TT 33: Correlated Electrons: Method Development 1

Time: Wednesday 9:30–12:45 Location: HSZ 201

TT 33.1 Wed 9:30 HSZ 201

Density functional perturbation theory with DFT+U in the mixed-basis framework — •Rolf Heid — Institute of Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology

DFT+U is a viable tool to improve description of materials, where the standard DFT exchange-correlation potentials fail to catch essential properties of electronic correlation. While phenomenological in nature, it is numerically efficient and also gives access to energy derivatives, e.g. forces and force constants. Most applications to lattice dynamics properties have been based on the direct method (supercells and forces), while the linear response approach has been rarely used.

Here I describe a combination of DFT+U and density functional perturbation theory (DFPT) in the framework of the mixed-basis approach, an efficient method based on norm-conserving pseudopotentials employing a combination of plane waves and tailored local functions for the expansion of the valence states. The DFPT extension of the mixed-basis method [1,2] has been extensively applied in the past. The present DFT+U implementation employs the fully rotationally invariant form [3] in its relativistic extension [4]. Its usefulness is demonstrated for compounds containing 3d or 4f/5f elements.

[1] R. Heid et al., Phys. Rev. B **60**, R3709 (1999).
[2] R. Heid et al., Phys. Rev. B **81**, 174527 (2010).
[3] A.I. Liechtenstein et al., Phys. Rev. B **52**, R5467 (1995).
[4] A. B. Shick et al., Europhys. Lett. **69**, 588 (2005).

TT 33.2 Wed 9:45 HSZ 201

TRILEX^2 approach: towards the calculation of realistic systems — •Evgeny A. Stepanov[1], Silke Biermann[2], and Alexander I. Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, Germany — [2]Centre de Physique Theorique, Ecole Polytechnique, Palaiseau, France

A theoretical description of strongly correlated realistic systems is a challenging issue. A state-of-art method that allows to obtain single-particle properties of a corresponding multi-band electronic problem is the dynamical mean field theory (DMFT). Starting from DMFT, it is known that a consistent calculation of two-particle susceptibilities can be done via a ladder diagram that necessarily contains local vertex corrections. However, a calculation of these vertices is the most complicated and time consuming part of numerical approaches that describe nonlocal collective effects diagrammatically beyond DMFT. In some cases, a description of collective electronic fluctuations can be performed in a much simpler way using the GW+DMFT theory. However, the GW+DMFT in its original form accounts for the screening of the local Coulomb interaction only in the charge channel. Thus, the effect of the magnetic fluctuations in the nonlocal self-energy is missing. Recently, some of us introduced a computationally inexpensive TRILEX^2 approach [PRB 100, 205115 (2019)] that describes nonlocal many-body effects in the GW+DMFT style, but allows for a simultaneous account for collective excitations in different (charge, spin, etc.) bosonic channels. Here, we apply this method to a multi-band Hubbard model to explore orbital and spin fluctuations.

TT 33.3 Wed 10:00 HSZ 201

Strong-coupling formula for momentum-dependent susceptibilities in dynamical mean-field theory — •Junya Otsuki[1], Kazuyoshi Yoshimi[2], Hiroshi Shinaoka[3], and Yusuke Nomura[4] — [1]Research Institute for Interdisciplinary Science, Okayama University, Okayama Japan — [2]Institute for Solid State Physics, University of Tokyo, Chiba, Japan — [3]Saitama University, Saitama, Japan — [4]University of Tokyo, Tokyo, Japan

Computing momentum-dependent susceptibilities in the dynamical mean-field theory (DMFT) requires solving the Bethe-Salpeter equation, which demands large computational cost. Exploiting the strong-coupling feature of local fluctuations, we derive a simplified formula that can be solved at a considerably lower cost [1]. This formula allows us to estimate an effective intersite interaction, which is reduced to a well-known formula in the strong-coupling limit, such as the kinetic exchange and RKKY interactions. We present some applications of this formula to demonstrate its validity and applicability.

[1] J. Otsuki, K. Yoshimi, H. Shinaoka, Y. Nomura, Phys. Rev. B **99**, 165134 (2019)

TT 33.4 Wed 10:15 HSZ 201

Fixed point and thermodynamic stability of DMFT — •Erik van Loon[1] and Friedrich Krien[2] — [1]University of Bremen, Bremen, Germany — [2]Jožef Stefan Institute, Ljubljana, Slovenia

We consider the hysteresis region and critical end point of the DMFT metal-insulator transition by analyzing the fixed point equation and the Landau free energy.

TT 33.5 Wed 10:30 HSZ 201

Bandwidth renormalization due to the intersite Coulomb interaction — Yann in 't Veld[1], •Malte Schüler[2,3], Tim Wehling[2,3], Mikhail Katsnelson[1], and Erik van Loon[2,3] — [1]Institute for Molecules and Materials, Radboud University — [2]Bremen Center for Computational Materials Science, University Bremen — [3]Institute for Theoretical Physics, University Bremen

The theory of correlated electrons is currently moving beyond the paradigmatic Hubbard U, towards the investigation of intersite Coulomb interactions. Recent investigations have revealed that these interactions are relevant for the quantitative description of realistic materials. Physically, intersite interactions are responsible for two rather different effects: screening and bandwidth renormalization. We use a variational principle to disentangle the roles of these two processes and study how appropriate the recently proposed Fock treatment of intersite interactions is in correlated systems. The magnitude of this effect in graphene is calculated based on cRPA values of the intersite interaction. We also apply the variational principle to benzene and find effective parameters comparable to those obtained by ab-initio density matrix downfolding.

TT 33.6 Wed 10:45 HSZ 201

Single-boson exchange decomposition of the vertex function — •Friedrich Krien[1,3], Angelo Valli[2,3], and Massimo Capone[3] — [1]Institut Jozef Stefan, Ljubljana, Slovenia — [2]TU Wien, Austria — [3]SISSA, Trieste, Italy

We present a decomposition of the four-point vertex function which imparts a physical interpretation of the vertex in terms of the exchange of bosons of three flavors. The proposed decomposition does not require the matrix inversion of the Bethe-Salpeter equation and avoids the vertex divergences intrinsic to the traditional parquet decomposition. We discuss parametrizations of the vertex function in terms of the Hedin three-leg vertex.

15 min. break.

TT 33.7 Wed 11:15 HSZ 201

Symmetric improved estimators for continuous-time quantum Monte Carlo — •Josef Kaufmann[1], Patrik Gunacker[1], Alexander Kowalski[2], Markus Wallerberger[1], Giorgio Sangiovanni[2], and Karsten Held[1] — [1]Institut für Festkörperphysik, TU Wien — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Continuous-time quantum Monte Carlo in the hybridization expansion is the current method of choice for solving the multiorbital Anderson impurity model. However, the results suffer from notoriously high noise at large Matsubara frequencies. Previously, this problem has been addressed e.g. by improved estimators [1]

We now go beyond this by deriving equations of motion for Green's functions symmetrically with respect to all time arguments. The resulting equations relate the one- and two-particle Green's function to correlators of up to six particles at four times [2], which can be computed by worm sampling [3, 4]. Finally, we arrive at self-energies and vertex functions that are practically noiseless at all frequencies.

This increase in precision leads to improved convergence behavior in dynamical mean-field theory calculations, as well as more reliable analytical continuation to real frequencies.

[1] H. Hafermann et al., PRB 85, 205106 (2012)
[2] J. Kaufmann, P. Gunacker et al., PRB 100, 075119 (2019)
[3] P. Gunacker et al., PRB 92, 155102 (2015)
[4] M. Wallerberger et al., CPC 235, 388 (2019)

TT 33.8 Wed 11:30 HSZ 201

Novel approach to non-local correlations: dual boson di-

agrammatic monte carlo — •Matteo Vandelli[1,2], Evgeny Stepanov[1], Angel Rubio[2], and Alexander Lichtenstein[1] — [1]Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

A long list of interesting physical phenomena arises due to strong interactions among electrons, but the mechanisms behind them are not fully understood yet. One of the most successful methods to deal with correlations is Dynamical Mean Field Theory (DMFT). However diagrammatic extensions are needed to capture non-local correlations. In particular dual theories are very promising, since they are based on an exact transformation. Recently Gukelberger et al. [PhysRevB.96.035152] have proven that the combination of Dual Fermion approach with diagrammatic Monte Carlo (DiagMC@DF) reproduces very accurately the results based on numerically exact Monte Carlo benchmarks. We expanded this scheme so that we could include non-local interactions appearing in the Extended Hubbard model. In order to achieve this goal, we combined diagrammatic Monte Carlo with Dual Boson approach (DiagMC@DB). The main advantage of this technique is that it can capture the interplay between competing instabilities. Furthermore the algorithm samples all the possible Feynman diagrams, as opposed to other diagrammatic approaches that arbitrarily select only some topologies.

TT 33.9 Wed 11:45 HSZ 201

Quantum Dynamics Made Fast: Achieving Linear Time-Scaling for Nonequilibrium Green Functions — •Niclas Schlünzen, Jan-Philip Joost, and Michael Bonitz — CAU Kiel, Germany

The accurate description of nonequilibrium dynamics in correlated quantum-many-body systems remains to be a driving force for current research in condensed-matter physics and beyond. Among others, the nonequilibrium Green functions (NEGF) method has proven to be a powerful tool to predict quantum dynamics[1]. However, NEGF simulations are computationally expensive due to their T^3 scaling with the simulation duration T . With the introduction of the generalized Kadanoff–Baym ansatz[2] (GKBA), T^2 scaling could be achieved for second order Born (SOA) selfenergies[3], which has substantially extended the scope of NEGF simulations. Recently[4], we could show that GKBA-NEGF simulations can be performed with order T^1 scaling for SOA and even *GW* selfenergies. Here, we show numerical results for various many-body approximations and demonstrate that tremendous computational speed-up can be achieved.

[1] K. Balzer and M. Bonitz, Lect. Notes Phys. **867** (2013)
[2] P. Lipavský *et al.*, Phys. Rev. B **34**, 6933 (1986)
[3] S. Hermanns *et al.*, Phys. Scr. **2012** 014036 (2012)
[4] N. Schlünzen *et al.*, submitted, arXiv:1909.11489

TT 33.10 Wed 12:00 HSZ 201

Functional renormalization group for a large Moiré unit cell — •Lennart Klebl, Dante Kennes, and Carsten Honerkamp — RWTH Aachen University, Aachen, Germany

Layers of two-dimensional materials arranged at a twist angle with respect to each other lead to enlarged unit cells with potentially strongly altered band structures, offering a new arena for novel and engineered many-body ground states. For the exploration of these, renormalization group methods are an appropriate, flexible tool that takes into account the mutual influence of competing tendencies. We show how the functional renormalization group known from simpler two-dimensional systems can be employed for large unit cells of Moiré superlattices, providing a description on the atomic scale and absorbing available ab-initio information on the model parameters. For the case of twisted bilayer graphene models, we explore the leading ordering tendencies depending on the band filling and the range of interactions. The results indicate a delicate balance between distinct magnetically ordered ground states.

TT 33.11 Wed 12:15 HSZ 201

Efficient simulation of the Dynamics in Two-Dimensional Quantum Spin Systems with Isometric Tensor Networks — •Sheng-Hsuan Lin and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

We introduce a numerical method to efficiently simulate the dynamical spin structure factor of two-dimensional quantum spin systems. The time evolution of truly two-dimensional systems is made possible using recently introduced isometric tensor network states [1]. We benchmark the algorithm by considering two paradigmatic models: First, we compare our results for the transverse field Ising model on square lattice with the prediction of spin wave theory. Second, we consider the Kitaev model on the honeycomb lattice and compare to the exact solution.

[1] arXiv preprint arXiv:1902.05100 (2019)

TT 33.12 Wed 12:30 HSZ 201

Orientational order parameters for arbitrary quantum systems* — •Michael te Vrugt and Raphael Wittkowski — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149 Münster, Germany

The concept of quantum-mechanical nematic order, which is important in systems such as superconductors, is based on an analogy to classical liquid crystals, where order parameters are obtained through orientational expansions. We generalize this method to quantum mechanics based on an expansion of Wigner functions. This provides a systematic framework for the derivation of quantum order parameters, which unifies all known types of quantum orientational order into one framework and has a natural connection to the classical case. Moreover, new order parameters allow to find new orientational quantum phases. The method is demonstrated for Fermi liquids and spin systems. In addition, we construct new order parameters for molecular systems that cannot be properly described with the usual nematic tensors.

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