TT 80: Correlated Electrons: (General) Theory 2

Time: Thursday 16:00–18:30 Location: H18

TT 80.1 Thu 16:00 H18

A novel solution of the Hubbard model: a generalized equation-of-motion approach to the underdoped cuprates puzzle — •Andrea Di Ciolo[1] and Adolfo Avella[1,2] — [1]Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno, I-84084 Fisciano (SA), Italy — [2]CNR-SPIN, UoS di Salerno, I-84084 Fisciano (SA), Italy

We solve the Hubbard model on a d-dimensional hypercubic lattice in the framework of the Composite Operator Method (COM) within a 4-pole approximation. This approach extends the 2-pole [1] and the 3-pole [2] schemes treating on equal footing both U and J scales of energy. The COM, which is based on the Green's function formalism, is highly tunable and expressly devised for the characterization of strongly correlated electronic states and the exploration of novel emergent phases. Motivated by the long-standing experimental challenge posed by the puzzling spectral properties of the underdoped cuprates, we adopt a basis of fields containing operators specifically designed to describe Hubbard electronic transitions dressed by nearest-neighbor spin fluctuations and to capture the effects of these latter on all electronic properties. The spin fluctuations play a crucial role in the mechanism of pseudogap formation and evolution as well as in the unconventional behavior of the Fermi surface, the spectral weights and the electronic dispersion. Thus, we exploit this non canonical, but very efficient, operatorial representation of correlated electrons to achieve a deeper understanding of the underdoped phase of cuprates.

[1] F. Mancini, and A. Avella, Adv. Phys. **53**, 537 (2004)
[2] A. Avella, Eur. Phys. J. B **87**, 45 (2014)

TT 80.2 Thu 16:15 H18

Multiplons in the two-hole excitation spectra of the Hubbard model — •Roman Rausch and Michael Potthoff — I. Institute for Theoretical Physics, University of Hamburg

Using the density-matrix renormalization group (DMRG) in combination with the Chebyshev polynomial expansion technique, we study the two-hole excitation spectra of the one-dimensional Hubbard model from $n = 2$ down to half-filling $n = 1$. Experimentally, this corresponds to the Auger Electron Spectroscopy (AES). The spectra reveal multiplon physics, i.e., the relevant final states are characterized by two (doublon), three (triplon), four (quadruplon) and more holes, potentially forming stable compound objects or resonances with finite lifetime. This multiplon phenomenology is analyzed by interpreting not only the local and k-resolved two-hole spectra, but also auxiliary three- and four-hole spectra, as well as by referring to effective low-energy models and employing a filter-operator technique. In addition, we compare with the elementary excitations of the Bethe ansatz, which in particular reveals the decay channels of the doublon into spinons and holons in one dimension. For all fillings with $n > 1$, the doublon lifetime is strongly k-dependent and even infinite at the Brillouin zone edges. This can be traced back to the "hidden" charge-SU(2) symmetry of the model. We briefly discuss how this k-dependence changes in two dimensions, by applying DMRG to small-radius cylinders, as well as extrapolating to larger systems by using cluster perturbation theory (CPT).

[1] R. Rausch, M. Potthoff, arXiv:1510.01162

TT 80.3 Thu 16:30 H18

Doping effects on the three-orbital spin-orbit-coupled Hubbard model — •Aaram J. Kim[1], Harald O. Jeschke[1], Philipp Werner[2], and Roser Valenti[1] — [1]Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Department of Physics, University of Fribourg, Chemin du Musée 3, 1700 Fribourg, Switzerland

We investigate doping effects in a spin-orbit-coupled three-orbital Hubbard model by means of the dynamical mean-field theory combined with the continuous-time quantum Monte Carlo method. Near 5/6-filling, the spin-orbit-coupled Mott insulator emerges as a consequence of the interplay between the relativistic spin-orbit term and the strong U interaction. In particular, we discuss the spectral properties of the hole-doped spin-orbit-coupled Mott insulator and its phase transitions as a function of interaction U and doping concentration. The two-particle correlation function is also studied to show the dynamic properties of the system. We discuss implications of the model results for real materials.

TT 80.4 Thu 16:45 H18

Hybrid-Space Density Matrix Renormalization Group applied to the Two-Dimensional Hubbard Model — •Georg Ehlers and Reinhard M. Noack — Philipps-University Marburg

We apply the hybrid-space density matrix renormalization group (DMRG) to the two-dimensional Hubbard model on a cylinder surface. The hybrid-space DMRG uses a momentum-space representation in the transverse and a real-space representation in the longitudinal direction. Utilizing the transverse momentum quantum number allows us to gain significant speedup and memory savings compared to real-space DMRG. Especially, the computational costs of the hybrid-space DMRG are almost independent of the cylinder circumference for fixed size of the truncated Hilbert space. We investigate ground state properties such as the behavior of the ground-state energy, pair-field correlations, and the appearance of stripes at intermediate coupling and weak doping. We find striped ground states generically, with the width of the stripes depending on the filling, the boundary conditions, and the width of the cylinder. Furthermore, we analyze the interplay between the different stripe configurations and the decay of the pairing correlations.

15 min. break

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Ground state phase diagram of the repulsive fermionic t-t' Hubbard model on the square lattice from weak-coupling — •Fedor Simkovic[1], Xuan-Wen Liu[2], Youjin Deng[2], and Evgeny Kozik[1] — [1]King's College London, Strand, London WC2R 2LS, UK — [2]University of Science and Technology of China, Hefei, Anhui 230026, China

We obtain a complete and exact in the weak-coupling limit ($U \to 0$) ground state phase diagram of the repulsive fermionic Hubbard model on the square lattice for filling factors $0 \leq n \leq 2$ and next nearest neighbour hopping amplitudes $0 \leq t' \leq 0.5$. Phases are distinguished by the symmetry and the number of nodes of the superfluid order parameter. The phase diagram is richer than may be expected and typically features states with a high —higher than that of the fundamental mode of the corresponding irreducible representation— number of nodes. The effective coupling strength in the Cooper channel λ, which determines the critical temperature T_c of the superfluid transition, is calculated in the whole parameter space and regions with high values of λ are identified. It is shown that besides the expected increase of λ near the Van Hove singularity line, joining the ferromagnetic and antiferromagnetic points, another region with high values of λ can be found at quarter filling and $t' = 0.5$ due to the presence of a line of nesting at $t' \geq 0.5$. The results can serve as benchmarks for controlled non-perturbative methods and guide the ongoing search for high-T_c superconductivity in the Hubbard model.

TT 80.6 Thu 17:30 H18

Nature of the many-body excitations in a quantum wire — •Oleksandr Tsyplyatyev — Institut für Theoretische Physik, Universität Frankfurt, Frankfurt, Germany

The natural excitations of an interacting one-dimensional system at low energy are hydrodynamic modes of Luttinger liquid, protected by the Lorentz invariance of the linear dispersion. We show that beyond low energies, where quadratic dispersion reduces the symmetry to Galilean, the main character of the many-body excitations changes into a hierarchy: calculations of dynamic correlation functions for fermions (without spin) show that the spectral weights of the excitations are proportional to powers of R^2/L^2, where R is a length-scale related to interactions and L is the system length. Thus only small numbers of excitations carry the principal spectral power in representative regions on the energy-momentum planes. We have analysed the spectral function in detail and have shown that the first-level (strongest) excitations form a mode with parabolic dispersion, like that of a renormalised single particle. The second-level excitations produce a singular power-law line shape to the first-level mode and multiple power-laws at the spectral edge. We have illustrated crossover to Luttinger liquid at low energy by calculating the local density of state through all energy

scales: from linear to non-linear, and to above the chemical potential energies.

[1] O. Tsyplyatyev et al., PRL **114**, 196401 (2015).
[2] O. Tsyplyatyev et al., arXiv:1508.07125.

TT 80.7 Thu 17:45 H18

Theoretical calculation of photoemission spectra for Ir-based perovskites — •Ekaterina Plotnikova[1], Krzysztof Wohlfeld[2], Kateryna Foyevtsova[3], and Jeroen van den Brink[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [2]Institute of Theoretical Physics, University of Warsaw, Pasteura 5, PL-02093 Warsaw, Poland — [3]University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1 Canada

The layered iridates, Ba_2IrO_4 and Sr_2IrO_4, have recently attracted a lot of attention due to their structural and electronic similarities to the layered cuprates. Nevertheless, due to the strong spin-orbit coupling in the iridates, their properties upon electron or hole doping *may* be substantially different than those of the high-T_C cuprates. As a first step in understanding the physics of the doped iridates, we calculate the photoemission spectra of layered iridates using a polaronic model and the self-consistent Born approximation. We compare the obtained spectra to those calculated using the density functional theory and to the experimental spectra obtained by ARPES on Ba_2IrO_4 and Sr_2IrO_4.

TT 80.8 Thu 18:00 H18

The shape of the Compton profile for metals — •Michael Sekania[1,2], Wilhelm H. Appelt[1,3], Diana Benea[4,5], Hubert Ebert[5], and Liviu Chioncel[1,3] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Andronikashvili Institute of Physics, Tamarashvili 6, 0177 Tbilisi, Georgia — [3]Augsburg Center for Innovative Technologies, University of Augsburg, D-86135 Augsburg, Germany — [4]Faculty of Physics, Babes-Bolyai University, Kogalniceanustr 1, Ro-400084 Cluj-Napoca, Romania and — [5]Department of Chemistry, Ludwig Maximilian University of Munich, Butenandstr. 5-13, D-81377 München, Germany

The electron momentum density and Compton profiles of weakly interacting metals are investigated in the framework of the density functional theory. The valence electrons contributions to the Compton profiles for different lattice symmetries are analyzed. We find that the shape of the Compton profiles can be modeled by the so-called q-Gaussian distribution recently proposed by Tsallis in the context of generalized canonical distributions. Our analysis shows that tails typically ignored in the conventional studies of the Compton profiles contain significant information about the electron momentum distribution in solids.

TT 80.9 Thu 18:15 H18

Rigorous Bounds on Pomeranchuk $l = 1$ Instabilities from Ward Identities — •Egor Kiselev[1], Mathias Scheurer[1], Jörg Schmalian[1,2], and Peter Wölfle[1,3] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, 76049 Karlsruhe, Germany — [2]Institute for Solid State Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]nstitut für Nanotechnologie, Karlsruher Institut für Technologie, D-76021 Karlsruhe, Germany

Pomeranchuk Instabilities signal spontaneous deformations of the Fermi surface. The shape of those deformations is parametrized by spherical harmonics $Y_{l,0}$, so that Pomeranchuk Instabilities can be classified by the number l. In the $l = 1$ case the Fermi surface is displaced by a small momentum and the instability results in spontaneously flowing spin or charge currents.

Using generalized Ward Identities it will be shown, that $l = 1$ Pomeranchuk Instabilities in the spin/charge sector cannot be caused by a locally spin/charge conserving interaction respectively. Since the general case of Coulomb interaction between electrons and ions conserves electronic spin and charge, it is concluded that $l = 1$ Pomeranchuk Instabilities can only occur, when relativistic physics is considered.

We discuss implications of our results for proposed emergent spin-orbit couplings, preemptive Pomeranchuk Instabilities near a ferromagnetic quantum critical point, and the low temperature Fermi liquid behaviour of ^{3}He.