid (NS) and supersolid (SS) phases as well as the corresponding phase transition. It was long proposed that vacancies and defects may play a crucial role in the formation of the supersolid phase. Hence we studied the incommensurability which is a measure of the net fraction of vacancies. For the NS phase we re-obtained the well-known thermal activation theory. However, the incommensurability in the SS displays a rather different behavior, which also suggests that the NS to SS transition is a commensurate-incommensurate transition.

TT 23.7 Wed 15:45 H 0104

Plateaux and supersolid phases in $SrCu_2(BO_3)_2$ — •Kai P. Schmidt, Julien Dorier, and Frederic Mila — Institute of Theoretical Physics, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

In a magnetic field, $SrCu_2(BO_3)_2$ displays magnetization plateaux at fractional fillings 1/8, 1/4 and 1/3. This work aims at a microscopic description of these plateaux, and investigate the behavior around these plateaux focussing on possible supersolid phases.

Using series expansion techniques, we have derived a realistic hard-core boson model which is dominated by long-range repulsive interactions and correlated hopping. We investigate the properties of this model by a classical approximation based on a spin representation. While the long-range interactions stabilize solid phases at fractional fillings (magnetization plateaux), the correlated hopping favours supersolid phases. This interplay between interactions and kinetics leads to a rich phase diagram with solid, superfluid, and supersolid competing phases.

TT 23.8 Wed 16:00 H 0104

Non-equilibrium Hubbard Model in an external, time-

dependent field — •Andreas Lubatsch and Johann Kroha — Physikalisches Institut, Universitaet Bonn, Germany

Mott-Hubbard insulating materials have the potential to be used for ultrafast electric switches, driven by an external laser field, because of the short relaxation times characteristic for strongly correlated systems. We consider the Hubbard model at half filling, driven by an external, stationary laser field. This electromagnetic field couples to the dipole moment of the charge distribution in the system, i.e. it induces an extra contribution to the hopping amplitude in the Hubbard Hamiltonian, periodic in time (photo-induced hopping). We generalize the dynamical mean-field theory (DMFT) to this non-equilibrium situation, employing a Floquet expansion of the electron density in terms of higher harmonics of the time-periodic hopping amplitude within the Keldysh formalism. We calculate the non-equilibrium electron distribution function, the density of states and the DC conductivity in the presence of the external laser field for laser frequencies above and below the Mott-Hubbard gap. The results demonstrate that the system can be switched from a Mott-Hubbard insulating state to a conducting state by the external field, which corresponds to photo-induced excitations into the upper Hubbard band.

TT 23.9 Wed 16:15 H 0104

Real-time evolution of the nonequilibrium Hubbard model — •Michael Möckel and Stefan Kehrein — LMU München, Department für Physik und Arnold Sommerfeld Center for Theoretical Physics, Theresienstraße 37, 80333 München

Recent experiments with cold atomic gases loaded onto optical lattices have opened up a new line of research into nonequilibrium properties of closed quantum systems. Motivated by these results we study the Hubbard model in infinite dimensions for a weak two-particle interaction $U\Theta(t)$ which is switched on instantaneously in time. We address the question of its real-time evolution by means of the flow equation technique and calculate the time-dependent momentum distribution function. After an initial buildup of a correlated distribution on a time scale set by U^{-1} a nonequilibrium transient state extends on a long time scale proportional to U^{-4}. It resembles an interacting Fermi liquid at zero temperature but its quasiparticle residuum mismatches the value for the correlated equilibrium state.

TT 23.10 Wed 16:30 H 0104

Non-thermal steady states after an interaction quench in the Falicov-Kimball model — •Martin Eckstein and Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

We present the exact solution of the Falicov-Kimball model after a sudden change of its interaction parameter using non-equilibrium dynamical mean-field theory. For different interaction quenches between the homogeneous metallic and insulating phases the system relaxes to a non-thermal steady state on time scales on the order of $\hbar$/bandwidth, showing collapse and revival with an approximate period of h/interaction if the interaction is large. We discuss the reasons for this behavior and provide a statistical description of the final steady state by means of generalized Gibbs ensembles.

TT 23.11 Wed 16:45 H 0104

Relaxation of a one-dimensional Mott insulator after a quantum quench — •Marcus Kollar and Martin Eckstein — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, 86135 Augsburg, Germany

We obtain the exact time evolution for a one-dimensional integrable fermionic Hubbard model after a sudden change of its interaction parameter, starting from either a metallic or a Mott-insulating state. In all cases the system relaxes to a new steady state, showing that the presence of the Mott gap does not inhibit relaxation. The properties of the final state are described by the fully constrained Gibbs ensemble. We discuss under which conditions such ensembles provide the correct statistical description of integrable systems in general.

15 min. break

TT 23.12 Wed 17:15 H 0104

Inhomogeneous solutions of the charge rotationally invariant Gutzwiller approach for the Hubbard model — •Falk Günther and Götz Seibold — BTU Cottbus, PO BOX 101344, 03013 Cottbus

We present a charge rotationally invariant Gutzwiller approach for the attractive Hubbard model. It is shown the formalism can be used to calculate homogeneous and inhomogeneous charge-ordered (CDW) and superconducting (SC) structures. Our formalism reproduces the correct degeneracy between CDW and SC phase in the half filled system. Restricting to on-site attraction we find that inhomogeneous structures e.g. anti-phase domain walls with regard to the SC order are only excitations of the system but never constitute the ground state of the model. In addition we present results for the Gutzwiller approximated extended Hubbard model including nearest neighbor repulsion, which allows for a competition between inhomogeneous CDW and SC textures.

TT 23.13 Wed 17:30 H 0104

Gutzwiller approach to phonon renormalization in the correlated SSH Model — •Ernst von Oelsen — Institut für Physik, BTU Cottbus, PBox 101344, 03013 Cottbus, Germany

The SSH Model [1] is supplemented with a Hubbard repulsion term in order to study the influence of electronic correlations on transitive phonon excitations. Our investigations are based on the time-dependent Gutzwiller approximation [2] and we restrict to the undimerized case. Eliminating double occupancy fluctuations via an anti-adiabaticity condition we obtain the quadratic fluctuations in the phonon and electronic density fields. Already on this level we find correlation-induced softening for small wave vectors which eventually induces an instability in addition to the Peierls nesting mechanism. In addition we show that inclusion of a Hubbard repulsion creates additional couplings between electrons and phonons beyond the bare transitive interaction. Finally we calculate the phonon self-energy which is compared with the uncorrelated case.

[1] W. P. Su and J. R. Schrieffer and A. J. Heeger, Phys. Rev. B **22**, 2099 (1980)

[2] G. Seibold and J. Lorenzana, Phys. Rev. Lett. **86**, 2605 (2001)

TT 23.14 Wed 17:45 H 0104

Rotationally invariant slave-boson formalism and momentum dependence of the quasiparticle weight — •Frank Lechermann[1], Antoine Georges[2], Gabriel Kotliar[3], and Olivier Parcollet[4] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Germany — [2]CPHT, École Polytechnique, Palaiseau, France — [3]Serin Physics Laboratories, Rutgers University, NJ, USA — [4]Service de Physique Théorique, CEA Saclay, Gif-Sur-Yvette, France

The rotationally invariant formulation of the slave-boson formalism is generalized to multiorbital models, with arbitrary interactions, crystal fields, and multiplet structure [1]. This allows for the study of multiplet effects on the nature of low-energy quasiparticles. Nondiagonal components of the matrix of quasiparticle weights can be calculated within this framework. When combined with cluster extensions of dynamical mean-field theory, this method renders it possible to address the effects of spatial correlations, such as the generation of the superexchange and the momentum dependence of the quasiparticle weight. The method is illustrated on several examples, including a two-dimensional single-band Hubbard model (within a two-site cellular dynamical mean-field approximation).

[1] F. Lechermann, A. Georges, G. Kotliar, and O. Parcollet, PRB **76** 155102 (2007).

TT 23.15 Wed 18:00 H 0104

Absence of fermionic quasi-particles in the BEC regime of the attractive Fermi gas — •Nils Lerch, Lorenz Bartosch, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

We calculate the effect of order parameter fluctuations on the fermionic single-particle excitations of the attractive Fermi gas in the BEC regime where the binding energy of the s-wave bound state is the largest energy scale. We show that in dimensions $D = 3$ the singular interaction between the fermions mediated by the gapless Bogoliubov-Anderson mode prohibits the existence of well-defined quasi-particles. We explicitly calculate the single-particle spectral function and show that in this case the quasi-particle residue and the density of states are logarithmically suppressed.

TT 23.16 Wed 18:15 H 0104

Self-masking of Fermi surface symmetry breaking in layered materials — •hiroyuki yamase — Max-Planck-Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Recently, a new type of spontaneous symmetry breaking, the d-wave type Fermi surface deformation (dFSD), the so-called Pomeranchuk instability, was found in various two-dimensional (2D) models such as t-J, Hubbard, and extended Hubbard. Such 2D systems are often realized in layered materials, where a small interlayer coupling exists. In this contribution, employing the bilayered model with a pure forward scattering interaction driving the dFSD instability, we study the stacking of the dFSD state along the z axis. Since the dFSD is characterized by breaking of the Ising symmetry, there are two possibile stacks, (+,+) and (+,–). We find that the latter "antiferromagnetic" configuration is usually favored and thus bulk symmetry breaking is hidden.

TT 23.17 Wed 18:30 H 0104

Influence of electronic correlations on the ground-state properties of CeN. — •Elena Voloshina[1] and Beate Paulus[2] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

The electron-correlation effects on the ground-state properties of CeN were studied by *ab initio* quantum-chemical methods. The $4f$-states of cerium were treated with $4f$-in-core pseudopotential derived by M. Dolg *et al.* for trivalent cerium (Ce^{11+}-PP) [1]. The approach which was used consists in the combination of two separate steps: 1) the ground-state Hartree-Fock calculations for the crystal; 2) application of the method of increments [2] to the studied system, which allows an expansion of bulk properties using the information from quantum-chemical calculations performed for finite cluster, in connection with the size-extensive coupled-cluster method. As it can be expected, for CeN correlation play a significant role: with Hartree-Fock method only a half of the experimental cohesive energy has been covered, whereas after correlation corrections the ground-state properties were shown to be in good agreement with the experimental data found in literature. The computed ground-state properties of CeN are compared with corresponding values obtained for LaN and GdN [3].

[1] M. Dolg, P. Fulde, W. Küchle, *et al.* J. Chem. Phys. 94, 3011 (1991). [2] H. Stoll, Phys. Rev. B 46, 6700 (1992). [3] S. Kaldova, M. Dolg, H.-J. Flad, *et al.* Phys. Rev. B 57, 2127 (1998).