TT 44: Correlated Electrons: Method Development

Time: Wednesday 15:00–19:00 Location: H7

TT 44.1 Wed 15:00 H7

Dynamical susceptibility in DMFT: a sparse QMC sampling approach — •Dominique Geffroy[1,2], Hiroshi Shinaoka[3], Jan Kuneš[2], Junya Otsuki[4], Markus Wallerberger[5], Emanuel Gull[5], and Kazuyoshi Yoshimi[6] — [1]Department of Condensed Matter Physics, MU Brno, Czech Republic — [2]Institute for Solid State Physics, TU Wien, Austria — [3]Department of Physics, Saitama University, Japan — [4]Department of Physics, Tohoku University, Japan — [5]University of Michigan, Ann Arbor, USA — [6]Institute for Solid State Physics, University of Tokyo, Japan

We discuss a new technique for the efficient sampling of two-particle correlation functions in the framework of dynamical mean-field theory. The approach is based on the expansion of the two-particle Green's function, based on the recently introduced "intermediate representation" basis [1,2]. We demonstrate that both the complex low-frequency structure, and the high-frequency tails are correctly described.

This sparse sampling can be used for the calculation of dynamic susceptibilities, after inversion of the Bethe-Salpeter equation. We present results in the context of the BEC to BCS crossover [3, 4] in the vicinity of the excitonic condensation in the two-band Hubbard model [5].

[1] H. Shinaoka, J. Otsuki et. al., Phys. Rev. B 96, 035147 (2017)
[2] H. Shinaoka, J. Otsuki et al., Phys. Rev. B 97, 205111 (2018)
[3] B. Zenker, D. Ihle et al., Phys. Rev. B 85, 121102(R) (2012)
[4] J. Kuneš, J. Phys.: Cond. Mat. 27, 333201 (2015)
[5] D. Geffroy, J. Kaufmann et al., arXiv 1808.08046 (2018)

TT 44.2 Wed 15:15 H7

Self-Consistent Ladder Dynamical Vertex Approximation — •Josef Kaufmann[1], Anna Kauch[1], Oleg Janson[1,2], and Karsten Held[1] — [1]Institute for Solid States Physics, TU Wien — [2]IFW Institute for Theoretical Solid State Physics, Dresden

The dynamical vertex approximation (DΓA) is a diagrammatic extension [1] of the dynamical mean-field theory (DMFT). In the so-called ladder-DΓA, one treats the irreducible vertex in the particle-hole channel as completely local and builds nonlocal ladder diagrams from it, which are then used as corrections to the DMFT self-energy. The local vertex is extracted from two-particle Green's functions, calculated by using continuous-time quantum Monte Carlo for an effective Anderson impurity model [2,3].

Traditionally, self-consistency has been mimicked by a so-called λ-correction. In this talk, we go a considerable step beyond and present a self-consistent formulation and solution of the DΓA equations, naturally fulfilling physical constraints, such as the asymptotics of the self-energy. The applicability is demonstrated in calculations for the Hubbard model on a square lattice and on a (geometrically frustrated) Kagome lattice.

[1] G. Rohringer *et al.*, Rev. Mod. Phys. 90, 025003 (2018)
[2] P. Gunacker *et al.*, Phys. Rev. B 92, 155102 (2015)
[3] J. Kaufmann *et al.*, Phys. Rev. B 96, 035114 (2017)

TT 44.3 Wed 15:30 H7

Predicting exact Green functions from perturbative solutions by a neural network — •Patryk Kubiczek and Alexander Lichtenstein — I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany

Green functions are building blocks for a plethora of many-body theories. While in many cases quantum Monte Carlo methods allow for a reliable calculation of Green functions for large interacting systems, they can still be hindered by the sign problem, especially in the real-time formulation. However, it is usually relatively inexpensive to get approximate solutions from a perturbation theory. We propose a new calculation scheme, in which a neural network is trained to predict exact Green functions from complementary perturbative solutions, as long as there exists an efficient method to generate a sufficiently large training set of exact solutions. We employ this scheme as an imaginary-time impurity solver for the dynamical mean field theory (DMFT) for the Hubbard model on a Bethe lattice.

TT 44.4 Wed 15:45 H7

Slave rotor approach to impurity models with ligand orbitals — •Jakob Steinbauer[1] and Silke Biermann[1,2,3] — [1]Ecole Polytechnique, Palaiseau, France — [2]Collège de France, Paris, France — [3]European theoretical spectroscopy facility, Europe

We propose a slave (spin/rotor) method for the solution of many-orbital quantum impurity problems, which maps the original problem with correlated and ligand orbitals onto one with an effective correlated shell only. This is particularly useful for the dynamical mean field theory treatment of transition metal oxides where the interactions between ligand states and d-states are all too often simply neglected. We derive a general formalism relying on an optimized effective model obtained from the variational principle of Feynman and Peierls and apply our method to a minimal 2-band model with orbitals of d and p character.

TT 44.5 Wed 16:00 H7

Fermion-boson vertex within Dynamical Mean-Field Theory — •Erik van Loon[1,2], Friedrich Krien[3,4], Hartmut Hafermann[5], Alexander Lichtenstein[3], and Mikhail Katsnelson[1] — [1]Radboud University, Nijmegen, the Netherlands — [2]University of Bremen, Bremen, Germany — [3]University of Hamburg, Hamburg, Germany — [4]SISSA, Trieste, Italy — [5]Huawei Technologies, Paris, France

In the study of strongly interacting electrons, correlations on the two-particle level are becoming accessible. These correlation functions are generally rather complicated and cumbersome objects that lack a clear physical intuition. In this work, we study a particular two-particle correlation function that does have a clear intuition: the fermion-boson vertex. It describes the response of the Green's function (self-energy) when an external field is applied. As such, it displays interesting behaviour when the metal-insulator transition is approached. We provide several perspectives on this object, including Ward identities, sum rules, analytical continuation, and its role in diagrammatic extensions of Dynamical Mean-Field Theory.

TT 44.6 Wed 16:15 H7

Spektra: An Online Tool for Analytic Continuation — •Khaldoon Ghanem — Max Max Planck Institute for Solid State Research, Stuttgart, Germany

The stochastic sampling method (StochS) is used for the analytic continuation of quantum Monte Carlo data from the imaginary axis to the real one. Due to its lack of explicit parameters and its potential of resolving sharp features, StochS provides a promising alternative to the commonly used maximum entropy method.

In earlier DPG talks, we presented an efficient algorithm of stochastic sampling that reduces the computational cost by orders of magnitude. We also showed that StochS has an implicit default model given by the discretization grid and provided a recipe for choosing this grid. We extended StochS into a gridless method (gStochS) by sampling the grid points from a default model and then extend gStochS to sample over a whole class of default models with different widths (eStochS).

In this talk, we review the aforementioned developments in a unifying framework where stochastic sampling methods are organized as a hierarchy of increasing power and cost. We present a highly-optimized implementation of all three methods: StochS, gStochS and eStochS, and make it accessible through an online interface. The user can simply upload data in a convenient format and submit calculations with few clicks. The computation is done remotely and results are available in seconds/minutes. The interface also facilitates comparing different results in order to apply our recipe for choosing the optimal hyperparameters, if needed.

TT 44.7 Wed 16:30 H7

Quantum Monte Carlo simulation of the chiral Heisenberg Gross-Neveu-Yukawa phase transition with a single Dirac cone — •Thomas C. Lang and Andreas M. Läuchli — University of Innsbruck, Austria

We present quantum Monte Carlo simulations for the chiral Heisenberg Gross-Neveu-Yukawa quantum phase transition of relativistic fermions with $N = 4$ Dirac spinor components subject to a repulsive, local four fermion interaction in 2+1d. Here we employ a two dimensional lattice Hamiltonian with a single, spin-degenerate Dirac cone, which exactly reproduces a linear energy-momentum relation for all finite size lattice momenta in the absence of interactions. This allows us to significantly reduce finite size corrections compared to the widely studied

honeycomb and π-flux lattices. A Hubbard term dynamically generates a mass beyond a critical coupling of $U_c = 6.76(1)$ as the system acquires antiferromagnetic order and SU(2) spin rotational symmetry is spontaneously broken. At the quantum phase transition we extract a self-consistent set of critical exponents $\nu = 0.98(1)$, $\eta_\phi = 0.53(1)$, $\eta_\psi = 0.18(1)$, $\beta = 0.75(1)$. We provide evidence for the continuous degradation of the quasi-particle weight of the fermionic excitations as the critical point is approached from the semimetallic phase. Finally we study the effective "speed of light" of the low-energy relativistic description, which depends on the interaction U, but is expected to be regular across the quantum phase transition. We illustrate that the strongly coupled bosonic and fermionic excitations share a common velocity at the critical point.

TT 44.8 Wed 16:45 H7

Critical energy spectrum of the chiral Ising Gross-Neveu-Yukawa field theory on the torus — •Michael Schuler[1], Stephan Hesselmann[2], Thomas C. Lang[1], Stefan Wessel[2], and Andreas M. Läuchli[1] — [1]Institute for Theoretical Physics, University of Innsbruck, Austria — [2]Institut für Theoretische Festkörperphysik, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany

We investigate the critical torus low-energy spectrum of the chiral Ising universality class with $N = 4$ component Dirac spinors in $2 + 1d$ from the strongly interacting t-V model of spinless fermions, which serves as a universal fingerprint of the associated critical Gross-Neveu-Yukawa field theory. We employ a combination of exact diagonalization and quantum Monte Carlo simulations to compute the critical energy spectra on finite-size clusters and extrapolate them to the thermodynamic limit. We show that the strong interaction between the spinor field and the scalar order-parameter field strongly influences the critical energy levels on the torus. Furthermore, we highlight the effect of different cluster shapes on the critical torus spectrum and illustrate that they can be interpreted by adding non-zero flux around the torus. In addition we estimate the renormalization of the Fermi velocity in the semimetallic (Dirac) phase from the behavior of the energy spectrum and extrapolate the observed linear renormalization to the critical point. Our investigation shows that precise knowledge of the spectrum even on small clusters already provides valuable insight into the properties of critical systems.

15 min. break.

TT 44.9 Wed 17:15 H7

News on tensor network algorithms — •Roman Orus — Donostia International Physics Center (DIPC)

In this talk I will make an overview of recent developments concerning the simulation of quantum lattice systems with tensor networks, focusing on systems in the thermodynamic limit. In particular, I will flash developments concerning: (i) results from infinite-PEPS for different models in the ruby, triangle-honeycomb and star lattices; (ii) a simple PEPS algorithm for arbitrary lattices; (iii) PEPO algorithms for 2d dissipative and finite-temperature systems, and (iv) the implementation of SU(2) symmetry via fusion trees and the study of a chiral Heisenberg ladder.

TT 44.10 Wed 17:30 H7

Tensor network algorithms for simulating real quantum materials — •Augustine Kshetrimayum[1], Matteo Rizzi[2], Roman Orus[3], Bella Lake[4], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Physics Department, Freie Universität Berlin, 14195 Berlin, Germany — [2]Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany — [3]Donostia International Physics Center, Paseo Manuel de Lardizabal 4, E-20018 San Sebastián, Spain — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

In this talk, I will present some results on how tensor network algorithms can be used to simulate real quantum materials. In particular, I will first talk about how PEPS can be used to simulate two-dimensional thermal states based on an annealing mechanism. I will give the examples of the Ising and the Bose Hubbard model on a square lattice. In the second part, I will discuss about the material $Ca_{10}Cr_7O_{28}$ that was recently discovered in the lab to be a quantum spin liquid. We study this material using a variant of PEPS known as the Projected Entangled Simplex State. We show that our numerical results nicely fit with the previously obtained experimental results.

TT 44.11 Wed 17:45 H7

Quantum dynamics via universal quantum gates emulated with matrix product states — •Constantin Meyer[1], Sebastian Paeckel[1], Robert Schade[2], Salvatore R. Manmana[1], and Thomas Köhler[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, Germany — [2]Institut für Theoretische Physik, Technische Universität Clausthal, Germany

As quantum-computation devices are currently under development, but have only a small number of qubits, it is interesting to ask whether one can emulate gate-based quantum computations for certain simple cases using a classical computer. Often, approaches based on exact diagonalizations and a complete representation of the states are used, which severely restrict the number of emulated qubits. Here, we use matrix-product states, which allow for the treatment of significantly more qubits. We implement the time evolution of a many-body Hamiltonian in this setup by formulating the Trotter decomposition via universal gates. The matrix-product operators of these gates are represented as finite-states machines. This allows us to test the reliability of the implemented emulator by comparing time evolutions to exact results.

TT 44.12 Wed 18:00 H7

Simulations in 2D using isometric Projected Entangled Pair States — •Sheng-Hsuan Lin and Frank Pollmann — Department of Physics, T42, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany

Projected Entangled Pair States (PEPS) have been proposed as a generalization of matrix-product states (MPS) to two-dimensional systems. However, numerical algorithms based on PEPS tend to be unstable due to the lack of a proper canonical form. This problem can be addressed by introducing a gauge fixing or constraint on local tensors. In our approach, we consider PEPS consisting of isometric tensors which then allow for efficient simulations. First, we benchmark an algorithm that variationally minimizes the energy within the manifold of isometric tensors by comparing to exact results. Second, we consider real time evolution and focus on dynamical correlations in a quantum spin system.

TT 44.13 Wed 18:15 H7

An fRG library for high performance computing — •Jannis Ehrlich[1,2], Daniel Rohe[3], and Carsten Honerkamp[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The functional renormalization group (fRG) is a versatile tool to investigate different aspects of correlated electron systems, for example the emergence and competition of ordering tendencies and their energy scales. Although the fRG enables an unbiased investigation of correlations without favouring a specific channel in contrast to Bethe-Salpeter equations, numerical implementations of the fRG easily become intricate and require sufficient testing. Hence the fRG has not been as widely used as other numerical schemes for correlated electrons. In order to facilitate an easier application, we present a fRG-library which can be used readily by simply specifying the model for investigation. The calculation of the fRG flow is done inside the fRG-library, which is parallelized by MPI and OpenMP. As a first example, we present the code performance obtained for the 2D Hubbard model with and without the recently developed Truncated Unity formalism. In addition, as a demonstration of the code versatility, we present the phase diagram of the 3D Hubbard model and first results of a Rashba model with Zeeman splitting.

TT 44.14 Wed 18:30 H7

Leading logarithmic approximation to the X-ray-edge model from a single-loop functional renormalization group approach — •Jan Diekmann and Severin Georg Jakobs — Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen

Numerous models for low-dimensional correlated systems (e.g. X-ray-edge model, Kondo model, one-dimensional metals) have logarithmic divergencies in different diagrammatic channels of the four-point function. Then the sum of all parquet diagrams with bare lines contains all leading logarithmic divergencies, cf. Ref. [1]. The functional renormalization group (FRG) in a single-loop truncation does not repro-

duce all parts of all parquet diagrams; recently, it was shown how a multi-loop extension of the FRG can achieve this [2]. However, in this talk we present a (purely Fermionic) single-loop FRG that reproduces identically the leading logarithmic result of Ref. [1] for the four-point function of the X-ray-edge model. Our FRG approximation accounts for the leading contribution of every parquet diagram and is closely related to the parquet approach of Ref. [1]. Indeed, certain technical steps in Ref. [1] can be understood as introducing an RG cut-off and solving the very single-loop FRG flow equation. We expect that our findings can be transferred to other models with logarithmic divergencies.

[1] B. Roulet, J. Gavoret, P. Nozières, Phys. Rev. **178**, 1072 (1969)
[2] F. B. Kugler, J. von Delft, Phys. Rev. Lett. **120**, 057403 (2018)

TT 44.15 Wed 18:45 H7

Learning multiple order parameters with interpretable machines — •Jonas Greitemann, Ke Liu, and Lode Pollet — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München

Machine learning shows promise for studying phase transitions many-body systems. However, most studies are tied to situations involving only one phase transition and one order parameter. Systems that accommodate multiple phases of coexisting and competing orders, which are common in condensed matter physics, remain largely unexplored from a machine learning perspective. We investigate the multiclassification of phases using Support Vector Machines (SVMs) and present a generic protocol for detecting hidden spin and orbital orders to learn multiple phases and their analytical order parameters. Our focus is on multipolar orders and their tensorial order parameters whose analytical form is extracted for tensors up to rank 6. Furthermore, we discuss an intrinsic parameter of SVM, the bias, which allows for a special interpretation in the classification of phases, and its utility in diagnosing the existence of phase transitions. We show that it can be exploited as an efficient way to explore the topology of unknown phase diagrams where the supervision is entirely delegated to the machine.