TT 84: Correlated Electrons: (General) Theory

Time: Thursday 9:30–13:15 Location: HSZ 304

TT 84.1 Thu 9:30 HSZ 304

Uniform Electron Gas Approximation for the Second Order Screened Exchange Energy — •Felix Hummel and Georg Kresse — University of Vienna, Austria

The second order screened exchange (SOSEX) energy is the leading order correction to the random phase approximation (RPA) of the correlation energy. Computing the SOSEX contribution from the Kohn-Sham or Hartree-Fock orbitals scales like N^5, making it considerably less practical than direct RPA, which can be implemented with an N^4 or even an N^3 scaling.

We approximate the exchange kernel by the respective kernel of the uniform electron gas. This allows for an approximation of the RPA+SOSEX energy with the favourable scaling of RPA. We believe, this captures the dominant part of the SOSEX contribution for many materials and we compare it with full RPA+SOSEX calculations.

TT 84.2 Thu 9:45 HSZ 304

Calculation of screened coulomb interaction in f electron systems: dynamical screening and role of self-consistency. — •Bernard Amadon[1], Thomas Applencourt[1], and Fabien Bruneval[2] — [1]CEA, DAM, DIF, F-91297 Arpajon, France — [2]CEA, DEN, Service de Recherches de Métallurgie Physique , F-91191 Gif-sur-Yvette, France

The combination of density functional theory in the local density approximation (LDA) and dynamical mean field theory (DMFT) [1] has been successful to describe localized or delocalized correlated electrons in condensed matter [2]. However, the accurate calculations of structural or spectral properties relies on the determination of the screened Coulomb interactions between correlated electrons. In the last ten years, the constrained Random Phase Approximation was developed to describe the screening of correlated electrons by non correlated electrons [3]. In this presentation, we will first discuss the calculation of the screened interaction for strongly correlated metals and insulating oxides with correlated f electrons. We will discuss the importance of dynamical screening and self-consistency. Then we show applications to DFT+DMFT calculations with a recent implementation [4].

[1] A. Georges et al., Rev. Mod. Phys. 68, 13 (1996)
[2] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006)
[3] F. Aryasetiawan et al Phys. Rev. B 70, 195104 (2004)
[4] B. Amadon, Journal of Phys.: Condens. Matter 24, 075604 (2012)

TT 84.3 Thu 10:00 HSZ 304

First multi-reference correlation treatment of bulk metals — •Elena Voloshina[1] and Beate Paulus[2] — [1]Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Freie Universität Berlin, 14195 Berlin, Germany

Existence of the *sp-d* hybridization of the valence band states of the *fcc* Ca and Sr in the vicinity of the Fermi level indicates that their electronic wave function can have a multi-reference (MR) character. We performed a wave function-based correlation treatment for these materials by means of the method of increments. As oppose to the single-reference correlation treatment (here: coupled cluster), which fails to describe cohesive properties in both cases, employing the MR averaged coupled pair functional one can achieve almost 100 % of the experimental correlation energy.

TT 84.4 Thu 10:15 HSZ 304

The puzzle of the basis-set for realistic calculations of correlated materials: The examples of Ni-heterostructures and Cuprates — •Giorgio Sangiovanni[1], Nicolaus Parragh[1], Philipp Hansmann[2], Stefan Hummel[3], Karsten Held[3], and Alessandro Toschi[3] — [1]Universität Würzburg — [2]Ecole Polytechnique, Paris — [3]Technische Universität Wien

The input for materials calculations done with dynamical mean field theory is a low-energy model defined on a small set of localized wave-functions constructed after the density functional theory step. The larger the energy window of the bands used in such a construction is, the more localized the resulting wave-functions will be. Since the assumption of a local Coulomb interaction is justified only if the orbitals of the minimal basis set considered as correlated are truly localized, the agreement with experiments is expected to improve upon including a higher number of relevant degrees of freedom. In the case of transition-metal oxides this would mean considering both the more correlated *d*- and the less correlated *p*-orbitals. In several cases, however, the agreement is surprisingly much better in the *d*-only case. We have shown that the physics arising from *d*-only and *dp* models for Ni-based heterostructures is indeed very dissimilar due to a different effect of the Hund's rule coupling in the two cases [1]. Analogous issues affect also theoretical predictions for Cuprates, for which the role of the *d-p* hybridization may appear at a first sight less relevant [2].

[1] N. Parragh, *et al.*, Phys. Rev. B **88**, 195116 (2013)
[2] P. Hansmann, *et al.*, *preprint* (2013)

TT 84.5 Thu 10:30 HSZ 304

One-particle irreducible functional approach: A route to diagrammatic extensions of the dynamical mean-field theory — •Georg Rohringer[1], Alessandro Toschi[1], Hartmut Hafermann[2], Karsten Held[1], Vladimir Anisimov[3,4], and Andrey Katanin[3,4] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Centre de Physique Théorique, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]Institute of Metal Physics, 620990, Ekaterinburg, Russia — [4]Ural Federal University, 620002, Ekaterinburg, Russia

We present an approach[1] which is based on the one-particle irreducible (1PI) generating functional formalism and includes electronic correlations on all length-scales beyond the local correlations of dynamical mean field theory (DMFT). This formalism allows us to unify aspects of the dynamical vertex approximation (DΓA) and the dual fermion (DF) scheme, yielding a consistent formulation of nonlocal correlations at the one- and two-particle level beyond DMFT within the functional integral formalism. In particular, the considered approach includes one-particle reducible contributions from the three- and more-particle vertices in the dual fermion approach, as well as some diagrams not included in the ladder version of DΓA. To demonstrate the applicability and physical content of the 1PI approach, we compare the diagrammatics of 1PI, DF and DΓA, as well as the numerical results of these approaches for the half-filled Hubbard model in two dimensions.

[1] G. Rohringer, A. Toschi, K. Held, V. I. Anisimov, and A. A. Katanin, Phys. Rev. B **88**, 115112 (2013)

TT 84.6 Thu 10:45 HSZ 304

Efficient real frequency solver for dynamical mean field theory — •Yi Lu[1,2] and Maurits W. Haverkort[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

We present an efficient exact diagonalization (ED) based real frequency solver for the general Anderson impurity problem and dynamical mean field theory (DMFT). It alleviates the exponential increasing Hilbert space encountered by conventional ED algorithms as a function of the number of bath sites. A specific bath geometry is realized upon which basis set optimization can be applied. The restricted Hilbert space allows calculations including a few hundred bath sites at moderate cost, which solve for spectral functions with energy resolution better than $1/\mathcal{O}(10^2)$ of the bandwidth. Good agreement with other methods including numerical renormalization group and continuous-time quantum Monte Carlo is obtained for model systems over a wide parameter space, with comparable or better accuracy at much lower computation cost. Dynamical quantities can be easily obtained on the real axis. We show several examples of DMFT calculations on transition metal oxides, including nickelates and related heterostructures.

TT 84.7 Thu 11:00 HSZ 304

Quasi-continuous-time impurity solver for the cluster dynamical mean-field theory with linear scaling in the inverse temperature — •Daniel Rost[1,2], Nils Blümer[1], and Fakher F. Assaad[3] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Graduate School Materials Science in Mainz, Johannes Gutenberg University, Mainz, Germany — [3]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Germany

We present an extension to cellular dynamical mean-field theory (CDMFT) of an recently developed unbiased quantum Monte Carlo (QMC) impurity solver for single-site DMFT [1]. The novel algorithm is based on a multigrid version of BSS-QMC [2,3], which yields Green

functions free of significant Trotter errors, and scales linearly with the inverse temperature $\beta = 1/T$ and cubically in the cluster size N. We use the superior scaling to explore ultra-low temperature regimes at moderate cluster sizes, not reachable with state-of-the-art continuous time QMC impurity solvers that scale cubically in β.

[1] D. Rost, F. Assaad and N. Blümer, PRE 87, 053305 (2013)
[2] E. Khatami et al., PRE 81, 056703 (2010)
[3] R. Blankenbecler, D. Scalapino, R. Sugar, PRD 24, 2278 (1981)

15 min. break.

TT 84.8 Thu 11:30 HSZ 304

Divergent precursors of the Mott metal-insulator transition in dynamical mean field theory and beyond — •T. Schäfer[1], G. Rohringer[1], O. Gunnarsson[2], S. Ciuchi[3], G. Sangiovanni[4], E. Gull[5], J. LeBlanc[6], P. Thunström[1], M. Wallerberger[1], and A. Toschi[1] — [1]Institute of Solid State Physics, Vienna University of Technology, Austria — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany — [3]Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, Italy — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [5]Department of Physics, University of Michigan, USA — [6]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Bulk electronic correlated systems can be often successfully studied by dynamical mean field theory (DMFT), which is able to properly describe the intrinsically non-perturbative phenomenon of the Mott-Hubbard metal-to-insulator transition (MIT). Recently it has been shown that the first hallmarks of the MIT can already be identified well inside the metallic regime in terms of divergences of the two-particle irreducible vertex [1].

In this talk the non-perturbative region of the Hubbard model's phase diagram beyond the first precursor line towards the MIT is explored in more detail and, eventually, the effects of the inclusion of short-ranged spatial correlations are discussed [2].

[1] T. Schaefer, G. Rohringer, O. Gunnarsson, S. Ciuchi, G. Sangiovanni, and A. Toschi, Phys. Rev. Lett. 110, 246405 (2013)
[2] T. Schaefer et al., in preparation

TT 84.9 Thu 11:45 HSZ 304

Stochastic Mode Sampling (SMS) - An Efficient Approach to the Analytic Continuation Problem — •Khaldoon Ghanem and Erik Koch — Computational Materials Science, German Research School for Simulation Sciences, Jülich, Germany

Stochastic sampling methods (SSMs) provide a promising alternative to the commonly used maximum entropy method (MEM) in solving the analytic continuation problem of non-negative quantities like the spectral function or the optical conductivity. SSMs assume a flat prior probability, which is the appropriate choice in the absence of any prior knowledge, while MEM unjustifiably biases the results toward a default model. On the other hand, SSMs can be exceedingly slow compared to MEM because of the large correlation times.

We present a new stochastic sampling method, *Stochastic Mode Sampling* (SMS). Instead of sampling the components of the solution directly, we sample the singular vectors (modes) of the kernel, which relates the data to the solution. In this basis, the sampled quantities are uncorrelated except for the coupling through the non-negativity constraint. The weaker this coupling, the more efficient the method, so we modify the kernel such that the coupling is minimized, thus reducing correlation times dramatically in comparison to other SSMs. We also show how to make SMS solutions converge as the discretization grid becomes larger and denser.

TT 84.10 Thu 12:00 HSZ 304

Fermionic functional renormalization group flows into antiferromagnetically ordered phases — •Stefan A. Maier and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany and JARA - FIT Fundamentals of Future Information Technology

In this talk, we report on purely fermionic functional renormalization group flows into antiferromagnetically ordered phases. Starting from the fRG one-loop flow equations, a hierarchy of approximations is devised. Interaction terms breaking the discrete time-reversal and translational symmetries are thereby successively neglected, whereas they remain broken on the one-particle level. In the course of these approximations, also an exchange parametrization is employed. For the spin-density wave (SDW) phase of a two-pocket model initially proposed by Chubukov *et al.* in Phys. Rev. B **78** 134512, the flow equations are then integrated numerically at the most approximate level of the hierarchy. This yields a SDW gap that is significantly reduced compared to mean-field theory, and the inclusion of the charge-density wave and singlet-pairing channels turns out to be crucial. The observed violation of the SU(2) Ward identity appears acceptable on a qualitative level, suggesting that the underlying approximations are physically meaningful.

TT 84.11 Thu 12:15 HSZ 304

Impurity solver based on Dynamical Density Matrix Renormalization Group — •Markus Greger and Marcus Kollar — Theoretische Physik III, Zentrum für Elektronische Korrelationen und Magnetismus, Universität Augsburg

We present a deconvolution-free extension of the dynamical density matrix renormalization group (DDMRG) for impurity problems. Our method is highly accurate in the low-energy sector and yields spectra that are comparable in resolution to the numerical renormalization group (NRG). The method is suitable as an impurity solver for multi-orbital dynamical mean-field theory (DMFT). We present results for the Green function, self-energy, and spin-susceptibility for multi-band Hubbard models, focusing on the effect of the Hund's rule coupling on these spectra at low-energies.

TT 84.12 Thu 12:30 HSZ 304

Low-energy singularities in the ground state of fermionic superfluids — •Benjamin Obert[1], Christoph Husemann[2], and Walter Metzner[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Carl Zeiss AG, Carl Zeiss Promenade 10, D-07745 Jena, Germany.

We analyze the effects of order parameter fluctuations on the ground state of fully gapped charge-neutral fermionic superfluids. The Goldstone mode associated with the spontaneously broken symmetry leads to a problem of coupled singularities in $d \leq 3$ dimensions. We derive a minimal set of one-loop renormalization group equations which fully captures the interplay of the singularities. The flow equations are based on a symmetry conserving truncation of a scale dependent effective action. We compute the low energy behavior of longitudinal, transverse and mixed order parameter correlations, and their impact on the fermionic gap. We demonstrate analytically that cancellations protecting the Goldstone mode are respected by the flow, and we present a numerical solution of the flow equations for the two-dimensional attractive Hubbard model.

TT 84.13 Thu 12:45 HSZ 304

Symmetry breaking with Projected Entangled Pair States — •Manuel Rispler and Norbert Schuch — Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

Projected Entangled Pair States (PEPS) have been introduced as a two-dimensional generalization of Matrix Product States and form a part of the larger class of Tensor Network States, which parametrize quantum states according to their entanglement structure. In this talk, we explain how the mechanism of symmetry breaking can be understood in the framework of PEPS models. We give examples and illustrate how perturbations give rise to the symmetry broken states. We further discuss how this allows to understand the entanglement spectrum as arising from a local Hamiltonian on the boundary of the system.

TT 84.14 Thu 13:00 HSZ 304

Critical Exponents of Strongly Correlated Fermion Systems from Diagrammatic Multi-Scale Methods — Andrey Antipov[1,2], Emanuel Gull[3], and •Stefan Kirchner[1,2] — [1]MPI for Physics of Complex Systems, Dresden — [2]MPI for Chemical Physics of Solids — [3]Department of Physics, University of Michigan

The dynamical mean field theory (DMFT) has become the standard tool in describing strongly correlated electron materials. While it captures the quantum dynamics of local fields, it neglects spatial correlations. To describe e.g. anti-ferromagnetism, unconventional superconductivity or frustration a proper treatment of non-local correlations is necessary. Diagrammatic multi-scale approaches offer an elegant option to accomplish this: the difficult correlated part of the system is solved using a non-perturbative many-body method, whereas 'easier', 'weakly correlated' parts of the problem are tackled using a secondary perturbative scheme. Here we employ such a method, the dual fermion approach, to problems of charge ordering in Falicov-Kimball model [1]

by constructing a systematic diagrammatic extension on top of DMFT. Near the critical point of the Falicov-Kimball model we study the interplay between charge excitations and long-range fluctuations. We show that such multi-scale approach is indeed capable of capturing the non mean-field nature of the critical point of the lattice model and correctly describes the transition to mean-field like behavior as the number of spatial dimensions increases.

[1] A. Antipov, E. Gull, S. Kirchner, arXiv:1309.5976(2013).