TT 63: Low-Dimensional Systems: 2D - Theory

Time: Thursday 9:30–13:00 Location: H21

TT 63.1 Thu 9:30 H21

Giant valley drifts in uniaxially strained monolayer MoS_2 — •Udo Schwingenschlögl, Qingyun Zhang, Yingchun Cheng, and Li-Yong Gan — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

Using first-principles calculations, we study the electronic structure of monolayer MoS_2 under uniaxial strain. We show that the energy valleys drift far off the corners of the Brillouin zone (K points), about 12 times the amount observed in graphene. Therefore, it is essential to take this effect into consideration for a correct identification of the band gap. The system remains a direct band gap semiconductor up to 4% uniaxial strain, while the size of the band gap decreases from 1.73 to 1.54 eV. We also demonstrate that the splitting of the valence bands due to inversion symmetry breaking and spin-orbit coupling is not sensitive to strain.

[1] Q. Zhang, Y. Cheng, L.-Y. Gan, and U. Schwingenschlögl, PRB **88**, 245447 (2013)

TT 63.2 Thu 9:45 H21

Coexistence of incommensurate magnetism and superconductivity in the two-dimensional Hubbard model — Hiroyuki Yamase[1,2], •Andreas Eberlein[1,3], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Department of Physics, Harvard University, Cambridge, USA

We analyze the competition of magnetism and superconductivity in the two-dimensional Hubbard model with a moderate interaction strength, including the possibility of incommensurate spiral magnetic order. Using an unbiased renormalization group approach, we compute magnetic and superconducting order parameters in the ground state. In addition to previously established regions of Néel order coexisting with d-wave superconductivity, the calculations reveal further coexistence regions where superconductivity is accompanied by incommensurate magnetic order.

TT 63.3 Thu 10:00 H21

Physical dipoles and second order perturbation theory for dipolar fermions in two dimensions — •Philipp Lange, Jan Krieg, and Peter Kopietz — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt/Main, Germany

By considering electric physical dipoles, we propose a new regularization for the Fourier transform of the interaction of dipolar fermions in two dimensions. Using this regularization, we calculate the self-energy, the renormalized chemical potential, and the renormalized Fermi surface of dipolar fermions in two dimensions in full second order perturbation theory.

TT 63.4 Thu 10:15 H21

Thermodynamics and renormalized quasiparticles in the vicinity of the dilute Bose gas quantum critical point in two dimensions — •Jan Krieg[1], Simon Streib[1], Dominik Strassel[2], Sebastian Eggert[2], and Peter Kopietz[1] — [1]Goethe-Universität Frankfurt, Deutschland — [2]Technische Universität Kaiserslautern, Deutschland

Using the functional renormalization group and quantum Monte Carlo methods we investigate the region close to the quantum critical point of a dilute two-dimensional boson gas in the normal phase. Decoupling the two-particle interaction in the particle-particle channel and using a simple truncation of the flow equations we derive the leading order logarithmic corrections to pressure, density, and entropy as well as to the effective mass and to the wavefunction renormalization. We find that recent experiments using cold atoms are in good agreement with our results.

TT 63.5 Thu 10:30 H21

Nonlocal density interactions on the honeycomb and bilayer square lattice — •Stefan Wessel and Michael Golor — Institute for Theoretical Solid State Physics, RWTH Aachen University

We consider an efficient scheme to perform sign problem-free determinantal quantum Monte Carlo simulations of Hubbard models with nonlocal density-density interactions on half-filled bipartite lattices, based on a bond-decoupling of the extended interaction terms. We apply our scheme to the Hubbard model on the square lattice bilayer with an interlayer repulsion, and present the ground state phase diagram within the accessible parameter region. In particular, for sufficiently strong interlayer tunneling, we observe the emergence of a direct dimer product state of mixed D-Mott and S-Mott character. We also examine the stability range of this state within strong-coupling perturbation theory. Furthermore, we consider the Hubbard model on the honeycomb lattice with next-nearest-neighbor interactions. Such an interaction is found to enhance both charge density and spin-current correlations within the semimetallic region. However, inside the accessible parameter region, they do not stabilize long-ranged charge density wave order nor a quantum spin Hall state, and the only insulating state that we observe exhibits long-range antiferromagnetism.

TT 63.6 Thu 10:45 H21

Spin spectral functions of a quantum spin liquid phase on the kagome lattice from quantum Monte Carlo — •Maximilian Lohöfer and Stefan Wessel — Institute for Theoretical Solid State Physics

We analyze the dynamical spin structure factor of a spin-$\frac{1}{2}$ XY-model on a kagome lattice with additional ring-exchange terms along the bow-tie plaquettes. This model is known to exhibit a quantum phase transition between a transverse ferromagnetic phase and a gapped Z_2 quantum spin liquid regime for strong ring-exchange interactions. We employ a combination of sign problem-free quantum Monte Carlo simulations and analytic continuation to study the evolution of the dynamical structure factor across the quantum phase transition in order to extract signatures for the spin liquid state in this non-trivial spin model.

TT 63.7 Thu 11:00 H21

Boson-fermion duality for corner entanglement entropies in free field theories — •Johannes Helmes[1,2], Lauren Hayward Sierens[2,3], Anushya Chandran[2], and Roger Melko[2,3] — [1]University of Cologne, Germany — [2]Perimeter Institute, Waterloo, Canada — [3]University of Waterloo, Canada

Subleading corrections to the prevalent area-law of (Rényi) entanglement entropies of critical quantum many-body systems are known to show universal behavior. For gapless systems a logarithmic correction arises from the presence of corners in the subsystem. Its coefficient is concretely related to the central charge of the stress tensor of the low-energy effective conformal field theory (CFT) and hence counts the underlying degrees of freedom. A surprising duality is revealed in these corner terms of an opening angle $\theta \lesssim \pi$ between free boson and Dirac fermion lattice field theories for reciprocal Rényi indices.

We compute the entanglement entropies via an exact lattice diagonalization supplemented by a numerical linked-cluster expansion. Using these data we show that the duality is also relatively robust for a corner with an opening angle of $\theta = \pi/2$. We furthermore apply our numerical treatment to a variety of other angles θ. The results confirm the scaling of the corner term with $(\theta - \pi)^2$ and shed light on the gradual dissolution of the duality in the limit of small angles.

15 min. break

TT 63.8 Thu 11:30 H21

High-performance functional renormalization group calculations for interacting fermions on the square lattice — •Julian Lichtenstein[1,2], David Sánchez de la Peña[1,2], Stefan A. Maier[1,2,3], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [2]JARA-FIT, Jülich-Aachen Research Alliance – Fundamentals of Future Information Technology — [3]Institute for Theoretical Physics, University of Cologne, Germany

The truncated unity functional renormalization group (TUfRG) approach is a novel functional renormalization group (fRG) variant. It is based on an exchange parametrization of the two-fermion interaction [1], while the structure of the equations is inspired by the singular-mode functional renormalization group put forward by Wang et al. [2]. On the basis of speedup data gained from our implementation we show that the TUfRG facilitates efficient calculations on a large num-

ber of multi-core CPUs. In this context, it will be illustrated that a separation of the underlying equations, as it is done in the TUfRG, is numerically advantageous. In order to discuss strong and weak points of this method, we compare data for the t,t' Hubbard model on the square lattice to those from other fRG methods. Furthermore, we analyze the effect of including longer ranged interactions in addition to the purely local Hubbard interaction.

This work was supported by DFG via RTG1995 'Quantum many-body methods in condensed matter systems'.

[1] C. Husemann and M. Salmhofer, PRB **79**, 195125 (2009)
[2] W. S. Wang et al., PRB **85**, 035414 (2012)

TT 63.9 Thu 11:45 H21

A functional Renormalization Group calculation with high wavevector resolution for extended Hubbard models on the honeycomb lattice — •David Sánchez de la Peña[1], Julian Lichtenstein[1], Stefan Maier[1,2], and Carsten Honerkamp[1] — [1]Institute for Theoretical Solid State Physics, RWTH-Aachen University, D-52056 Aachen, Germany and JARA Fundamentals of Future Information Technologies — [2]Institute for Theoretical Physics, Cologne University, D-50937 Cologne, Germany

Extended Hubbard models on the honeycomb lattice exhibit a rich variety of ordering tendencies at low energies, which manifest themselves as instabilities of the normal state respect to the inclusion of electron-electron interactions. In an attempt to describe the low-energy properties of real materials with such a honeycomb structure, like graphene, we analyze the arising ordering tendencies and corresponding critical scales as a function of doping and interaction parameters. For that matter, we employ a truncated unity functional Renormalization Group treatment (TUfRG), which allows for an unbiased investigation of the competing instabilities arising in the effective low-energy theory starting from a given set of bare Coulomb interactions. Being based on channel decomposed flow equations, the wavevector resolution that can be achieved is much higher than that of N-patch fRG schemes, which also allows the inclusion of a weakly screened long-range Coulomb tail in the bare interactions.

This work was supported by the DFG-SPP 1459 'Graphene'.

TT 63.10 Thu 12:00 H21

Frequency-dependent interactions in a two-patch model — •Timo Reckling and Carsten Honerkamp — Institute for Theoretical Solid State Physics, RWTH Aachen University, 52056 Aachen, Germany

We study a two-patch model for interacting fermions with the functional Renormalization Group (fRG). The goal is to gain insight into the frequency dependence of the effective interaction that is generated in the fRG flow. In our model each interaction component g_i depends on three bosonic transfer frequencies or 3 fermionic frequencies that determine the loop contributions on the r.h.s. of the fRG equations. We discuss the applicability of simplified ansatzes like Lorentzians to describe the frequency dependencies. Moreover, we analyze the influence of the frequency dependence on the critical scales of the flows to strong coupling.

This work is supported by the DFG-RTG 1995 "Quantum many-body methods in condensed matter systems".

TT 63.11 Thu 12:15 H21

Efficiency of the Hybrid Quantum Monte Carlo Method for Hubbard type models. — •Stefan Beyl, Fakher F. Assaad, and Florian Goth — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

The Hybrid Quantum Monte Carlo method has the potential advantage of reaching very large system sizes for Hubbard type models since it can scale linearly with the euclidean volume. Here we argue that the performance of the method is strongly dimension dependent. In the one-dimensional case, the fact that the fermion matrix has no zeros leads to a stable algorithm which scales more efficiently than generic auxiliary field method. In two dimensions the fermionic matrix has zeros thereby leading to a breakdown of ergodicity. We propose to use a complex Hubbard Stratonovich transformation to avoid this problem.

TT 63.12 Thu 12:30 H21

Spontaneous breaking of particle-hole-symmetry on a Lieb-lattice — •Johannes S. Hofmann[1], Thomas C. Lang[2,1], Martin Bercx[1], and Fakher F. Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Institute for Theoretical Physics, University of Innsbruck, Austria

We study the t-V-model of spinless fermions on a two dimensional Lieb-lattice at half filling, using both exact diagonalization and continuous-time Quantum Monte Carlo (QMC) methods. The non-interacting model supports a Dirac cone as well as a flat band at the Fermi level. While the flatness is protected by the sub-lattice symmetry, a flat band is also highly susceptible to interaction effects. We find that nearest neighbor Coulomb repulsion leads to spontaneous breaking of the sub-lattice symmetry due to the formation of a charge density wave. In principle, this allows to further investigate the model away from half filling without introducing a sign problem to the QMC. We analyze the critical temperature of the phase transition and study its dependence on the interaction strength.

TT 63.13 Thu 12:45 H21

Finite-Temperature Sensitivity of Entanglement Spectra and Their Numerical Reconstruction from Rényi Entropies — •Wilfried Michel, Peter Broecker, and Simon Trebst — University of Cologne, Germany

Entanglement spectra provide deep insight into the entanglement structure of quantum many-body systems, in particular in the presence of (chiral) topological order. Here we discuss numerical approaches to reconstruct the n lowest eigenvalues of the entanglement spectrum from the first n Rényi entropies including characteristic polynoms, maximum entropy techniques, and a power method. We further discuss the stability of the entanglement spectrum in the presence of thermal fluctuations.

We illustrate our findings for the one-dimensional $S = 1/2$ quantum Heisenberg model in a ladder geometry, which exhibits a quantum phase transition from a symmetry protected phase to a trivial phase.