TT 9: CE: (General) Theory 1

Time: Monday 14:00–18:15 Location: HSZ 201

TT 9.1 Mon 14:00 HSZ 201

Non-equilibrium self-energy-functional theory — •Matthias Balzer and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Hamburg

Using standard perturbation theory to all orders, the grand potential of a system of strongly correlated electrons can be expressed as a functional of the self-energy such that the physical self-energy is a stationary point. Non-perturbative approximations can be constructed by restricting the domain of the self-energy functional $\Omega[\Sigma]$ to a subspace of trial self-energies spanned by an exactly solvable reference system [1]. This comprises approximations, such as the dynamical mean-field theory (DMFT) and the variational cluster approximation (VCA).

Here we show that this concept can be extended straightforwardly to the non-equilibrium case. Green's functions and self-energies have to be defined on the three-branch Keldysh-Matsubara contour in the complex time plane [2], and Ω must be reinterpreted accordingly. The resulting variational scheme is extremely general and provides a rederivation of non-equilibrium DMFT [3], for example.

To discuss practical issues relevant for a numerical implementation of a non-equilibrium VCA, we consider in a first step a coupling of Hubbard-type reference systems consisting of two sites only. Different initial states will be considered, e.g. an uncorrelated Neel state or a correlated singlet state, to study the time evolution of spin correlations.

[1] M. Potthoff, Eur. Phys. J. B 32, 429 (2003).
[2] M. Wagner, Phys. Rev. B 44, 6104 (1991).
[3] J. Freericks et al., Phys. Rev. Lett. 97, 266408 (2006).

TT 9.2 Mon 14:15 HSZ 201

Efficient Legendre representation of Many-Particle Green's functions — •Lewin Boehnke[1], Frank Lechermann[1], Michel Ferrero[2], and Olivier Parcollet[3] — [1]1. ITP, Universität Hamburg, D-20355 Hamburg, Germany — [2]CPhT, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]IPhT, CEA/DSM/IPhT-CNRS/URA 2306 CEA-Saclay, F-91191 Gif-Sur-Yvette, France

Even though a way of obtaining frequency and wave-vector-dependent lattice susceptibilities within the dynamical mean-field theory (DMFT) is known for some years [1], only very few calculations were actually performed. A reason therefore is the numerically expensive handling of the two-particle Green's function with respect to three slowly decaying frequency variables. Within quantum Monte-Carlo (QMC) methods, the latter fact renders the accumulation lengthly and leads to numerical instabilities in the further use of the obtained many-particle objects.

We propose tailored representation of the one- and two-particle Green's function for an accurate QMC accumulation within the class of continuous-time impurity solvers [2,3] for the DMFT approximation, based on the expansion of fermionic degrees of freedom in Legendre polynomials. This leads to a substantial increase in performance, allowing for the efficient calculation of spin and charge susceptibilities for canonical models as well as realistic materials over wide ranges of temperature, doping and interaction strength.

[1] V. Zlatić and B. Horvatić, Solid State Commun. **75**, 263 (1990).
[2] A.N. Rubtsov and A.I. Lichtenstein, JEPT Lett. **80**, 61 (2004).
[3] P. Werner, A. Comanac, L. de' Medici, et al., PRL **97**, 76405 (2006).

TT 9.3 Mon 14:30 HSZ 201

Numerical correlation-energy functional for lattice density-functional theory: A systematic approach to the ground-state properties of strongly correlated systems — •Matthieu Saubanere and Gustavo Pastor — Institut für Theoretische Physik Heinrich-Plett-Str. 40 D-34132 Kassel

We present an accurate method to determine ground-state properties of strongly-correlated electrons described by lattice-model Hamiltonians. In lattice density-functional theory (LDFT) the basic variable is the one-particle density matrix γ. From the HK theorem, the ground state Energy $E_{gs}[\gamma_{gs}] = \min_\gamma E[\gamma]$ is obtained by minimizing the energy over all the representable γ. The energy functional can be divided into two contributions: the kinetic-energy functional, which linear dependence on γ is exactly known, and the correlation-energy functional $W[\gamma]$, which approximation constitutes the actual challenge. Within the framework of LDFT, we develop a numerical approach to $W[\gamma]$, which involves the exact diagonalization of an effective many-body Hamiltonian of a cluster surrounded by an effective field. This effective Hamiltonian depends on the density matrix γ. In this talk we discuss the formulation of the method and its application to the Hubbard and single-impurity Anderson models in one and two dimensions. The accuracy of the method is demonstrated by comparison with the Bethe-Ansatz solution (1D), density-matrix renormalization group calculations (1D), and quantum Monte Carlo simulations (2D).

TT 9.4 Mon 14:45 HSZ 201

Effective models for gapped phases of strongly correlated quantum lattice models — Hong Yu Yang and •Kai Phillip Schmidt — Lehrstuhl für Theoretische Physik I, TU Dortmund, 44221 Dortmund, Germany

We present a robust scheme to derive effective models non-perturbatively for quantum lattice models when at least one degree of freedom is gapped. A combination of graph theory and the method of continuous unitary transformations (gCUTs) is shown to efficiently capture all zero-temperature fluctuations in a controlled spatial range. The gCUT can be used either for effective quasi-particle descriptions or for effective low-energy descriptions in case of infinitely degenerate subspaces. We illustrate the method for 1d and 2d lattice models yielding convincing results in the thermodynamic limit. Various extensions and perspectives of the gCUT are discussed.

TT 9.5 Mon 15:00 HSZ 201

Lower energy bounds for condensed matter systems — •Robert Hübener, Thomas Barthel, and Jens Eisert — Universität Potsdam

Greens function methods, known e.g. from quantum chemistry, allow to calculate lower energy bounds for bosonic and fermionic models in the thermodynamic limit. In the context of condensed matter physics, they can be used to complement variational methods, e.g. DMRG, which generally provide upper bounds. The tightness of the lower bounds depends on the level of compliance with so called N-representability conditions. In this talk we discuss technical aspects, like the formulation of the optimization problem as a semidefinite program, as well as the underlying issue of N-representability. Applications will be demonstrated.

15 min. break

TT 9.6 Mon 15:30 HSZ 201

Spectra and kinks in the electronic dispersion of charge-transfer systems — •Markus Greger, Marcus Kollar, and Dieter Vollhardt — Theoretische Physik III, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg

We investigate kinks in the effective dispersion of correlated multi-band systems, concentrating on the perovskite geometry. Previously it was shown that the one-band Hubbard model exhibits kinks due to an entirely electronic mechanism [1], which is different from conventional mechanisms such as the coupling between electrons and phonons or other bosonic modes. Here we demonstrate the applicability of this mechanism in the case of the Emery model (two/three-band Hubbard model) for hole-doped cuprate compounds. We solve these multi-band models within dynamical mean-field theory using the numerical renormalization group (NRG), which is ideally suited to resolve spectral features at comparably low energy, including kinks. We discuss in detail the construction of the effective impurity Hamiltonian and the corresponding Wilson chains within the NRG procedure for such multi-band models.

[1] K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke and D. Vollhardt, Nature Physics 3, 168 (2007).

TT 9.7 Mon 15:45 HSZ 201

Loschmidt echo and work distribution in isolated many-body systems after a global quench — •Marcus Kollar[1], Malte Lehmann[2], and Eric Lutz[2] — [1]Theoretical Physics III, University of Augsburg, 86135 Augsburg — [2]Department of Physics, University of Augsburg, 86135 Augsburg

For a sudden quench of the Hamiltonian of an isolated quantum system there is a relation between (i) the distribution of the performed work and (ii) the Loschmidt echo, which is a measure of the overlap

of the initial and the time-evolved state, but which is notoriously difficult to measure. We derive an uncertainty relation for the widths of these two functions and argue that for global quenches in many-body systems both functions are typically Gaussians, thus fulfilling their uncertainty relation as an equality. This suggests that it may be possible to measure the Loschmidt echo via the experimentally more easily accessible work distribution.

TT 9.8 Mon 16:00 HSZ 201

Non-Fermi-liquid signatures in the Hubbard model due to van Hove singularities — •Sebastian Schmitt — Theoretische Physik II, Technische Universität Dortmund

We consider the Hubbard model within the single-site dynamical mean-field theory (DMFT) on lattices which exhibit a van Hove singularity in the vicinity of the Fermi level. Analytical treatment of the lattice summation reveals a non-analytic contribution of the van Hove singularity to the local effective medium (Weiss field). This leads to a non-Fermi liquid self-energy and transport properties within a full numerical solution of the DMFT on a two-dimensional square lattice with nearest- and next-nearest-neighbor hoppings. At temperatures on the order of the low-energy scale T_0 an unusual maximum emerges in the imaginary part of the self-energy which is renormalized toward the Fermi level for finite doping. At zero temperature this double-well structure is suppressed but an anomalous energy dependence of the self-energy remains. The asymptotic low-temperature behavior of the resistivity changes from Fermi liquid to non-Fermi liquid behavior as function of doping. The results are also discussed regarding their relevance for quantum cluster approximations and high-temperature cuprate superconductors.

TT 9.9 Mon 16:15 HSZ 201

Dimensional aspects of antiferromagnetism: dynamical mean-field theory versus direct quantum Monte Carlo — •Elena V. Gorelik[1], Theresa Paiva[2], Richard Scalettar[3], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Instituto de Fisica, Universidade Federal do Rio de Janeiro, Brazil — [3]Department of Physics, UC Davis, USA

Although the dynamical mean-field theory (DMFT) is well established for strongly correlated fermions, it is clear that nonlocal correlations will modify all DMFT results. Thus, the recently revealed [1] antiferromagnetic (AF) signatures in the double occupancy D of fermions on a cubic lattice could shift to lower T or the DMFT scenario might even break down. The situation should be worse in 2 dimensions, for which the Mermin-Wagner theorem excludes AF order at $T > 0$.

However, our DMFT predictions for $D(T)$ in the square-lattice agree with direct quantum Monte Carlo (QMC) results [2] within 10%. In 3 dimensions, we find nearly exact agreement between DMFT and QMC both at large T and for $T \lesssim T_{\rm N}^{\rm DMFT}$. The primary effect of nonlocal correlations is a smoothing of the DMFT curves at $T \gtrsim T_{\rm N}^{\rm DMFT}$.

Somewhat surprisingly, $T_{\rm N}^{\rm DMFT}$ is much more relevant for the AF signatures in $D(T)$ than the true $T_{\rm N}$. Thus, magnetism is more local in many respects than previously assumed, and real-space DMFT is well-suited for addressing inhomogeneous 3-dimensional systems.

[1] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).
[2] Th. Paiva, R. Scalettar, M. Randeria, and N. Trivedi, Phys. Rev. Lett. **104**, 066406 (2010).

TT 9.10 Mon 16:30 HSZ 201

New routes to frustration and the suppression of antiferromagnetic signatures — •Nils Blümer and Elena Gorelik — Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany

An established route for studying frustration effects in Hubbard-type models is the addition of frustrating bonds to a bipartite lattice. In particular, one can tune from the square towards the triangular lattice by adding hopping along one diagonal per plaquette with amplitude $t' \in [0, t]$ (for square-lattice hopping t). While this tuning exposes frustration effects, it also changes the coordination ($4 \leq Z \leq 6$), i.e., affects the energy scales and, thereby, all observables in all phases.

We complement the above model with an additional inter-plane hopping $t_z = \sqrt{t^2 - t'^2}$; then $t' \in [0, t]$ tunes between the cubic and the triangular lattice at constant $Z_{\rm eff} = 6$. Our quantum Monte Carlo based dynamical mean-field calculations at half filling ($n = 1$) show that the recently suggested signature [1] of antiferromagnetic (AF) correlations, an enhanced double occupancy at strong coupling, is suppressed (proportional to t'^2) even before the AF order breaks down; in contrast, nonmagnetic phases are unaffected. This confirms our strong-coupling picture [1] quantitatively and should be useful for cold-atom experiments.

[1] E. V. Gorelik, I. Titvinidze, W. Hofstetter, M. Snoek, and N. Blümer, Phys. Rev. Lett. **105**, 065301 (2010).

15 min. break

TT 9.11 Mon 17:00 HSZ 201

Non-Abelian SU(N) symmetries applied to matrix product states — •Andreas Weichselbaum and Jan von Delft — Ludwig Maximilians University, Munich, Germany

We generalized our numerical framework of matrix product states (MPS) from arbitrary Abelian to non-abelian quantum symmetries. It is based on the simple observation that Clebsch Gordan coefficient spaces can be split off in a tensor product like fashion for all objects relevant within MPS, and is thus applicable to the numerical or density matrix renormalization group (NRG or DMRG, respectively). As an example, I will present results on a generalized SU(3) symmetric Anderson impurity model within the numerical renormalization group based on the explicit treatment of U(1)⊗SU(2)⊗SU(3) and $\mathrm{SU}(2)^{\otimes 4}$ symmetries. This model of a fully screened S=3/2 spin Anderson model was suggested recently as the effective microscopic Kondo model for Fe impurities in gold or silver.

TT 9.12 Mon 17:15 HSZ 201

The Crooks relation in optical spectra - universality in work distributions for weak local quenches — •Markus Heyl and Stefan Kehrein — Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany

We show that work distributions and non-equilibrium work fluctuation theorems can be measured in optical spectra for a wide class of quantum systems. We consider systems where the absorption or emission of a photon corresponds to the sudden switch on or off of a local perturbation. For the particular case of a weak local perturbation, the Crooks relation establishes a universal relation in absorption as well as in emission spectra. Due to a direct relation between the spectra and work distribution functions this is equivalent to universal relations in work distributions for weak local quenches. As two concrete examples we treat the X-ray edge problem and the Kondo exciton [1].

[1] M. Heyl and S. Kehrein, arXiv:1006.3522

TT 9.13 Mon 17:30 HSZ 201

Tunnelling matrix elements with Gutzwiller wave functions — •Andrea Di Ciolo, Luca F. Tocchio, and Claudius Gros — Institut fuer Theoretische Physik, Goethe Universitaet Frankfurt, Frankfurt Am Main, Germany.

We use a generalized Gutzwiller approach [N. Fukushima, et al., Phys. Rev. B 72, 144505 (2005)], in order to study projected particle (hole) excitations for superconducting systems and systems with antiferromagnetic (AFM) order. As in the standard Gutzwiller scheme [M. C. Gutzwiller, Phys. Rev. Lett. 10, 159 (1963); F. C. Zhang, et al., Supercond. Sci. Tech. 1, 36 (1988)] the effects of the strong electronic correlations are given via the suppression of the site double occupancy; for our computations it is helpful to consider a lattice with a reservoir site unaffected by this suppression of the double occupancy.

In this approach we obtain the probabilities for the tunnelling of a particle (hole) into the projected state [A. Di Ciolo, et al., arXiv:1010.5055] . Our results are due only to the physical properties of the trial state and not to the choice of a specifical Hamiltonian: in this sense, they are model-independent but not universal, because they rely on the features of the chosen Gutzwiller wave function (projected Fermi Sea, BCS superconductor, AFM...)

The accuracy and the reliability of our analytical approximation is tested using the Variational Monte Carlo. Possible comparisons with tunnelling experiments will be discussed.

TT 9.14 Mon 17:45 HSZ 201

Simulations of excitons in coupled quantum dots — •Alexander Stark[1], Philipp Schneider[1], Sergey Grishkevich[1,2], and Alejandro Saenz[1] — [1]Humboldt-Universität, Berlin, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

We present the extension of our program code for two atoms in optical lattices to excitons in coupled quantum dots, i.e. quantum dot

molecules. To obtain the eigenvalues and the corresponding wave functions we are using a full configuration-interaction approach based on an one particle B-Spline basis for the radial part and spherical harmonics for the angular part of the wave function. The double well confinement potential is treated in full dimensionality. This allows us to handle variably confined lateral and vertical coupled quantum dots. The separation of the dots can be adjusted from box-like unified dots to nearly full separated individual dots. The interaction between the electron and the hole can be also varied arbitrarily, including the repulsive electron-electron Coulomb potential and possible shielding effects. Further, to study quantum dot molecules in different materials the effective masses of the particles can be set to corresponding values. The next step is to include a time-dependent perturbation and to study the dynamics of the exciton. First results of the calculations are presented.

TT 9.15 Mon 18:00 HSZ 201

Competing chiral and multipolar electric phases in the extended Falicov-Kimball model — •Bernd Zenker[1], Holger Fehske[1], and Cristian Daniel Batista[2] — [1]Ernst-Moritz-Arndt Universität Greifswald, Greifswald, Germany — [2]Los Alamos National Laboratory, Los Alamos, USA

We study the effects of interband hybridization within the framework of an extended Falicov-Kimball model with itinerant c and f electrons. An explicit interband hybridization breaks the U(1) symmetry associated with the conservation of the difference between the total number of particles in each band. As a result, the degeneracy between multipolar electric and chiral orderings is lifted. We analyze the weak- and strong-coupling limits of the c-f electron Coulomb interaction at zero temperature, and derive the corresponding mean-field quantum phase diagrams at half-filling for a model defined on a square lattice.