TT 16: Correlated Electrons: Method Development

Time: Wednesday 9:30–13:15 Location: H10

Invited Talk TT 16.1 Wed 9:30 H10

Multimethod, multimessenger approaches to models of strong correlations — •Thomas Schäfer — Max Planck Research Group "Theory of Strongly Correlated Quantum Matter" (SCQM), Max Planck Institute for Solid State Research, Stuttgart, Germany

The Hubbard model is the paradigmatic model for electronic correlations. In this talk I present a general framework for the reliable calculation of its properties, which we coined multi-method, multi-messenger approach. I will illustrate the power of this approach with three recent studies: (i) an extensive synopsis of arguably all available finite-temperature methods for the half-filled Hubbard model on a simple square lattice in its weak-coupling regime, fully clarifying the impact of spin fluctuations and tracking their footprints on the one- and two-particle level, (ii) a complementary subset of those applied to the Hubbard model on a triangular geometry, exhibiting the intriguing interplay of geometric frustration (magnetism) and strong correlations (Mottness) and (iii) a multi-method study of a model for magnetism in infinite-layer nickelates. These examples may work as a blueprint of similar future studies of strongly correlated systems.

TT 16.2 Wed 10:00 H10

Random phase approximation for gapped systems: Role of vertex corrections and applicability of the constrained random phase approximation — •Erik van Loon[1], Malte Rösner[2], Mikhail Katsnelson[2], and Tim Wehling[3] — [1]Lund University, Lund, Sweden — [2]Radboud University, Nijmegen, the Netherlands — [3]University of Bremen, Bremen, Germany

The many-body theory of interacting electrons poses an intrinsically difficult problem that requires simplifying assumptions. For the determination of electronic screening properties of the Coulomb interaction, the random phase approximation (RPA) provides such a simplification. Here we explicitly show that this approximation is justified for band structures with sizable band gaps. This is when the electronic states responsible for the screening are energetically far away from the Fermi level, which is equivalent to a short electronic propagation length of these states. The RPA contains exactly those diagrams in which the classical Coulomb interaction covers all distances, whereas neglected vertex corrections involve quantum tunneling through the barrier formed by the band gap. Our analysis of electron-electron interactions provides a real-space analogy to Migdal's theorem on the smallness of vertex corrections in electron-phonon problems. An important application is the increasing use of constrained RPA calculations of effective interactions. We find that their usage of Kohn-Sham energies accounts for the leading local (excitonic) vertex correction in insulators.

TT 16.3 Wed 10:15 H10

Consistency of potential energy in the diagrammatic vertex approximation — •Julian Stobbe and Georg Rohringer — Institute of Theoretical Physic, University of Hamburg, 20355 Hamburg, Germany

In the last decades, dynamical mean field theory (DMFT) and its diagrammatic extensions have been successfully applied to describe local and nonlocal correlation effects in correlated electron systems. Unfortunately, both of them suffer from intrinsic inconsistencies which lead to a violation of the Pauli principle (and related sum rules) as well as the conservation laws of the system. This limits the predictive power of these approaches as fundamental observables such as the kinetic and/or potential energies are not unambiguously defined. Here, we will discuss an approach to overcome the ambiguity in the calculation of the potential energy within the ladder dynamical vertex approximation (DΓA) by introducing an effective mass renormalization parameter in both the charge and the spin susceptibility of the system. The applicability of the method is then demonstrated on the half filled single-band Hubbard model on a three-dimensional cubic lattice. Furthermore, the solution method will be discussed, since the new method requires careful consideration of finite approximation of infinite Matsubara sums.

TT 16.4 Wed 10:30 H10

Vertex divergences in the Anderson impurity model - From real to imaginary frequencies — •Michael Meixner[1], Johannes Halbinger[2], Seung-Sup Lee[3], Fabian Kugler[4], Patrick Chalupa-Gantner[5], Alessandro Toschi[5], Jan von Delft[2], and Thomas Schäfer[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Munich, Germany — [3]Department of Physics and Astronomy, National University, Seoul, South Korea — [4]Department of Physics and Astronomy, Rutgers University, Piscataway, NJ, USA — [5]Institute for Solid State Physics, TU Wien, Vienna, Austria

Generalized susceptibilities not only are at the heart of calculating momentum- and frequency-dependent response functions, but can also provide direct physical insights into local magnetic moment formation and Kondo screening. In particular, recent literature has investigated the implications of divergences of the irreducible vertex function on the Matsubara axis in the charge and particle-particle channels on the physics of the Anderson impurity model. In this study we examine the divergent properties of the two-particle irreducible vertex function in the Anderson impurity model employing the numerical renormalization group (NRG). In a first step data is benchmarked against state of the art results from continuous-time quantum Monte Carlo on the imaginary frequency axis. In a second step NRG allows us to access not only imaginary frequencies but also real frequencies via the Keldysh contour at very low temperatures and without analytic continuation.

TT 16.5 Wed 10:45 H10

Exact continuum representation of long-range interacting systems — •Andreas Alexander Buchheit[1], Torsten Kessler[1], Peter Schuhmacher[2], and Benedikt Fauseweh[2] — [1]Saarland University, 66123 Saarbrücken, Germany — [2]German Aerospace Center (DLR), 51147 Cologne, Germany

Continuum limits are a powerful tool in the study of many-body systems, yet their validity is often unclear when long-range interactions are present. In this work, we rigorously address this issue and put forth an exact representation of long-range interacting lattices that separates the model into a term describing its continuous analogue, the integral contribution, and a term that fully resolves the microstructure, the lattice contribution. For any system dimension, any lattice, any power-law interaction and for linear, nonlinear, and multi-atomic lattices, we show that the lattice contribution can be described by a differential operator based on the multidimensional generalization of the Riemann zeta function, namely the Epstein zeta function. Our representation provides a broad set of tools for studying the analytical properties of the system and it yields an efficient numerical method for the evaluation of the arising lattice sums. We benchmark its performance by computing classical forces and energies in three important physical examples, in which the standard continuum approximation fails: Skyrmions, defects in ion chains, and spin waves in a pyrochlore lattice with dipolar interactions. We demonstrate that our method exhibits the accuracy of exact summation at the numerical cost of an integral approximation.

TT 16.6 Wed 11:00 H10

Exotic phases in long-range interacting quantum lattices — Andreas A. Buchheit[1], •Torsten Kessler[1], Peter K. Schuhmacher[2], and Benedikt Fauseweh[2] — [1]Saarland University, Saarbrücken, Germany — [2]German Aerospace Center (DLR), Cologne, Germany

We provide a rigorous analysis of the effects of power-law long-range interactions on the phase diagram of a multi-dimensional quantum spin lattice. Starting from the discrete Hamiltonian, we use the recently developed singular Euler-Maclaurin expansion and derive an exact and parameter-free field theory that fully captures the effects due to the inherent discreteness of the lattice. For any lattice and any system dimension, we derive analytic expressions for the phase boundaries to ferromagnetic and anti-ferromagnetic phases and outline their dependence on the exponent of the power-law interaction and of the system dimension.

TT 16.7 Wed 11:15 H10

SU(2)-symmetric tensor network study of the classical Heisenberg model — •Philipp Schmoll[1], Augustine Kshetrimayum[1,2], Jens Eisert[1,2], Roman Orus[3,4,5], and Matteo

Rizzi[6,7] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Helmholtz Center Berlin, 14109 Berlin, Germany — [3]Donostia International Physics Center, E-20018 San Sebastián, Spain — [4]Ikerbasque Foundation for Science, E-48013 Bilbao, Spain — [5]Multiverse Computing, E-20014 San Sebastián, Spain — [6]Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), 52425 Jülich, Germany — [7]Institute for Theoretical Physics, University of Cologne, D-50937 Köln, Germany

The classical Heisenberg model in two spatial dimensions constitutes one of the most paradigmatic spin models, taking an important role in statistical and condensed matter physics to understand magnetism. Despite its paradigmatic character controversies remain whether the model exhibits a phase transition at finite temperature. In this work, we make use of state-of-the-art tensor network approaches, representing the classical partition function in the thermodynamic limit over a large range of temperatures. By implementing an SU(2) symmetry in our tensor network, we are able to handle very large bond dimensions, which is crucial in detecting phase transitions. With decreasing temperatures, we find a rapidly diverging correlation length, whose behaviour is apparently compatible with the two main contradictory hypotheses known in the literature, namely a finite-T transition and asymptotic freedom, though with a slight preference for the second.

15 min. break

TT 16.8 Wed 11:45 H10

Matrix-product-state-based band-Lanczos solver for quantum cluster approaches — Sebastian Paeckel[1,2], Thomas Köhler[3], Salvatore R. Manmana[4], and •Benjamin Lenz[5] — [1]Arnold Sommerfeld Center of Theoretical Physics, University of Munich, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany — [3]Department of Physics and Astronomy, Uppsala University, Sweden — [4]Institute for Theoretical Physics, Georg August University of Göttingen, Germany — [5]Institut de minéralogie, de physique des matériaux et de cosmochimie (IMPMC), Sorbonne University, Paris, France

We present a matrix-product-states-based band-Lanczos method as a solver for quantum cluster techniques. Based on a traditional band-Lanczos technique for the calculation of the cluster Green's function, we introduce and motivate different convergence criteria and discuss their impact on the stability of the results at the example of the variational cluster approximation. The capabilities of this method to calculate the self-energy functional are demonstrated for Hubbard-like models on different cluster geometries. Finally, we show a finite-size scaling of order parameters using cluster sizes, which are out of reach for traditional exact-diagonalization-based solvers.

TT 16.9 Wed 12:00 H10

Hierarchical equations of motion approach to open quantum system dynamics: Matrix product state formulation in twin space — •Yaling Ke[1], Raffaele Borrelli[2], and Michael Thoss[1] — [1]Institute of Physics, Albert-Ludwig University Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany — [2]DISAFA, Università di Torino, I-10095 Grugliasco, Italy

The hierarchical equations of motion (HEOM) approach is a numerically exact method to study the dynamics of open quantum systems with non-perturbative system-environment interaction and non-Markovian memory at finite temperatures. Although considerable progress has been made over the past few decades to extend the applicability of the HEOM approach, the numerical cost is still very expensive for reasonably large systems.

In this contribution, we present the twin-space formulation of the HEOM approach in combination with the matrix product state representation for open quantum systems coupled to a hybrid fermionic and bosonic environment. The key ideas of the approach are a reformulation of a set of differential equations for the auxiliary density matrices into a time-dependent Schrödinger-like equation for an augmented multi-dimensional wave function as well as its tensor decomposition into a product of low-rank matrices. The new approach facilitates accurate simulations of non-equilibrium quantum dynamics in larger and more complex open quantum systems with both factorized and correlated initial conditions.

TT 16.10 Wed 12:15 H10

Single-boson-exchange-fRG application to the two-dimensional Hubbard model at weak coupling — Sarah Heinzelmann[1], Kilian Fraboulet[1], Pietro Bonetti[2], Aiman Al-Eryani[1], Demetrio Vilardi[2], •Alessandro Toschi[3], and Sabine Andergassen[1] — [1]Eberhard Karls Universität Tübingen — [2]Max Planck Institut Stuttgart — [3]Technische Universität Wien

We illustrate the computational advantages of the recently introduced single-boson exchange (SBE) formulation for the one-loop functional renormalization group (fRG) applied to the two-dimensional Hubbard model. We present a detailed analysis of the physical susceptibilities and their evolution with temperature and interaction strength, both at half filling and finite doping. We find that the rest functions describing the corrections beyond the SBE contributions play a negligible role in the weak coupling regime. The SBE formulation of the fRG flow hence allows for a substantial reduction of the numerical effort in the treatment of the two-particle vertex function, paving a promising route for future multiboson and multiloop extensions.

TT 16.11 Wed 12:30 H10

Connecting real- and imaginary-frequency axis for two-particle many-body propagators — •Selina Dirnböck[1], Sebastian Huber[1], Seung-Sup Lee[2,3], Fabian Kugler[4], Jan von Delft[3], Karsten Held[1], and Markus Wallerberger[1] — [1]TU Wien, Austria — [2]Seoul National University, South Korea — [3]Ludwig-Maximilians-Universität München, Germany — [4]Rutgers University, New Jersey, USA

Two-particle response functions are a centerpiece of quantum many-body physics, relating both to experiment, where they can be observed as susceptibilities, and to theory, where they form the basis of advanced self-consistent field theories. Yet, due to their size and complex structure, they are challenging to handle numerically.

Recently, two advances have been made to tackle this problem: firstly, the intermediate representation together with an overcomplete basis (IR+OB), which provides a highly efficient compression of propagators in imaginary frequency, and secondly, partial spectral functions (PSFs), which allow for the efficient evaluation in real frequency, by, for example, using the numerical renormalization group (NRG).

In this talk, we connect these two approaches: we show that the IR+OB and PSFs are intimately connected. We also show that the two-particle propagator obtained from NRG/PSFs on the real-frequency axis can be compressed efficiently using IR+OB on imaginary-frequency axis, reducing the memory demand by more than three orders of magnitude. Finally, we use the guidance from PSFs to develop a physical regularization scheme for the IR+OB.

TT 16.12 Wed 12:45 H10

Trie-based ranking of quantum many-body states — •Markus Wallerberger and Karsten Held — TU Wien, Vienna, Austria

Ranking bit patterns – finding the index of a given pattern in an ordered sequence – is a major bottleneck scaling up numerical quantum many-body calculations, as fermionic and hard-core bosonic states translate naturally to bit patterns. Traditionally, ranking is done by bisectioning search, which has poor cache performance on modern machines.

We instead propose to use tries (prefix trees), thereby achieving a two- to ten-fold speed-up in numerical experiments with only moderate memory overhead. For the important problem of ranking permutations, the corresponding tries can be compressed. These compressed "staggered" lookups allow for an additional speed-up while retaining the memory requirements of prior algorithms based on the combinatorial number system.

We use these improvements to go to larger system sizes for which three-and four-point propagators can be computed.

TT 16.13 Wed 13:00 H10

Tetranacci polynomials in solid state phyics — •Nico Leumer — IPCMS, CNRS, Strasbourg

In mesoscopic physics, state of the art theoretical research relies not solely but to large extend on numerical investigations. Naturally, support from analytical side is important whenever possible, in particular to appeal physical intuition. For the first time, I will introduce to a broader audience so called Tetranacci polynomials, which offer a generic technique to analytic diagonalize a variety of model Hamiltonians for finite system size and when open/free boundary conditions are imposed. As perspective, this approach is applicable on discrete physical (sub-) systems owing at least two degrees of freedom per atom, such as the Kitaev chain or the 1d Rashba-nanowire in magnetic field positioned on superconducting substrate. The use extends

further to the famous Su-Schrieffer-Heeger model or to topological trivial tight-binding chains having nearest and next nearest neighbor hopping. In my presentation, I elaborate that Tetranacci polynomials extend Bloch's theorem and how they are related to eigenvectors and eigenvalues. Within the frame drawn by the illustrative example of the X-Y-chain in transverse magnetic field, I demonstrate how previous diagonalization approaches are recovered by the more general Tetranacci technique. The final part of my presentation is devoted to an overview of physically distinct systems hosting Tetranacci polynomials and their common spectral features overlooked in earlier studies.

[1] N. Leumer et al., J. Condens. Matter Phys. 32 445502 (2020)
[2] N. Leumer et al., Phys. Rev. B 103, 165432 (2021)