TT 13: Correlated Electrons: Method Development I

Time: Monday 15:00–18:30 Location: HSZ/0101

TT 13.1 Mon 15:00 HSZ/0101

Real-Frequency Dynamical Mean-Field Theory Without Broadening Inside the Self-Consistency Cycle — •Aleksandrs Zacinskis[1], Frank T. Ebel[2], Sina Shokri[1], Lukas Hellman[1], Fabian B. Kugler[3], Karsten Held[2], and Maurits W. Haverkort[1] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Institute of Solid State Physics, TU Wien — [3]Institute for Theoretical Physics, University of Cologne

Dynamical mean-field theory has become one of the central frameworks for studying strongly correlated electron systems. Real-frequency implementations offer a major advantage by providing direct access to spectral properties without the need for analytic continuation. Most current real-frequency implementations work slightly off the real axis and evaluate $G(\omega+i\Gamma)$ instead of $G(\omega)$, which introduces an artificial broadening and can lead to systematic errors. We present a strictly real-frequency method with zero broadening inside the self-consistency cycle, addressing both the Dyson equation and the "improved estimator" self-energy [PRB 105, 245132]. Our formulation allows the self-energy to be extracted directly from the continued-fraction representation of the impurity Green's function, as obtained from Krylov bases in Lanczos methods, Wilson chains in NRG, or Kernel Polynomial methods. This method completely removes the need for artificial broadening and is applicable to all real-frequency impurity solvers. We compare the zero-broadening self-energy to its finite-broadening counterpart obtained with Exact Diagonalization solver, demonstrating the impact of broadening on accuracy and various quantities.

TT 13.2 Mon 15:15 HSZ/0101

Bath parameterization and multi-orbital physics in cluster DMFT — •Diego Florez-Ablan[1], Carlos Mejuto-Zaera[2], and Massimo Capone[1] — [1]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [2]Univ Toulouse, CNRS, Laboratoire de Physique Théorique, Toulouse, France.

Quantum embedding methods such as cluster dynamical mean-field theory (CDMFT) require accurate and reliable impurity solvers and a controlled treatment of the bath in order to be predictive for correlated materials. Building on an efficient selected configuration interaction impurity solver, a systematic analysis of bath discretization effects is presented for one- and two-orbital Hubbard models within Hamiltonian-based CDMFT, focusing on the impact of bath size and parameterization on the zero-temperature Mott transition and on possible tendencies towards symmetry-broken solutions. The study shows that, while large baths yield relatively robust results for the single-band half-filled Hubbard model, small baths can display a non-negligible dependence on parameterization, and that in the two-orbital case some quantitative sensitivity to bath parametrization persists.

Building on this benchmark, the same CDMFT machinery is applied to investigate the Hund metal regime of the two-band Hubbard model, which is relevant for the description infinite-layer nickelates, with the goal of assessing the effects of short-range spatial fluctuations on Hund-driven correlations and how they affect the stability of the Hunds metal phase in the presence of a crystal-field splitting.

TT 13.3 Mon 15:30 HSZ/0101

Uncovering correlated topological phases via a cluster-diagrammatic approach — •Félix Fossati and Evgeny Stepanov — CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Topological phases exhibit remarkable properties, including protected conducting edge states and robustness against local perturbations. Most studies of topological phenomena have focused on the non-interacting limit, where complete topological classification can be done using a single-particle band structure. While topological properties are known to be robust against weak interactions and disorder, a fundamental question remains: can electronic correlations themselves induce topological phases starting from a trivial non-interacting system? In this work, we address this question by extending the diagrammatic D-TRILEX method to a two-site cluster DMFT reference system. This approach therefore enables capturing short-range correlations non-perturbatively, while treating long-range correlations diagrammatically beyond the cluster DMFT level. We apply our method to the one-dimensional Hubbard model and demonstrate that, by tuning the strength of the non-local Coulomb interaction, our approach captures the formation of both the bond-order-wave (BOW) and the charge-density-wave (CDW) states. We show that the BOW phase can be mapped onto the Su-Schrieffer-Heeger model, while the combined CDW+BOW state corresponds to a Rice-Mele model. The non-trivial topological character of these interaction-induced phases is confirmed by the presence of localised edge states.

TT 13.4 Mon 15:45 HSZ/0101

Cluster extension of the DMF^{2}RG and application to the $2d$ Hubbard model — •Marcel Krämer[1,2,3], Michael Meixner[3], Kilian Fraboulet[3], Demetrio Vilardi[3], Pietro Bonetti[4], Nils Wentzell[5], Alessandro Toschi[2], and Sabine Andergassen[1,2] — [1]Institute of Information Systems Engineering, TU Wien, Vienna, Austria — [2]Institute for Solid State Physics, TU Wien, Vienna, Austria — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Department of Physics, Harvard University, Cambdrige, USA — [5]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

The DMF^{2}RG has been introduced to overcome the weak-coupling limitation of the fermionic functional renormalization group (fRG). This approach builds on the idea of exploiting the dynamical mean-field theory (DMFT) as starting point for the fRG flow, thus capturing local non-perturbative correlations via DMFT together with perturbative non-local correlations generated during the flow. We show how non-local non-perturbative correlations can be incorporated in the DMF^{2}RG scheme by employing solutions of non-local extensions of DMFT as a starting point of the flow. The one-loop fRG flow equations are formulated within the single-boson exchange decomposition (SBE), which classifies diagrams contributing to the two-particle vertex in terms of interaction reducibility and has been proven to be a powerful bosonization scheme. We illustrate the ability of this approach to capture non-local non-perturbative correlations in the $2d$ Hubbard model and summarize latest methodological advances.

TT 13.5 Mon 16:00 HSZ/0101

Exact t_{2g}^n super-exchange Hamiltonians for complex orbital ordering — •Amit Chauhan, Xue-Jing Zhang, and Eva Pavarini — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a general approach for studying complex orbital ordering in t_{2g}^n correlated systems. The first step consists in building exact super-exchange (SE) Hamiltonians [1-4], projected onto irreducible tensor components. The technique we adopt is suitable both for analytic and efficient numerical calculations. Next, we obtain the total energy- which includes SE, spin-orbit and crystal-field contributions- via a variational Ansatz for the many-body wavefunction. The total energy is then optimized in the chosen parametric space to find the spin and orbitally ordered ground state. Finally, SE theory is combined with DFT+DMFT calculations via an order parameter decomposition scheme. Results for paradigmatic cases are presented.

[1] X.-J. Zhang, E. Koch, E. Pavarini, PRB **105**, 115104 (2022).
[2] X.-J. Zhang, E. Koch, E. Pavarini, PRB **102**, 035113 (2020).
[3] X.-J. Zhang, E. Koch, E. Pavarini, PRB **106**, 115110 (2022).
[4] A. Chauhan, X.-J. Zhang, E. Pavarini (in preparation).

TT 13.6 Mon 16:15 HSZ/0101

Dimer Hubbard operators and their applications — •Jie Xiong and Silke Biermann — CPhT, Ecole Polytechnique, Palaiseau, France

Hubbard operators, introduced in the 1960s as projectors between atomic many-body eigenstates [1], serve as quasiparticle operators that naturally represent the lower and upper Hubbard bands. They also provide one of the earliest systematic approaches for calculating Green's functions in the Hubbard model. Extending this approach, we construct quasiparticle operators for the dimer Hubbard model and propose a general framework for analyzing quasiparticle operators in interacting many-body systems with periodic boundary conditions. As an application, we derive the equations of motion for the dimer Hubbard operators and compute Green's functions for finite benchmark models. Our findings suggest broad prospects for extending the quasiparticle-operator construction to larger correlated systems and

exploring its potential applications in topological phases.
[1] J. Hubbard, Proc. R. Soc. Lond. A 276, 238 (1963).

15 min. break

TT 13.7 Mon 16:45 HSZ/0101

Non-perturbative effects of short-range spatial correlations at the two-particle level — •Michael Meixner[1], Matthias Reitner[2], Thomas Schäfer[1,3], and Alessandro Toschi[2] — [1]Max-Planck-Institute for Solid-State Research, Stuttgart, Germany — [2]TU Wien, Vienna, Austria — [3]University of Trieste, Trieste, Italy

Non-local correlations have a strong impact on the electronic dynamics of the square lattice Hubbard model. Specifically, the Mott metal-insulator transition (MIT) occurs at lower interactions when including spatial correlations to the local model via cellular dynamical mean field theory (CDMFT). We present the Bethe-Salpeter equation (BSE) of the charge response and corresponding Ward identities applicable to the CDMFT. The scheme is employed to study the impact of real space bosonic correlations between the impurity sites onto the lattice thermodynamic derivatives such as the charge response. Firstly, we report the occurrence of the break down of self-consistent perturbation theory in the charge channel by observation of the divergence of the irreducible vertex. This is, we find, a precursor of the thermodynamic instability of CDMFT and the corresponding suppression of the charge response at the metal-insulator transition. Secondly, for both phenomena, we underline the essential role of next-neighbour spin correlations.

TT 13.8 Mon 17:00 HSZ/0101

Promising properties of Ghost Gutzwiller Ansatz: from Mott insulators to correlated antiferromagnets — •Antonio Maria Tagliente[1], Michele Fabrizio[1], and Carlos Mejuto-Zaera[2] — [1]International School for Advanced Studies (SISSA) — [2]Laboratoire de Physique Théorique, CNRS, Université de Toulouse, UPS

The ghost Gutzwiller wavefunction is a recently proposed variational Ansatz that generalizes the traditional Gutzwiller wavefunction. It consists of a Slater determinant defined in an enlarged Hilbert space that is variationally projected into the physical one. This wavefunction is therefore naturally capable of describing Hubbard bands and coexisting quasiparticle peaks.

Here, we present several results obtained through this wavefunction treated with the so-called Gutzwiller approximation.

We begin by showing that the wavefunction can describe genuine paramagnetic Mott insulators, whose finite spin susceptibility has remained elusive using other methods. A metal lead in contact with such a Mott insulator can directly reveal the spinon excitations responsible for the paramagnetic behavior, which emerge at the interface as a heavy-fermion band.

We finally demonstrate that the ghost Gutzwiller wavefunction can stabilize a correlated antiferromagnet with spin-unpolarized Hubbard bands but polarized spinons. This solution contains much more entanglement than the conventional dynamical mean-field one, and might be more representative of an actual correlated antiferromagnet in finite dimensions.

TT 13.9 Mon 17:15 HSZ/0101

Fluctuating field theory description of collective instabilities in the doped Hubbard model — •Erik Linnér[1,2], Laura Torchia[1], Silke Biermann[2,3,4], and Massimo Capone[1,5] — [1]International School for Advanced Studies (SISSA), Trieste, Italy — [2]CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, Palaiseau, France — [3]Collège de France, Paris, France — [4]European Theoretical Spectroscopy Facility, Palaiseau, France — [5]CNR-IOM, Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche, Trieste, Italy

Fluctuating field theory is a recently developed method for the description of competing collective fluctuations in correlated electron systems, able to account for spin, charge, and superconducting instabilities. On the basis of a variational principle, the method allows to explicitly account for the leading collective modes and their interplay, with access to electronic and spectroscopic properties. Extending its prior application to the Hubbard model at half-filling, we investigate its description of the doped Hubbard model, accounting for various spin instabilities. Interestingly, unlike for Néel ordering which dominates near half-filling, we show that the phase structure of the fluctuating fields for collective instabilities with arbitrary ordering vector $\mathbf{Q}$ become important. Within the method, the incommensurate spin ordering driven by doping is associated with a phase structure expressing the modulation of the ordering relative the underlying lattice geometry. Thus, we observe the method, despite its weak-coupling rot, gives an efficient tool to investigate the phase diagram beyond mean-field theory.

TT 13.10 Mon 17:30 HSZ/0101

Competing instabilities for models with non-local and retarded interactions: a functional renormalization group perspective — •Kilian Fraboulet[1,2,3], Aiman Al-Eryani[4], Marcel Gievers[5], Sarah Heinzelmann[3], Friedrich Krien[5], and Sabine Andergassen[2,5] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institute of Information Systems Engineering, TU Wien, 1040 Vienna, Austria — [3]Institute for Theoretical Physics and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [4]Institute for Theoretical Physics III, Ruhr-Universität Bochum, 44801 Bochum, Germany — [5]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The functional renormalization group is an established approach to study competing orders in many-electron systems in an unbiased manner, notably with a bosonization technique called single-boson exchange formalism. The resulting fRG approach, referred to as single-boson exchange fRG, is used to analyze competing orders in the 2D extended Hubbard model, especially the growth of the charge-density wave instability when the nearest-neighbor Coulomb repulsion increases. Finally, I will show how one can, using the single-boson exchange fRG, efficiently design a temperature flow (where the temperature is used as flow parameter) for models involving retarded interactions with electron-phonon couplings, such as the Hubbard-Holstein model.

TT 13.11 Mon 17:45 HSZ/0101

Finite-difference parquet method and the strong-coupling pseudogap — Jae-Mo Lihm[1,2], Dominik Kiese[3], Seung-Sup B. Lee[2], and •Fabian B. Kugler[4,3] — [1]Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Seoul National University, Seoul, Korea — [3]Flatiron Institute, New York, USA — [4]University of Cologne, Cologne, Germany

We present the finite-difference parquet method [1], a two-particle diagrammatic approach with nonperturbative input. It takes the fully irreducible two-particle vertex from a reference solution while requiring only its full vertex explicitly. Using dynamical mean-field theory (DMFT) as a reference, this yields a reformulation of the parquet dynamical vertex approximation circumventing ill-behaved two-particle irreducible vertices. We use this method to investigate the pseudogap phase of the underdoped Hubard model. Our numerical results are consistent with diagrammatic Monte Carlo simulations and shed new light on the microscopic mechanism of the strong-coupling pseudogap: With dominant short-ranged antiferromagnetic spin fluctuations, we find an enhanced electron-paramagnon scattering amplitude crucial for the pseudogap opening. The form of this enhancement, reflected in the real part of the Hedin vertex, requires strong local correlations from DMFT as well as nonlocal correlations in multiple two-particle channels from solving the parquet equations.
[1] https://arxiv.org/abs/2505.20116

TT 13.12 Mon 18:00 HSZ/0101

Strong-coupling functional renormalization group: non-Fermi liquid physics in the infinite-U Hubbard model — Jonas Arnold, Peter Kopietz, and •Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

Exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within an operator formalism without using functional integrals. This simple insight allows us to apply unbiased FRG methods directly to strongly correlated electron systems with projected Hilbert spaces. Here, we use this approach to compute the electronic spectral function of the Hubbard model at infinite on-site repulsion where many-body states involving doubly occupied lattice sites are eliminated from the physical Hilbert space. For a square lattice with nearest-neighbor hopping we find that the finite-temperature electronic spectrum evolves from a Fermi liquid at low densities to an incoherent non-Fermi liquid at larger densities. Both at high and low densities, the volume of the Fermi surface is not constrained by Luttinger's theorem.

TT 13.13 Mon 18:15 HSZ/0101

Nagaoka kinetic ferromagnetism in the infinite-U Hubbard model — •Jonas Arnold, Peter Kopietz, and Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

We present a study of the infinite-U Hubbard model using an extension of the functional renormalization group (FRG) that works directly with non-canonical fermionic operators. Thus the projected Hilbert space is incorporated exactly, yielding an unbiased diagrammatic method that works in the thermodynamic limit, suitable to capture the long range physics of the strongly correlated electrons. We discuss the magnetic phase diagram for the full range of hole doping. Upon increasing the density, we identify a paramagnetic ground-state, followed by an antiferromagnetic stripe order and finally Nangaoka's kinetic ferromagnetism at high densities. The dynamical susceptibilities reveal the evolution of a paramagnon band into a diffusive continuum with increasing electron density.