TT 91: Correlated Electrons: Method Development

Time: Thursday 15:00–18:15 Location: H 0104

TT 91.1 Thu 15:00 H 0104

Changes in fRG critical scales due to frequency-dependence in a two-patch model — •Timo Reckling and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany

The frequency dependence of the running interactions has become an object of interest in various recent implementations of the functional Renormalization Group (fRG) for low-dimensional fermionic lattice models. In order to understand the main effects and to set up a simpler testbed for approximations, we study a two-patch g-ology model. We analyze the influence of the frequency dependence of the effective two-particle interaction on the critical scales of the flows to strong coupling. To this end the effective interaction which is generated in the fRG flow is parametrized by four interaction components $g_{1,2,3,4}$ each of which depend on three 3 fermionic Matsubara frequencies. Reducing this dependence on three frequencies defines various approximations, with the static approximation as the most drastic one. We can also switch the frequency dependence on and off in different channels which contain distinct loop contributions on the right hand side of the fRG flow equations. This allows us to gain constructive insight into how the frequency-(in)dependent multi-channel interplay determines the critical scales for ordering instabilities.

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TT 91.2 Thu 15:15 H 0104

Full frequency and momentum parametrization of the two-particle vertex in functional RG for fermionic lattice models — •Cornelia Hille[1], Agnese Tagliavini[1,2], Alessandro Toschi[2], Sabine Andergassen[1], and Carsten Honerkamp[3] — [1]Universität Tübingen, Tübingen, Deutschland — [2]Technische Universität Wien, Wien, Österreich — [3]RWTH Aachen, Aachen, Deutschland

The functional renormalization group (fRG) provides an unbiased method to investigate competing instabilities in fermionic lattice models. So far fRG applications succeeded in describing the qualitative phase diagrams for the perturbative coupling regime of various classes of one-band and multi-band models. However, quantitative predictions, e.g. about energy scales or susceptibilities, were not truly controlled because the full parameter dependence of the two-particle vertex had to be simplified for the sake of numerical feasibility, mostly by disregarding the frequency dependence of the vertex which rendered the selfenergy hard to include. Here we show how combining the vertex parametrization guided by the high frequency asymptotics and the expansion of the momentum dependences in terms of form factors results in a significant improvement of the implementation. By including the selfenergy and the susceptibility flow, we can directly compute physical observables that stand the comparison with other methods. With our unbiased implementation, we can systematically investigate the corrections to previous fRG approximations in the 2D-Hubbard model.

TT 91.3 Thu 15:30 H 0104

Phase transitions with a fully consistent second order functional renormalization group scheme — •Lisa Markhof[1], Björn Sbierski[2], Volker Meden[1], and Christoph Karrasch[2] — [1]Inst. for Theory of Stat. Phys., RWTH Aachen, Germany — [2]Dept. of Phys., FU Berlin, Germany

The functional renormalization group (fRG) is a versatile tool to tackle interacting many-body systems [1]. Recently, starting from the generic flow equations, the "extended coupled-ladder approximation" (eCLA) for specific models has been developed which is exact up to second order in the interaction [2,3], while still being feasible from a computational point of view. We here employ this scheme to study phase transitions in models of spinless fermions. Using a channel decomposition and exploiting the structure of the bare interaction, all second order terms can be included while keeping the number of flow equations managable. In contrast to other fRG schemes used earlier to investigate phase transitions [1], the self-energy feedback is fully contained as well. It is furthermore possible to incorporate a feedback of the vertex flow. In this approximation, the fRG captures phase transitions in one-dimensional tight-binding chains at half filling, which are inaccessible to a lowest order fRG scheme. We apply the eCLA to models in real space; a similar approach has been used in [4] in momentum space.

[1] W. Metzner et al., Rev. Mod. Phys. **84**, 299 (2012)
[2] F. Bauer et al., Phys. Rev. B **89**, 045128 (2014)
[3] L. Weidinger et al., Phys. Rev. B **95**, 035122 (2017)
[4] S. Sbierski and C. Karrasch, arXiv:1710.06373

TT 91.4 Thu 15:45 H 0104

Truncated unity functional renormalization group for multiband systems with spin-orbit coupling — •Giulio Schober[1], Jannis Ehrlich[1,2], Timo Reckling[1], and Carsten Honerkamp[1] — [1]RWTH Aachen University, Aachen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Although the functional renormalization group (fRG) is by now a well-established method for investigating correlated electron systems, it is still undergoing significant technical and conceptual improvements. In particular, the motivation to optimally exploit the parallelism of modern computing platforms has recently lead to the development of the "truncated unity" functional renormalization group (TU-fRG). Here, we review this fRG variant, and we provide its extension to multiband systems with spin-orbit coupling. Furthermore, we discuss some aspects of the implementation and outline opportunities and challenges ahead for predicting the ground state ordering and emergent energy scales for a wide class of quantum materials.

TT 91.5 Thu 16:00 H 0104

Charge dynamics of the antiferromagnetically ordered Mott insulator — •Xing-Jie Han[1], Yu Liu[2,3], Zhi-Yuan Liu[4], Xin Li[1], Jing Chen[1], Hai-Jun Liao[1], Zhi-Yuan Xie[5], B Normand[5], and Tao Xiang[1,6] — [1]Institute of Physics, Chinese Academy of Sciences — [2]LCP, Institute of Applied Physics and Computational Mathematics, Beijing — [3]Software Center for High Performance Numerical Simulation, Chinese Academy of Engineering Physics — [4]Institute of Theoretical Physics, Chinese Academy of Sciences — [5]Department of Physics, Renmin University of China — [6]Collaborative Innovation Center of Quantum Matter, Beijing

We introduce a slave-fermion formulation in which to study the charge dynamics of the half-filled Hubbard model on the square lattice. In this description, the charge degrees of freedom are represented by fermionic holons and doublons and the Mott-insulating characteristics of the ground state are the consequence of holon-doublon bound-state formation. The bosonic spin degrees of freedom are described by the antiferromagnetic Heisenberg model. Within this framework and in the self-consistent Born approximation, we perform systematic calculations of the average double occupancy, the electronic density of states, the spectral function and the optical conductivity. Qualitatively, our method reproduces the lower and upper Hubbard bands, the spectral-weight transfer into a coherent quasiparticle band at their lower edges and the renormalisation of the Mott gap, which is associated with holon-doublon binding, due to the interactions of both quasiparticle species with the magnons.

TT 91.6 Thu 16:15 H 0104

Efficient Bethe-Salpeter equations' inversion in dynamical mean-field theory — •Agnese Tagliavini[1,3], Stefan Hummel[2], Nils Wentzell[5], Sabine Andergassen[3], Alessandro Toschi[4], and Georg Rohringer[1] — [1]Institute for Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Physics of Nanostructured Materials, Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [3]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [4]Russian Quantum Center, 143025 Skolkovo, Russia — [5]Institut de Physique Théorique (IPhT), CEA, CNRS, 91191 Gif-sur-Yvette, France

Quantum many-body calculations of two-particle Greens' and vertex functions represent a very important, but also highly demanding task. Hence, a particular effort has been recently devoted to develop novel algorithmic procedures aimed at saving both memory and computational time. In this talk, we present two efficient and numerically stable asymptotic-based algorithms designed to correctly determine the local two-particle irreducible vertex in all scattering channels by means of

the inversion of the corresponding Bethe-Salpeter equations. The latter operation is, in fact, a fundamental step in diagrammatic extensions of DMFT like the Dynamical Vertex Approximation (DΓA). The two algorithms have been tested, and critically compared, for the single-band 3D Hubbard model in the vicinity of the Mott transition, where the asymptotic structures of the vertex functions become dominant.

TT 91.7 Thu 16:30 H 0104

Fractional quantum Hall effect in the interacting Hofstadter model via tensor networks — Matthias Gerster[1], •Matteo Rizzi[2], Pietro Silvi[1,3], Marcello Dalmonte[4], and Simone Montangero[1,5,6] — [1]ICQS & IQST, Ulm University, Germany — [2]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [3]Institute for Theoretical Physics, University of Innsbruck, Austria — [4]Abdus Salam ICTP, Trieste, Italy — [5]Theoretische Physik, Universität des Saarlandes, Saarbrücken, Germany — [6]Dipartimento di Fisica e Astronomia, Università di Padova, Italy

We show via tensor network methods that the Harper-Hofstadter Hamiltonian for hard-core bosons on a square geometry supports a topological phase realizing the $\nu - 1/2$ fractional quantum Hall (FQH) effect on the lattice. We address the robustness of the ground-state degeneracy and of the energy gap, measure the many-body Chern number, and characterize the system using Green functions, showing that they decay algebraically at the edges of open geometries, indicating the presence of gapless edge modes. Moreover, we estimate the topological entanglement entropy by taking a combination of lattice bipartitions that reproduces the topological structure of the original proposals by Kitaev and Preskill, and Levin and Wen. The numerical results show that the topological contribution is compatible with the expected value $\gamma = 1/2$. Our results provide extensive evidence that FQH states are within reach of state-of-the-art cold-atom experiments.

[1] Gerster *et al.*, Phys. Rev. B **96**, 195123 (2017)

15 min. break.

TT 91.8 Thu 17:00 H 0104

Identifying the pairing mechanism in strontium ruthenate via renormalization — •Mario Fink and Ronny Thomale — Institut für Theoretische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The superconducting state of strontium ruthenate Sr_2RuO_4 has mysteriously succeeded in defying any valid theory and the identification of its gap function for more than twenty years. Even the results of different experimental techniques seem to contradict each other when trying to pinpoint the order parameter. Former theories aiming at a description in terms of a time-reversal symmetry broken (chiral) state were experimentally disproven by the non-existence of edge currents. Our calculations are based on a more complete single-particle model that does not only incorporate the on-site spin-orbit interaction but also more extended non-local spin-orbit coupling terms which are evaluated in all d-orbitals. Using a combined weak-coupling and functional renormalization group approach we integrate out the high-energy degrees of freedom to identify the gap functions for a set of realistic interaction parameters. Motivated by recent experimental results showing a strong increase of the critical temperature under uniaxial pressure, we also explore the consequences of breaking the lattice symmetry D_{4h} down to D_{2h}.

TT 91.9 Thu 17:15 H 0104

Applications of time-dependent full configuration interaction quantum monte carlo — •Kai Guther[1], Werner Dobrautz[1], Olle Gunnarsson[1], and Ali Alavi[1,2] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Cambridge, Cambridge, United Kingdom

We employ the full configuration interaction quantum monte carlo [1] method to compute spectral functions of correlated electron systems by the means of complex time evolution [2] in combination with a Maximum Entropy Method [3] analytic continuation approach.

We discuss the dependence of the resulting spectral functions on the chosen complex time contour and simulation parameters and discuss the effect of the stochastic approximation. We study the effect of the chosen integrator for the time-evolution on a few examples and conclude that a second-order Runge-Kutta integrator is well-suited for our application. We discuss possible applications in a self-consistent DMFT scheme.

[1] G. H. Booth, A. J. W. Thom, and A. Alavi, The Journal of Chemical Physics 131, 054106 (2009)
[2] K. Guther, W. Dobrautz, O. Gunnarsson, A. Alavi, arXiv:1709.00218
[3] M. Jarrell and J. Gubernatis, Phys. Rep. 269, 133 (1996)

TT 91.10 Thu 17:30 H 0104

Having Monte Carlo decide which part of the weight to calculate: eigenstates-sampling in CTQMC — •Alexander Kowalski[1], Andreas Hausoel[1], Patrik Gunacker[2], and Giorgio Sangiovanni[1] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

Continuous-time quantum Monte Carlo algorithms are numerically exact methods for the solution of the Anderson impurity model often employed in DMFT calculations for strongly correlated electron systems. In the hybridization expansion CT-QMC algorithm, the local part of the system is solved exactly, which usually takes up most of the calculation time due to the exponential scaling of the local Hilbert space with the number of orbitals. A commonly used improvement is the use of conserved quantities to block-diagonalize the local Hamiltonian. We investigated the possibility of additionally sampling outer states separately in the Monte Carlo simulation, either grouped by the blocks of the Hamiltonian or individually.

We describe the details of the new Monte Carlo procedure, such as the modified updates we use to ensure ergodic and efficient sampling, as well as the influence on the average sign.

Using our implementation, we performed multi-orbital calculations at low temperatures and discuss the performance of the new method compared to conventional sampling.

TT 91.11 Thu 17:45 H 0104

Hybrid quantum Monte Carlo simulations of the two dimensional half-filled Su-Schrieffer-Heeger (SSH) model — •Stefan Beyl, Martin Hohenadler, Florian Goth, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Su-Schrieffer-Heeger (SSH) model describes electrons interacting with quantum phonons via a bond coupling. While the model is understood in detail in one dimension, no systematic results are available in two dimensions. Here, we use the Hybrid Quantum Monte Carlo (HQMC) method to simulate the model on the square lattice without a sign problem. We determine the phase diagram and discuss the advantages and challenges of HQMC in the context of electron-phonon systems.

TT 91.12 Thu 18:00 H 0104

Functional renormalisation group for quantum critical metals in $d = 2$ — •Matthew Trott and Chris Hooley — SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, Fife, KY16 9SS, United Kingdom

We present a novel functional renormalisation group calculation for quantum critical metals in two spatial dimensions. We utilise soft frequency regulators to stop the suppression of particle-hole excitations in an attempt to consistently describe Landau damping and non-Fermi liquid effects. Additionally we track bosonic interactions up to sextic coupling to elucidate the fixed point structure.