TT 86: Correlated Electrons: (General) Theory 2

Time: Thursday 9:30–13:00 Location: H 3005

TT 86.1 Thu 9:30 H 3005

A dual-fermion analysis of the Anderson-Hubbard model — •Patrick Haase[1], Shuxiang Yang[2], Thomas Pruschke[1], Juana Moreno[2], and Mark Jarrell[2] — [1]Georg-August Universität Göttingen — [2]Louisiana State University

We apply the recently-developed dual-fermion method for disordered interacting systems to the Anderson-Hubbard model. This method treats both disorder and interaction on equal footing, takes into account non-local correlations systematically, and thus represents a significant extension over the single-site mean-field description. We analyze the metal-insulator transition as well as the anti-ferromagnetic transition of the three-dimensional cubic lattice, by looking at both the one- and two-particle quantities, like the local Green function and the conductivity.

TT 86.2 Thu 9:45 H 3005

Antiferromagnetic phase transition in the Hubbard model from diagrammatic multi-scale perspective — •Daniel Hirschmeier[1], Hartmut Hafermann[2], Emanuel Gull[3], Alexander Lichtenstein[1], and Andrey Antipov[3] — [1]Universität Hamburg, I. Institut für Theoretische Physik, Hamburg, Deutschland — [2]University of Michigan, Ann Arbor, USA — [3]Institut de Physique Theorique (IPhT), Gif-sur-Yvette, France

We have studied the phase diagram of the antiferromagnetic transition of the Hubbard model in three dimensions, employing the ladder dual fermion approach. This diagrammatic extension of dynamical mean field theory embeds the non-local correlations into the problem and allowed us to extract universal, Heisenberg like critical exponents of the spin susceptibility and the correlation length for large and intermediate values of the Coulomb repulsion. This critical behaviour is coincident with the opening of a gap in the density of states, reflecting a relation between single- and two-particle quantities. Furthermore we discuss the impact of the gap in the density of states on the critical properties of the phase transition.

TT 86.3 Thu 10:00 H 3005

Gutzwiller variational wave function for a two-orbital Hubbard model on a square lattice — •Kevin zu Münster — Philipps University, Marburg, Germany

Gutzwiller variational wave functions can be evaluated exactly in infinite dimensions by the introduction of a gauge in the variational parameters. We present the generalization of this method for multiorbital systems and its application to a finite-dimensional lattice. We show numerical results for a two-dimensional Hubbard model with p_x-p_y symmetry. A variation of the underlying Fermi surface leads to features like Pomerantchuk instabilities or a change of the Fermi surface topology.

TT 86.4 Thu 10:15 H 3005

Interplay between Point-Group Symmetries and the Choice of the Bloch Basis in Multiband Models — •Stefan A. Maier[1] and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52056 Aachen, Germany — [2]Member of JARA-FIT, Jülich-Aachen Research Alliance–Fundamentals of Future Information Technology

We analyze the point-group symmetries of generic multiband tight-binding models with respect to the transformation properties of the effective interactions. While the vertex functions in the orbital language may transform non-trivially under point-group operations, their point-group behavior in the band language can be simplified by choosing a suitable Bloch basis. We show that, for a large class of models, a natural Bloch basis exists, in which the vertex functions in the band language transform trivially under all point-group operations [cf. our article in *Symmetry*, **5(4)**, 313 (2013)]. As a consequence, the point-group symmetries can be used to reduce the computational effort in perturbative many-particle approaches, such as the functional renormalization group.

TT 86.5 Thu 10:30 H 3005

Towards high-performance functional renormalization group calculations for interacting fermions — •Julian Lichtenstein[1], Stefan A. Maier[1], Carsten Honerkamp[1,2], Edoardo Di Napoli[3], and Daniel Rohe[4] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA-FIT, Jülich-Aachen Research Alliance–Fundamentals of Future Information Technology — [3]AICES, RWTH Aachen University, Germany — [4]Forschungszentrum Juelich GmbH, Juelich, Germany

We show that the flow equations of the singular-mode functional renormalization group (SM-FRG) approach put forward by Wang et al. [1] can be derived from an exchange parametrization of the two-fermion interaction [2] by introducing an additional approximation. Furthermore, we present a new variant of the SM-FRG, in which, unlike in the original variant, the interaction is represented in a unique way. We then discuss the applicability of the approximation made in addition to an exchange parametrization. Finally, we argue that the approximation made facilitates more efficient multiband calculations on a larger number of multi-core CPUs.

[1] Wang et al., *Phys. Rev. B* **85**, 035414 (2012).
[2] C. Husemann and M. Salmhofer, *Phys. Rev. B* **79**, 195125 (2009)

TT 86.6 Thu 10:45 H 3005

Summing parquet diagrams via the functional renormalization group: x-ray problem revisited[1] — •Philipp Lange, Casper Drukier, Anand Sharma, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt

We present a simple and efficient method for summing so-called parquet diagrams of fermionic many-body systems with competing instabilities using the functional renormalization group. Our method is based on partial bosonization of the interaction using multi-channel Hubbard-Stratonovich transformations. A straightforward truncation of the resulting flow equations retaining only the frequency-independent parts of the two-point and three-point functions amounts to solving coupled Bethe-Salpeter equations for the effective interaction to leading logarithmic order. We apply our method to the x-ray problem and derive the singular frequency dependence of the x-ray response function and the particle-particle susceptibility. Our method can be applied to various other problems involving strong fluctuations in more than one scattering channel.

[1] G. D. Mahan, Phys. Rev. 163, 612 (1967).

TT 86.7 Thu 11:00 H 3005

Steps towards the application of two-particle irreducible functional renormalization group — •Jan Frederik Rentrop[1,2], Severin Georg Jakobs[1,2], and Volker Meden[1,2] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University, Germany — [2]JARA FIT - Fundamentals of Future Information Technology, 52056 Aachen, Germany

Functional renormalization group (RG) is an established method for the investigation of non-relativistic correlated quantum many-body problems in low dimensions. Commonly, the functional RG flow equations are derived in generating functional formalism and formulated for one-particle irreducible (1PI) vertex functions. However, generating functionals have long been written in a 2PI form as well. Based on these, proposals for 2PI functional RG schemes have been made. These mainly differ from one another with respect to the introduction of the flow parameter. It is remarkable that hardly any calculations for particular systems employing these proposed schemes have been published. Having performed toy model calculations for the quantum anharmonic oscillator, our recent work aims for a study of the single impurity Anderson model in equilibrium. The goal of this talk is to place 2PI schemes into a broader context (how they relate to other methods) and to present some data to evaluate the performance of the 2PI schemes in comparison to other schemes, in particular 1PI ones.

15 min. break.

TT 86.8 Thu 11:30 H 3005

From infinite to two dimensions through the functional renormalization group — •Ciro Taranto[1], Sabine Andergassen[2], Johannes Bauer[3], Karsten Held[1], Andrey Katanin[4], Walter Metzner[5], Georg Rohringer[1], and Alessandro Toschi[1] — [1]Institute for solid state physics, Vienna University of Technology, Austria — [2]Institute for theoretical physics and CQ center for collective quantum phenomena, University of Tübingen, Germany —

[3]Department of Physics, Harvard University, Usa — [4]Institute of metal Physics, Ural Federal University, Ekatrinburg, Russia — [5]Max Planck institute for Solid State research, Stuttgart, Germany

We present a novel scheme for an unbiased and non-perturbative treatment of strongly correlated fermions. The proposed approach combines two of the most successful many-body methods, i.e., the dynamical mean field theory (DMFT) and the functional renormalization group (fRG). Physically, this allows for a systematic inclusion of non-local correlations via the flow equations of the fRG, after the local correlations are taken into account non-perturbatively by the DMFT. To demonstrate the feasibility of the approach, we present numerical results for the two-dimensional Hubbard model at half-filling.

TT 86.9 Thu 11:45 H 3005

Correlated starting points for the functional renormalization group — •Nils Wentzell[1,2,3], Ciro Taranto[3], Andrey Katanin[4,5], Alessandro Toschi[3], and Sabine Andergassen[1,2] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria — [2]Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [3]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [4]Institute of Metal Physics, Kovalevskaya Str., 18, 620990, Ekaterinburg, Russia — [5]Ural Federal University, 620002, Ekaterinburg, Russia

We present a general frame to extend functional renormalization group (fRG) based computational schemes by using an exactly solvable *interacting* reference problem as starting point for the RG flow. The systematic expansion around this solution accounts for a non-perturbative inclusion of correlations. Introducing auxiliary fermionic fields by means of a Hubbard-Stratonovich transformation, we derive the flow equations for the auxiliary fields and determine the relation to the conventional weak-coupling truncation of the hierarchy of flow equations. As a specific example we consider the dynamical mean-field theory (DMFT) solution as reference system, and discuss the relation to the recently introduced DMF^{2}RG and the dual-fermion formalism.

TT 86.10 Thu 12:00 H 3005

The virial theorem within many-body extensions of density functional theory — •Andreas Östlin[1,2], Wilhelm Appelt[2,3], Liviu Chioncel[2,3], and Levente Vitos[1,4,5] — [1]Applied Materials Physics, Department of Materials Science and Engineering, KTH Royal Institute of Technology, Stockholm SE-100 44, Sweden — [2]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [4]Department of Physics and Materials Science, Uppsala University, P.O. Box 516, SE-75120 Uppsala, Sweden — [5]Research Institute for Solid State Physics and Optics, Wigner Research Center for Physics, Budapest H-1525, P.O. Box 49, Hungary

The virial theorem provides a relation between kinetic and potential energies for a large range of physical systems, and almost has the status of a conservation law. We investigate the fulfillment of the virial theorem for electronic structure calculations, in the framework of Density Functional Theory (DFT) both within the Local Density Approximation (LDA) and its Dynamical Mean Field Theory extension (LDA+DMFT). We demonstrate its validity for metals.

TT 86.11 Thu 12:15 H 3005

Quantum electrodynamical time-dependent density functional theory on a lattice — •Mehdi Farzanehpour[1] and Ilya Tokatly[1,2] — [1]Nano-Bio Spectroscopy group and ETSF Scientic Development Centre, Departamento de Fisica de Materiales, Universidad del Pais Vasco UPV/EHU, E-20018 San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain

We present a rigorous formulation of the time-dependent density functional theory for interacting lattice electrons strongly coupled to cavity photons. We start with an example of one particle on a Hubbard dimer coupled to a single photonic mode, which is equivalent to the single mode spin-boson model or the quantum Rabi model. For this system we prove that the electron-photon wave function is a unique functional of the electronic density and the expectation value of the photonic coordinate, provided the initial state and the density satisfy a set of well defined conditions. Then we generalize the formalism to many interacting electrons on a lattice coupled to multiple photonic modes and prove the general mapping theorem. We also show that for a system evolving from the ground state of a lattice Hamiltonian any density with a continuous second time derivative is locally v-representable.

TT 86.12 Thu 12:30 H 3005

Inverse Mean Field theories — •Peter Schmitteckert — Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Methods based on many particle wave functions are naturally suited to describe strongly correlated quantum system and enable the description of non-perturbative problems. However, an intuitive description of many particle wave functions is often lacking. In contrast, mean field (MF) theories cannot treat interaction effects rigorously, but provide simple pictures within a single particle framework. In mean field theories one typically introduces a mean field decoupling of the Hamiltonian which is then solved within a single particle description. Here we go the other direction. We first solve for a many particle wave function, which is then used to construct a corresponding MF description. Specifically we discuss different strategies to construct a suitable mean field theory, which can then be used to discuss the physical problem. Finally we address the problem of describing time dependent phenomena of correlated quantum systems within an inverse MF description.

TT 86.13 Thu 12:45 H 3005

Reduced density matrix functional theory via a wave function based approach — •Robert Schade[1], Peter Bloechl[1], and Thomas Pruschke[2] — [1]Institute for Theoretical Physics, Clausthal University of Technology, Clausthal, Germany — [2]Institute for Theoretical Physics, University of Goettingen, Goettingen, Germany

We propose a new method for the calculation of the electronic and atomic structure of correlated electron systems based on reduced density matrix functional theory (rDMFT). The density matrix functional is evaluated on the fly using Levy's constrained search formalism. The present implementation rests on a local approximation of the interaction reminiscent to that of dynamical mean field theory (DMFT). This wave function based approach can be integrated into the existing DFT framework by making use of natural orbitals.

Financial support by the DFG Research Unit FOR 1346 "Dynamical Mean-Field Approach with Predictive Power for Strongly Correlated Materials" is gratefully acknowledged.