TT 61: Correlated Electrons: (General) Theory 1

Time: Thursday 9:30–13:00 Location: H18

TT 61.1 Thu 9:30 H18

Collective magnetic excitations in correlated systems: self-consistent dual boson approach — Friedrich Krien[1], Evgeny Stepanov[2], Erik van Loon[2], Andrey Katanin[3], Mikhail Katsnelson[2], Alexey Rubtsov[4], and •Alexander Lichtenstein[1] — [1]University of Hamburg — [2]Radboud University Nijmegen — [3]Institute of Metal Physics, Ekaterinburg — [4]Moscow State University

We propose an efficient dual boson scheme for correlated magnetic systems, which extends the local dynamical mean-field theory to non-local interactions and collective excitations. The theory is fully self-consistent both on the one and on the two-particle level, thus describing the formation of collective magnetic modes as well as the renormalization of electrons and magnons spectra on equal footing. The method employs exact solution of effective impurity model consists of both fermion and spin-boson hybridization functions. We show that the theory is naturally described by a dual Luttinger-Ward functional and obeys the relevant conservation laws for magnetic excitations. We compare numerical results for the Hubbard model with non-local magnetic interactions with extended DMFT solution.

TT 61.2 Thu 9:45 H18

Ab-initio study of the finite temperature magnetism in iron and nickel II — •Andreas Hausoel[1], Michael Karolak[1], Ersoy Sasioglu[2], Alexander Lichtenstein[3], Karsten Held[4], Andrey Katanin[5], Alessandro Toschi[4], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Peter Grünberg Institut, Forschungszentrum Jülich — [3]Institut für Theoretische Physik, Universität Hamburg — [4]Institute of Solid State Physics, TU Wien — [5]Institute of Metal Physics, Ekaterinburg

The calculation of the ferromagnetic transition temperature of itinerant ferromagnets like iron and nickel has been a very hard problem for theory ever since. This is due to the interplay between strong local interactions and the itinerant character of the electrons. Here we show fully ab-initio DFT+DMFT calculations for bcc-iron and fcc-nickel, using the numerically exact Continuous Time Quantum Monte Carlo method in hybridization expansion. We consider the full cubic Coulomb interaction from cRPA. By discussing the effects of commonly used approximations (density-density and Slater-Kanamori) we find, that the magnetic ordering mechanisms in iron and nickel are very different.

TT 61.3 Thu 10:00 H18

Towards an efficient algorithmic combination of functional renormalization group and dynamical mean field theory — •Demetrio Vilardi[1], Nils Wentzell[2,3], Agnese Tagliavini[2,3], Ciro Taranto[1,3], Alessandro Toschi[2], Sabine Andergassen[3], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Vienna University of Technology, Vienna, Austria — [3]University of Tübingen, Tübingen, Germany

We present the advancements in the implementation of a recently proposed scheme for a non-perturbative treatment of strongly correlated fermion systems. This approach, called DMF^{2}RG, combines the local strong-coupling treatment of dynamical mean field theory (DMFT) and the non-local one of functional renormalization group (fRG). In our improved algorithmic implementation the full frequency dependence of the local DMFT vertex is retained in the flow. We show results for the one band 2D Hubbard model and compare them against other techniques.

TT 61.4 Thu 10:15 H18

Susceptibility calculations using a multi-orbital general CT-QMC solver for DMFT — •Julian Musshoff[1,2], Amin Kiani[1], and Eva Pavarini[1] — [1]Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, Germany — [2]Institute for Theory of Statistical Physics RWTH Aachen University, 52074 Aachen, Germany

Susceptibilities describe the response of a system to an external perturbation, and are therefore essential to compare theoretical calculations with experiments. We use a general continuous-time quantum Monte Carlo solver for dynamical mean-field theory to calculate generalized local susceptibilities. The method is applicable to strongly correlated materials with multi-orbital Hamiltonians. We calculate and store the susceptibilities in a compact form by using a Legendre polynomial representation. Furthermore we extend the local susceptibilities to lattice susceptibilities using the Bethe-Salpeter equation. In the talk we show magnetic susceptibility results for a representative system, $VOMoO_4$.

TT 61.5 Thu 10:30 H18

Analytic Continuation of Quantum Monte Carlo Data: Stochastic Sampling Method — •Khaldoon Ghanem and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

We apply Bayesian inference to the analytic continuation of quantum Monte Carlo (QMC) data from the imaginary axis to the real axis. Demanding a proper functional Bayesian formulation of any analytic continuation method leads naturally to the stochastic sampling method (StochS) as the Bayesian method with the simplest prior, while it excludes the maximum entropy method and Tikhonov regularization.

We present a new efficient algorithm for performing StochS that reduces computational times by orders of magnitude in comparison to earlier StochS methods. We apply the new algorithm to a wide variety of typical test cases: spectral functions and susceptibilities from DMFT and lattice QMC calculations. Results show that StochS performs well and is able to resolve sharp features in the spectrum.

TT 61.6 Thu 10:45 H18

Competition of multiplet and spin-orbit splitting in open-shells — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich

To study the trends in the spectra of open-shells across the periodic table, we perform density functional calculations for atoms and ions. We collect the Slater-Condon and spin-orbit parameters from the resulting self-consistent radial wave functions and potentials. To make these easily accessible, we provide a simple least squares fitting formula in the spirit of Slater's rules. Given these parameters we calculate the many-body spectra in *LS*-, intermediate-, and *jj*-coupling. To assess the relative importance of Coulomb and spin-orbit interactions, we estimate the width of the spectra by calculating the eigen-energy variance of the corresponding Hamiltonian using a simple formula that does not require diagonalizing a complicated many-body Hamiltonian.

TT 61.7 Thu 11:00 H18

High-order diagrammatic expansion for the Gutzwiller wave function — Marc Alexander and •Marcus Kollar — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg

Variational wave functions can provide insights into the physics of correlated electrons, but even the evaluation of static expectation values is notoriously difficult for many-body Hamiltonians. Usually stochastic or perturbative calculations are required, except for a few exact solutions in one or infinite dimensions. For the single-band Hubbard model a diagrammatic formulation for expectation values with the Gutzwiller wave function was developed [1,2], involving the same Feynman diagrams as ϕ^4 field theory. The Feynman diagrams for the latter problem can be generated by computer [3], which we convert and evaluate to high order for the Gutzwiller wave function. Possible applications to equilibrium and nonequilibrium problems are discussed.

[1] W. Metzner, Z. Phys. B. **77**, 253 (1989)
[2] F. Gebhard, PRB **41**, 9452 (1990)
[3] H. Kleinert et al., PRE **62**, 1537 (2000)

15 min. break

TT 61.8 Thu 11:30 H18

Efficient implementation of the parquet equations – role of the reducible vertex function and its kernel approximation — •Gang Li[1], Nils Wentzell[1,2], Petra Pudleiner[1], Patrik Thunström[1], and Karsten Held[1] — [1]nstitute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria — [2]Institut für Theoretische Physik and CQ Center for Collective Quantum Phenomena, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany

We present an efficient implementation of the parquet formalism which

respects the asymptotic structure of the vertex functions at both single- and two-particle levels in momentum- and frequency-space. We identify the two-particle reducible vertex as the core function which is essential for the construction of the other vertex functions. This observation stimulates us to consider a two-level parameter-reduction for this function to simplify the solution of the parquet equations. The resulting functions, which depend on fewer arguments, are coined "kernel functions". With the use of the "kernel functions", the open boundary of various vertex functions in the Matsubara-frequency space can be faithfully satisfied. We justify our implementation by accurately reproducing the dynamical mean-field theory results from momentum-independent parquet calculations. The high-frequency asymptotics of the single-particle self-energy and the two-particle vertex are correctly reproduced, which turns out to be essential for the self-consistent determination of the parquet solutions. The current implementation is also feasible for the dynamical vertex approximation.

TT 61.9 Thu 11:45 H18

High-frequency aysmptotics of the local vertex function: algorithmic implementations — •Agnese Tagliavini[1,2], Nils Wentzell[1,2], Gang Li[2], Ciro Taranto[2,3], Georg Rohringer[2], Karsten Held[2], Alessandro Toschi[2], and Sabine Andergassen[1] — [1]Institut für Theoretische Physik, Eberhard Karls Universität, 72076 Tübingen, Germany — [2]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [3]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany

Local vertex functions are a crucial ingredient of several forefront many-body algorithms in condensed matter physics. However, the full treatment of their frequency dependence poses a huge limitation to the numerical performance. A significant advancement requires an efficient treatment of the high-frequency asymptotic behavior of the vertex functions. We here provide a detailed diagrammatic analysis of the high-frequency asymptotic structures and their physical interpretation. Based on these insights, we propose a frequency parametrization, which captures the whole high-frequency asymptotics for arbitrary values of the local Coulomb interaction and electronic density. We present its algorithmic implementation in many-body solvers based on parquet-equations as well as functional renormalization group schemes and assess its validity by comparing our results for the single impurity Anderson model with exact diagonalization calculations.

TT 61.10 Thu 12:00 H18

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). We focus here on additional approximations to the exact density-matrix functional in the local approximation and evaluate their performance.

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TT 61.11 Thu 12:15 H18

Entanglement-Continuous Unitary Transformations — •Serkan Sahin and Román Orús — Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

In this talk we present a new algorithm for quantum many-body systems using continuous unitary transformations (CUT) and tensor networks (TNs). With TNs we are able to approximate the solution to the flow equations that lie at the heart of continuous unitary transformations. We call this method Entanglement-Continuous Unitary Transformations (eCUT). It allows us to compute expectation values of local observables as well as tensor network representations of ground states and low-energy excited states. An implementation of the method is shown for 1d systems using matrix product operators. We show preliminary results for the 1d transverse-field Ising model to demonstrate the feasibility of the method.

TT 61.12 Thu 12:30 H18

Towards an improved duality between tensor network states and AdS spacetime — •Charalampos Papadopoulos and Román Orús — Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

The conjectured AdS/CFT Correspondence, which states that a Conformal Field Theory (CFT) in Minkowski spacetime has a gravity dual in an asymptotically Anti-de Sitter space (AdS), is one of the best understood examples of the holographic principle, and has important applications in condensed matter physics. Tensor Networks (TNs) are a efficient way to calculate low-energy properties for strongly-correlated quantum many-body systems. The Multi-scale Entanglement Renormalization Ansatz (MERA) is a specific TN for a efficient description of critical quantum systems (CFTs). It was recently suggested that the MERA provides naturally a discretization of AdS spacetime on a lattice. It is however known that a conventional MERA can not reproduce the so-called "Bousso Bound", also called holographic entropy bound, which is a bound on the bulk entropy in spacetime. In this context, our aim is to generalize the proposed AdS/MERA correspondence to a more general AdS/TN duality, where the Bousso bound is satisfied. Progress in this direction as well as connections to strongly correlated systems will be discussed.

TT 61.13 Thu 12:45 H18

DMRG Application in Binary Tree Tensor Networks with Non-Abelian Symmetries — •Claudius Hubig and Ulrich Schollwöck — Department für Physik, LMU München, Germany

The density matrix renormalisation group (DMRG) algorithm and the underlying matrix product state (MPS) state representation have become the workhorse of numerical solid state physics in one dimension. Generalisations to two and more dimensions have been realised as general tensor networks. Of these, binary tree tensor networks preserve most of the favourable properties of MPS while already allowing for a strikingly different entanglement structure. This is in particular relevant in the context of dynamical mean-field theory, where DMRG-based solvers have been employed recently, but were hindered by the one-dimensional structure of MPS.

This contribution discusses the implementation and performance behaviour of DMRG and related methods for binary tree tensor networks which identically conserve both abelian and non-abelian symmetries, such as $U(1)_{\text{Charge}}$ and $SU(2)_{\text{Spin}}$. Numerical exploitation of these symmetries directly leads to large speed-ups and further simplifies parallelisation over many cores.