TT 24: Correlated Electrons: (General) Theory 2

Time: Wednesday 9:30–13:00 Location: HSZ 301

TT 24.1 Wed 9:30 HSZ 301

Finite-Temperature Variational Cluster Approach (VCA) — •Gang Li, Maximilian Kiesel, and Werner Hanke — Institute for Theoretical Physics and Astrophysics, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The Variational Cluster Approach (VCA) proliferates the many-body physics, contained in an exact solution of a "reference system", i.e. a cluster, in a controlled manner to the infinite-system size limit of strongly correlated lattice models. This approach has been found for the 2D single-band Hubbard model to reproduce salient features of the ($T = 0$) ground-state phase diagram [1], single-particle excitations [2] and, most recently, two-particle, i.e. magnetic excitations [3]. Here, we describe an implementation of the continuous-time QMC technique as a "cluster solver". This new method allows to consider finite temperature properties as well as a significantly large number of electronic (orbital) degrees of freedom in the underlying many-body model.

[1]. M. Aichhorn, E. Arrigoni, M. Potthoff, W. Hanke, Phys. Rev. B. **74**, 024508 (2006).

[2] M. Aichhorn, E. Arrigoni, Z. B. Huang, W. Hanke, Phys. Rev. Lett. **99**, 257002 (2007).

[3] S. Brehm, E. Arrigoni, M. Aichhorn, W. Hanke, arXiv: 0811.05213 (21.11.08).

TT 24.2 Wed 9:45 HSZ 301

The Dynamical Vertex Approximation: spatial correlations beyond Dynamical Mean Field Theory — •Alessandro Toschi[1], Andrey Katanin[2,3], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Austria — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Institute of Metal Physics, Ekaterinburg, Russia

Progress in going beyond the purely local description of the Dynamical Mean Field Theory (DMFT) has been recently obtained through cluster extensions of the method, which include spatial correlations within the cluster size. Long-range spatial correlations may be, however, of vital importance: They are responsible for a rich variety of phenomena, ranging from magnons and screening of the Coulomb interaction to quantum criticality. Our new diagrammatic approach, coined "Dynamical Vertex Approximation" (DΓA)[1,2], provides for a systematic treatment of the effects of long-range spatial correlations beyond DMFT. Specifically, we use the DΓA with a Moriyaesque λ correction for studying the impact of antiferromagnetic fluctuations on the spectral function in the whole phase diagram of the Hubbard model in three[1] and intwo dimensions[2,3] . The diagrammatic nature of DΓA, moreover, makes the algorithm well suited for a generalization to the more realistic case of multi-band Hamiltonians.

[1] A. Toschi, A. Katanin, and K. Held, Phys. Rev. B, **75**, 045118 (2007).

[2] K.Held, A. Katanin, and A. Toschi, Prog. Theo. Phys. Suppl, **176**, in print (arXiv: 0807.1860).

[3] A. Katanin, A. Toschi, and K. Held, arXiv:0808.0689 submitted to Phys. Rev. B

TT 24.3 Wed 10:00 HSZ 301

Long-range correlations beyond DMFT: the ladder dual fermion approach — •Hartmut Hafermann[1,3], Alexei N. Rubtsov[2], Mikhail I. Katsnelson[3], and Alexander I. Lichtenstein[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, Moscow State University, 119992 Moscow, Russia — [3]Institute for Molecules and Materials, Radboud University of Nijmegen, 6525 ED Nijmegen, The Netherlands

The dual fermion approach is a systematic perturbative extension of dynamical mean-field theory to describe the physics of strongly correlated lattice fermions. We generalize the approach to include long-range correlations via a ladder approximation to the self-energy. The method is applied to the two-dimensional Hubbard model. While the mean-field solution fails to describe the physics in the vicinity of the antiferromagnetic instability, the ladder approximation recovers good agreement to quantum Monte-Carlo results. Inclusion of the long-range correlations leads to the formation of a pseudogap in the local density of states.

TT 24.4 Wed 10:15 HSZ 301

Analytic Continuation of Quantum Monte Carlo Data by Stochastic Analytic Inference — •Sebastian Fuchs[1,2], Mark Jarrell[2], and Thomas Pruschke[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen — [2]Center for Computation and Technology, Louisiana State University, Baton Rouge, LA 70803, USA

The maximum entropy method is the standard tool for the analytic continuation of imaginary-time quantum Monte Carlo data. It uses arguments of Bayesian logic to obtain the most probable energy spectrum given the imaginary-time input data.

In the past efforts where made to provide an alternative to this standard approach [2]. It was proposed to perform an average over a wide range of spectra using Monte Carlo techniques instead of selecting a single spectrum. So far, the method lacked a rigorous rule to eliminate a free regularization parameter inherent in the algorithm.

We propose an algorithm that is based on Bayesian inference. It utilizes Monte Carlo simulations to both calculate a weighted average of possible spectra and to provide a strict criterion for the elimination of the regularization parameter.

Our implementation is based on the libraries of the ALPS project [3]. ALPS is an open source effort providing libraries and simulation codes for strongly correlated quantum mechanical systems.

[1] M. Jarrell, G. E. Gubernatis, Phys. Rep. **269**, 133 (1996).

[2] A. Sandvik, PRB **57**, 10287 (1998); K. Beach, cond-mat/0403055

[3] `http://alps.comp-phys.org`

Invited Talk TT 24.5 Wed 10:30 HSZ 301

Theory of time-resolved optical and photoemission spectroscopy for correlated electron systems — •Marcus Kollar — Theoretische Physik III, Universität Augsburg, 86135 Augsburg

In pump-probe experiments the real-time dynamics of interacting electrons is measured by first driving the sample out of equilibrium with a pump pulse, and then probing its state with a second pulse after a controlled time delay. In time-resolved (TR) optical spectroscopy the reflected electrical field is measured, whereas in TR photoemission spectroscopy the spectrum of the emitted electrons is analyzed. These experimental signals can be related to the two-time optical conductivity and to the real-time electronic Green function, respectively. Both quantities can be calculated using nonequilibrium dynamical mean-field theory (DMFT), which maps an interacting lattice system onto an effective time-dependent single-site problem. TR optical spectroscopy has the advantage of full time resolution [1], whereas TR photoemission spectroscopy provides momentum resolution of the electronic Green functions but suffers from some energy-time uncertainty restrictions [2]. We present explicit results for the Falicov-Kimball model [1,2], for which we model the pump excitation by a sudden parameter change in the Hamiltonian [3]. We identify characteristic signatures in the experimental signals, e.g., for as-yet-unobserved electronic collapse-and-revival oscillations, the type of which are well-known from cold atom experiments.

[1] M. Eckstein and M. Kollar, Phys. Rev. B **78**, 205119 (2008).

[2] arXiv:0809.4282; [3] Phys. Rev. Lett. **100**, 120404 (2008).

15 min. break

TT 24.6 Wed 11:15 HSZ 301

Adiabatic parameter change across the metal-insulator transition in the Falicov-Kimball model — •Martin Eckstein and Marcus Kollar — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg, 86153 Augsburg

We obtain the exact time evolution of the fermionic Falicov-Kimball model during a slow variation of the interaction parameter, using dynamical mean-field theory (DMFT) for nonequilibrium. For this purpose we adapt the DMFT equations which were derived for a sudden interaction quench [1] and solve them numerically. We analyze the dependence of the excitation energy on the ramp speed in the adiabatic limit, and find different power laws when the system is driven within the insulating phase, within the metallic phase, or between the two phases. Possible reasons for this behavior are discussed.

[1] M. Eckstein and M. Kollar, Phys. Rev. Lett. **100**, 120404 (2008).

TT 24.7 Wed 11:30 HSZ 301

Time evolution of correlations in strongly interacting fermions after a quantum quench — •Salvatore R. Manmana[1], Stefan Wessel[2], Reinhard M. Noack[3], and Alejandro Muramatsu[2] — [1]Institute of Theoretical Physics (CTMC), EPF Lausanne, CH-1015 Lausanne, Schweiz — [2]Institut für Theoretische Physik III, Universität Stuttgart — [3]Fachbereich Physik, Philipps-Universität Marburg

Using the adaptive time-dependent density matrix renormalization group, we study the time evolution of density correlations of interacting spinless fermions on a one-dimensional lattice after a sudden change in the interaction strength. Over a broad range of model parameters, the correlation function exhibits a characteristic light-cone-like time evolution representative of a ballistic transport of information. Such behavior is observed both when quenching an insulator into the metallic region and also when quenching within the insulating region. However, when a metallic state beyond the quantum critical point is quenched deep into the insulating regime, no indication for ballistic transport is observed. Instead, stable domain walls in the density correlations emerge during the time evolution, consistent with the predictions of the Kibble-Zurek mechanism.

TT 24.8 Wed 11:45 HSZ 301

Influence of orbital degeneracy on the two particle spectral function — •Berlinson Dominikus Napitu[1,2] and Jamal Berakdar[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle — [2]Institut für Physik- Heinrich-Damerow-Strasse 4 Halle (Saale)

We studied the evolution of two particle spectral function of the orbitally degenerate Hubbard model with the same and different bandwidth. The calculation of single particle spectra is based on dynamical mean field theory (DMFT) together with quantum monte carlo (QMC) while for two particle spectra the ladder approximation is implemented. The influence of temperature is also considered.

TT 24.9 Wed 12:00 HSZ 301

Band formation vs. local correlations: NiO — •T. Haupricht[1], R. Gierth[1], J. Weinen[1], S. G. Altendorf[1], A. Hendricks[1], Y.-Y. Chin[1,2], Z. Hu[1], J. Gegner[1], H. Fujiwara[1], D. Regesch[1], H. H. Hsieh[3], H.-J. Lin[2], C. T. Chen[2], and L. H. Tjeng[1] — [1]Institute of Physics II, University of Cologne, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Chung Cheng Institute of Technology, National Defense University, Taoyuan, Taiwan

Modeling the electronic structure of NiO is a true theoretical challenge. Even though the general agreement between the experimental valence-band photoemission (PES) spectrum of NiO and the results of a single-site cluster configuration interaction calculation is very good, some structures in the spectrum remain unexplained. These shortcomings have been recognized already when looking at the Ni 2p core level spectra, and were attributed to so-called non local screening effects involving neighboring Ni clusters [v. Veenendaal et al., PRL 70 (1993)]. We therefore set out to measure the valence band PES of NiO impurities in MgO thin films. Comparing the NiO impurity valence band spectrum to that of bulk NiO we find that there are indeed remarkable differences. On the other hand we find that the correspondence of the experimental NiO impurity valence band and the result of the cluster calculation is very good. We also compare our experimental data to the results of recent LDA+DMFT calculations [Kuneš at al., PRL 99 (2007); Kuneš at al., PRB 75 (2007); Taguchi et al., PRL 100 (2008)] with reasonable results but also showing characteristic discrepancies.

TT 24.10 Wed 12:15 HSZ 301

Pseudogap phase in hole-doped high-temperature superconductors — •Steffen Sykora and Klaus W. Becker — Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden

One of the most important unsolved problems in the understanding of copper-oxide superconductors is the pseudogap phase which is a most unusual state of matter. ARPES experiments have revealed a gap-like behavior on parts of the Fermi surface, leaving a non gapped segment known as Fermi arc around the diagonal of the Brillouin zone. Two main interpretations of the origin of the pseudogap have been proposed: either the pseudogap is a precursor to superconductivity, or it arises from another order competing with superconductivity. In this paper, the pseudogap phase is investigated in the framework of a novel renormalization scheme. We present results for the one-particle spectral function $A_{\mathbf{k}}(\omega)$ near the Fermi level for different values of wave vector $\mathbf{k}$, doping and temperature. The results show an excellent agreement with recently puplished ARPES measurements. The origin of the pseudogap will be discussed.

TT 24.11 Wed 12:30 HSZ 301

Renormalization approach to the two-dimensional Periodic Anderson Model — •Alexander Mai and Klaus W. Becker — Institut für Theoretische Physik, TU Dresden

Despite the success of numerical methods in the treatment of strongly correlated electron systems, analytical approaches are still needed to obtain a deeper understanding of the underlying physics. We apply the Projector-based Renormalization Method (PRM) to the Periodic Anderson Model (PAM) in two dimensions to study the valence transition in heavy fermion systems and its dependence on the different model parameters. In order to investigate superconductivity we extend the model by adding a conduction electron phonon coupling. We discuss the superconducting solution with respect to the different parameters of the model and the valence transition in the PAM.

TT 24.12 Wed 12:45 HSZ 301

Ab initio correlated electronic structure of Cu oxide and Fe-As compounds: a quantum chemical perspective — •Liviu Hozoi, Mukul Laad, and Peter Fulde — Max-Planck-Institut fuer Physik komplexer Systeme, Dresden

Wavefunction-based methods from modern quantum chemistry are applied to the study of the electronic structure of correlated transition-metal compounds. Whereas the correlation treatment is performed in direct-space, a k-space representation can be obtained later on after accounting for the (strong) short-range correlations. In some cases, a balanced treatment of the short-range interactions, onsite and intersite, is essential for achieving even a qualitatively correct picture.

In cuprates, we find that the Fermi surface (FS) of the hole doped material evolves from small hole pockets in the deeply underdoped region to one with both hole- and electron-like sheets at slightly higher doping and to a large FS consistent with Luttinger's theorem at still higher hole concentrations. Our results offer a route toward a resolution of the controversy generated by the apparent inconsistency between Shubnikov-deHaas measurements and the Luttinger sum rule for underdoped cuprates, as well as with recent Hall-effect data suggesting an electron-like Hall constant for hole doped cuprates at low T.

The multiorbital correlated electronic structure of the recently discovered Fe-As superconducting compounds is also discussed. We compute the ground-state for the undoped case and provide new insight into the nature of doped holes and electrons.