TT 5: Correlated Electrons: Method Development

Time: Monday 9:30–13:15 Location: HSZ 204

TT 5.1 Mon 9:30 HSZ 204

Generalized Bogoliubov-Hartree-Fock theory for the Hubbard model — •Chris Koschenz[1] and Carsten Timm[1,2] — [1]Institute of Theoretical Physics, TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

We present the phase diagram of the Hubbard model on the square lattice up to a four-site unit cell derived via a generalized Bogoliubov-Hartree-Fock theory. Our approach allows to study magnetic ordering, charge ordering, and superconductivity on the same footing and gives additional information about the so-called mixed phases [1]. These phases emerge in parameter ranges where the system is potentially strongly affected by fluctuations and cannot be described by any set of usual Hartree-Fock states (Slater determinants) [1,2]. Furthermore, we show how to obtain the self-consistent set of order parameters by straightforward unrestricted global minimization of the appropriate Landau functional [3]. This method allows us to study the coexistence and competition of various magnetic orders and can be used to study the possibility of additional phase transitions in the coexistence regime. [1] E. Langmann and M. Wallin, J. Stat. Phys. **127**, 825 (2007) [2] V. Bach *et al.*, J. Stat. Phys. **76**, 3 (1994) [3] R. Agra *et al.*, Eur. J. Phys. **27**, 407 (2006)

TT 5.2 Mon 9:45 HSZ 204

Competing instabilities with fRG in highly symmetric triangular lattice Hubbard models — •Hannes Braun — Max Planck Institute for Solid State Research

Motivated by, e.g., simulations via cold atomic gases and twisted multilayer transition metal dichalcogenides, we consider Hubbard models with SU(N)*SU(M) symmetry. Such highly symmetric systems with additional degrees of freedom offer possibilities for novel types of symmetry-broken phases and their competition. To analyse the competing correlated phases of the resulting Hubbard models, we generalise the functional Renormalization Group (fRG) approach for correlated fermionic systems to efficiently incorporate the high symmetries. The truncated unity fRG provides us with unbiased fluctuation diagnostics and allows us to analyse the interplay between charge, spin, and pairing instabilities on equal footing. We present the new set of SU(N)*SU(M)-symmetric fRG equations and first results for the two-dimensional Hubbard model on the triangular lattice.

TT 5.3 Mon 10:00 HSZ 204

Functional renormalization group without functional integrals — Peter Kopietz, Rüdiger Krämer, and •Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

We show that exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within a Hamiltonian operator formalism without using functional integrals. This can be useful for teaching FRG methods to students unfamiliar with functional integrals and also opens new possibilities for applying FRG methods to quantum systems with projected Hilbert spaces such as quantum spin models or strongly interacting fermionic lattice models. In particular, by representing the Hubbard model and the $t-J$-model in terms of so-called Hubbard X-operators we construct a new strong-coupling FRG approach to these models.

TT 5.4 Mon 10:15 HSZ 204

Reduced basis modeling of quantum spin systems based on DMRG — •Paul Brehmer[1], Michael Herbst[2], Matteo Rizzi[3,4], Benjamin Stamm[5], and Stefan Wessel[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Applied and Computational Mathematics, RWTH Aachen University, 52062 Aachen, Germany — [3]FZ Jülich GmbH, Institute of Quantum Control, Peter Grünberg Institut (PGI-8), 52425 Jülich, Germany — [4]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany — [5]Institute of Applied Analysis and Numerical Simulation, University of Stuttgart, 70569 Stuttgart, Germany

Within the reduced basis modeling approach, an effective low-dimensional subspace of a quantum many-body Hilbert space is constructed in order to investigate, e.g., the ground-state phase diagram. The basis of this subspace is built from solutions of snapshots, i.e., ground states corresponding to particular and well-chosen parameter values. Here, we show how a greedy strategy to assemble the reduced basis and thus to select the parameter points can be implemented based on density-matrix-renormalization-group (DMRG) calculations. Once the reduced basis is computed, observables required for the computation of phase diagrams can be computed with a computational complexity independent of the underlying Hilbert space for any parameter value. We illustrate the efficiency and accuracy of this approach for different one-dimensional quantum spin-S models with both $S = 1/2$ and $S = 1$, including anisotropic as well as biquadratic exchange interactions, leading to rich quantum phase diagrams.

TT 5.5 Mon 10:30 HSZ 204

Novel degrees of freedom in cluster Mott insulators — •Vaishnavi Jayakumar and Ciarán Hickey — Institute for Theoretical Physics, University of Cologne, Germany

The Hubbard model provides a playground for investigating the physics of a wide range of strongly correlated systems. An important feature of these systems is the Mott insulating phase, where at half-filling, an electron gets localised on a single lattice site. In this work, we study cluster Mott insulators – where electrons are now localised on clusters of sites. To that end, we study an extended Hubbard-Kanamori model on a plethora of clusters with multiple orbitals per site, at different electron fillings. We then explore different regimes of interplay between strong correlations and hopping within these clusters, and the effective degrees of freedom that emerge. It is seen, for example, that high ground-state degeneracies are possible that are due to a combination of both spatial and orbital symmetries. We further include crystal field splitting and spin-orbit coupling to bring our model closer to real materials. Once a blueprint for these building blocks has been established, the clusters can be connected through inter-cluster terms, giving rise to potentially novel Hamiltonians.

TT 5.6 Mon 10:45 HSZ 204

Numerical linked cluster expansions for the ordered low-field phase of the transverse-field Ising model — •Matthias Mühlhauser, Max Hörmann, and Kai Phillip Schmidt — Institute for Theoretical Physics I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We present a hypergraph approach to numerical linked cluster expansions (NLCEs) in the low-field limit of the transverse-field Ising model (TFIM) where the Z2-Symmetry of the TFIM is spontaneously broken and the ground state is magnetically ordered.

Conventional NLCEs in this limit are performed as site expansions where the magnetic order of the ground state is taken into account by longitudinal boundary fields on the graphs.

Here, using an isospectral dual description of the TFIM where the ordered phase is mapped to an effective (symmetry unbroken) polarized phase in the dual desciption, we demonstrate that a straightforward hypergraph expansion can be executed so that no boundary fields are necessary. This allows us to obtain competitive results for the ground-state energy of the ordered low-field phase of the TFIM.

TT 5.7 Mon 11:00 HSZ 204

Projective cluster-additve block-diagonalisation method — •Max Hörmann and Kai Phillip Schmidt — Institut für Theoretische Physik I, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen

We present an efficient block-diagonalisation method that only relies on the lowest eigenvectors and eigenvalues and allows for a linked-cluster expansion. The method is applied to a low-field expansion of the transverse-field Ising model on the square lattice. Both the single spin-flip and bound-state dispersion is calculated perturbatively and non-perturbatively. The origin of the breakdown of the non-perturbative linked-cluster expansion for the bound-state dispersion at a critical field value is discussed and potential solutions to overcome this problem are examined.

15 min. break

TT 5.8 Mon 11:30 HSZ 204

Series expansions with multiple quasi-particle types for the

dual Dicke-Ising model — •Andreas Schellenberger, Lea Lenke, and Kai Phillip Schmidt — FAU Erlangen-Nürnberg, Erlangen, Deutschland

The established approach of perturbative continuous unitary transformations (pCUT) constructs effective quantum many-body Hamiltonians in a perturbative series that conserve the number of one quasi-particle type. We extend the pCUT method to similarity transformations – dubbed pcst^{++} – allowing for multiple quasi-particle-types with complex-valued energies. This enlarges the field of application to closed and open quantum many-body systems with unperturbed operators corresponding to arbitrary superimposed ladder spectra. To illustrate the new possibility of the pcst^{++} method to specifically tackle interacting light-matter systems, we discuss the dual Dicke-Ising model. We determine low-energy spectral properties and investigate potential conversion processes between different quasi-particle types.

TT 5.9 Mon 11:45 HSZ 204

Series expansions in open and non-Hermitian quantum many-body systems with multiple quasi-particle types — •Lea Lenke, Andreas Schellenberger, and Kai Phillip Schmidt — FAU Erlangen-Nürnberg

The established approach of perturbative continuous unitary transformations (pCUT) constructs effective quantum many-body Hamiltonians in a perturbative series that conserve the number of one quasi-particle type. We extend the pCUT method to similarity transformations – dubbed pcut^{++} – allowing for multiple quasi-particle-types with complex-valued energies. This enlarges the field of application to closed and open quantum many-body systems with unperturbed operators corresponding to arbitrary superimposed ladder spectra. To this end a generalized counting operator is combined with the quasi-particle generator for open quantum systems recently introduced by Schmiedinghoff and Uhrig [1]. The pcut^{++} then yields model-independent quasi-particle conserving effective Hamiltonians and Lindbladians allowing a linked-cluster expansion similar to the conventional pCUT method. We illustrate the application of the pcut^{++} method by discussing representative open and non-Hermitian quantum systems. [1] G. Schmiedinghoff and G. S. Uhrig, arXiv:2203.15532 [cond-mat.quant-ph].

TT 5.10 Mon 12:00 HSZ 204

Multi-scale space-time ansatz for correlation functions of quantum systems — •Hiroshi Shinaoka[1], Markus Wallerberger[2], Yuta Murakami[3], Kosuke Nogaki[4], Rihito Sakurai[1], Philipp Werner[5], and Anna Kauch[2] — [1]Department of Physics, Saitama University, Saitama 338-8570, Japan — [2]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [3]Center for Emergent Matter Science, RIKEN, Wako, Saitama 351-0198, Japan — [4]Department of Physics, Kyoto University, Kyoto 606-8502, Japan — [5]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland

Correlation functions of quantum systems are central objects in quantum field theories, which may be defined in high-dimensional space-time domains. The numerical treatment of these objects suffers from the curse of dimensionality, which hinders the application of sophisticated many-body theories to interesting problems.

In this talk, we propose a quantum-algorithms-inspired Multi-Scale Space-Time Ansatz (MSSTA) for correlation functions of quantum systems [1]. The space-time dependence is mapped to auxiliary qubit (S = 1/2 spin) degrees of freedom describing exponentially different length scales, and the ansatz assumes a separation of length scales. We numerically verify the ansatz for various equilibrium and nonequilibrium systems and show essential building blocks of diagrammatic equations, such as convolutions or Fourier transforms are formulated in the compressed form using tensor networks.

[1] H. Shinaoka et al., arXiv:2210.12984v2

TT 5.11 Mon 12:15 HSZ 204

Efficient flow equations for dissipative systems — •Gary Schmiedinghoff and Götz S. Uhrig — Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Open quantum systems provide an essential theoretical basis for the development of novel quantum technologies, since any real quantum system inevitably interacts with its environment. Lindblad master equations capture the effect of Markovian environments. Closed quantum systems can be treated using flow equations with the particle conserving generator. We generalize this generator to non-Hermitian matrices and open quantum systems governed by Lindbladians, comparing our results with recently proposed generators by Rosso et al. In comparison, we find that our advocated generator provides an efficient flow with good accuracy in spite of truncations.

TT 5.12 Mon 12:30 HSZ 204

Dynamical mean-field study of a photon-mediated ferroelectric phase transition — •Katharina Lenk[1], Jiajun Li[2,3], Philipp Werner[2], and Martin Eckstein[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, 22607 Hamburg — [2]Department of Physics, University of Fribourg, 1700 Fribourg Switzerland — [3]Paul Scherrer Institute, Condensed Matter Theory, PSI Villigen, Switzerland

The interplay of light and matter gives rise to intriguing cooperative effects in quantum many-body systems. This is even true in thermal equilibrium, where the electromagnetic field can hybridize with collective modes of matter, and virtual photons can induce interactions in the solid. Here, we treat these light-mediated interactions using dynamical mean-field theory. We consider a minimal model of a two-dimensional material that couples to a surface plasmon polariton mode of a metal-dielectric interface. Within the mean-field approximation, the system exhibits a ferroelectric phase transition that is unaffected by the light-matter coupling. Bosonic dynamical mean-field theory provides a more accurate description and reveals that the photon-mediated interactions enhance the ferroelectric order and stabilize the ferroelectric phase.

TT 5.13 Mon 12:45 HSZ 204

Energy correlations of excited states in localization landscape theory — •Torsten Weber, Johannes Dieplinger, Christoph Forster, Lucas Resch, Ferdinand Evers, and Klaus Richter — Universität Regensburg, Regensburg, Deutschland

The localization landscape method, first described in [1], is a method that enables the prediction of the localization regions of eigenfunctions of a localized system. Additionally, the method gives a prediction of the energy of low-lying localized eigenfunctions by defining an effective potential from the landscape function [2]. This energy prediction, although providing good results for low energy eigenfunctions, ceases to work for higher energy states. Studying the method for a one-dimensional disordered system we observe a characteristic form of the ratio of the predicted eigenvalue by the landscape method and the actual eigenvalue for this region of the spectrum. We provide a possible explanation for this behaviour by extending the method leading to the energy prediction by including excited states of the effective potential. By harnessing the universal technique of quantifying excited states by counting nodes we observe a correspondence of the n-th excited states with the n-th repetition of a substructure of the characteristic behaviour described above. We go further to also find an analytic estimate for the structures.

[1] M. Filoche and S. Mayboroda, PNAS 109, 14761 (2012)
[2] D. N. Arnold et al., SIAM Journal on Scientific Computing, 41(1) (2019)

TT 5.14 Mon 13:00 HSZ 204

Extended quasiparticle Padé approximation for non-Fermi liquids — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

The extended quasiparticle picture is adapted to non-Fermi systems by suggesting a Padé approximation which interpolates between the known small scattering-rate expansion and the deviation from the Fermi energy. The first two energy-weighted sum rules are shown to be fulfilled independent of the interpolating function. For various models of one-dimensional Fermions scattering with impurities the quality of the Padé approximation for the spectral function is demonstrated and the reduced density matrix or momentum distribution is shown to be reproduced not possessing a jump at the Fermi energy. Though the two-fold expansion is necessary to reproduce the spectral function and reduced density it is shown that for the description of transport properties the extended quasiparticle approximation is sufficient. The T-matrix approximation leads to the delay time as the time two particles spend in a correlated state. This contributes to the reduced density matrix and to an additional part in the conductivity which is presented at zero and finite temperatures. Besides a localization at certain impurity concentrations, the conductivity shows a maximum at small temperatures interpreted as onset of superconducting behaviour

triggered by impurities. The Tan contact reveals the same universal behaviour as known from electron-electron scattering.

[1] arXiv:2208.11971