TT 10: Correlated Electrons: (General) Theory 1

Time: Monday 15:00–18:15 Location: H 3010

TT 10.1 Mon 15:00 H 3010

Enhanced Perturbative Continuous Unitary Transformation — •Holger Krull, Nils A. Drescher, and Götz S. Uhrig — TU Dortmund, Theoretical Physics I, 44221 Dortmund, Germany

We present an enhanced version of continuous unitary transformations (CUTs) to derive effective models perturbatively and non-perturbatively for quantum lattice models. The underlying idea is to expand the Hamiltonian and the generator of the flow equation in the expansion parameter. The operators are described in second quantization. For the method to be efficient, it is essential to keep track of the relevant contributions according to their order in the expansion parameter. This enhanced perturbative CUT (epCUT) allows us to determine effective Hamiltonians to high order. In contrast to perturbative CUT, the expansion around unperturbed Hamiltonians with non-equidistant spectrum is possible. In addition, we found that the set of differential flow equations of the epCUT can be integrated non-perturbatively leading to a robust extrapolation similar to self-consistent diagrammatic techniques. This directly evaluated epCUT (deepCUT) provides robust results even for relatively large expansion parameter as long as the relevant processes with a spatial range up to the correlation length are included. The epCUT and the deepCUT are illustrated for the $S = \frac{1}{2}$ antiferromagnetic Heisenberg ladder and for an extension with alternating rung couplings implying a non-equidistant unperturbed spectrum. The results for the ground state energy (order 17/16) and the dispersion (order 15/13) are presented.

TT 10.2 Mon 15:15 H 3010

Spectral properties of one-dimensional spin systems using deepCUT — •N. A. Drescher, H. Krull, T. Fischer, and G. S. Uhrig — TU Dortmund, Theoretical Physics I, 44221 Dortmund

Directly evaluated enhanced perturbative continuous unitary transformations (deepCUT) are a novel scheme to systematically derive effective low-energy models for many-particle Hamiltonians. Founded on high-order perturbative expansion techniques (epCUT), deepCUTs generate robust results beyond perturbation theory. We use them to decouple ground state and low-lying excitations of one dimensional spin systems. From the effective Hamiltonian, dispersion and bound states can be obtained. Applying the same unitary transformation to observables, we calculate spectral weights and the dynamical spin structure factor for the one and two quasi-particle channel at $T = 0$.

We illustrate the deepCUT method by an analysis of the antiferromagnetic S=$\frac{1}{2}$ Heisenberg ladder compound $(C_7(D,H)_{10}N)_2CuBr_4$. We compare our results for dispersion and spectral weight with inelastic neutron scattering data. Predictions for S=0,1 spectral densities and bound states relevant for various scattering experiments are presented.

TT 10.3 Mon 15:30 H 3010

DMFT study of correlated systems in d+p basis sets utilizing a continuous time algorithm — •Nicolaus Parragh, Giorgio Sangiovanni, Alessandro Toschi, Philipp Wissgott, Philipp Hansmann, and Karsten Held — Institut für Festkörperphysik, TU Wien

Ab-initio calculations for strongly correlated materials are nowadays very often performed within the LDA+DMFT scheme, a combination of local density approximation and dynamical mean field theory. Within this approach, a key point is which bands to keep when defining the low energy Hamiltonian for which DMFT self-consistency is performed. We show how the inclusion of p-bands (typically coming from Oxygen ligands on top of the transition metal d-orbitals) in the DMFT cycle affects the physics of the system. This has implications for current research in, e.g., iron and copper based superconductors. We use continuous-time Quantum Monte Carlo algorithm to solve the auxiliary impurity problem and focus on the role of SU(2)-symmetric interactions.

TT 10.4 Mon 15:45 H 3010

Electronic correlation at the two-particle level — •Thomas Schaefer[1], Georg Rohringer[1], Alessandro Toschi[1], Giorgio Sangiovanni[1], Olle Gunnarsson[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology, Austria — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Electronic correlated systems can often be successfully described by dynamical mean field theory (DMFT). If DMFT is applied to finite-dimensional systems it is self-consistent at the one-particle level. Extensions of DMFT based upon the systems' two-particle properties have been developed such as the dynamical vertex approximation (DΓA) [1] or the dual fermion approach [2]. In addition, the understanding and the calculation of two-particle quantities are crucial within DMFT to compute momentum-dependent response functions that can be compared directly with experiments. As hitherto the investigation of local and non-local two-particle properties has been merely sporadic, we provide a systematic analysis of the reducible and irreducible two-particle vertex functions by applying DMFT and the dynamical cluster approximation (DCA) to the two-dimensional Hubbard model.

[1] A. Toschi, A. A. Katanin, and K. Held, Phys. Rev. B 75, 045118 (2007).

[2] A. N. Rubtsov, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 77, 033101 (2008).

TT 10.5 Mon 16:00 H 3010

Dynamics in the Ising field theory after a quantum quench — •Dirk Schuricht[1,2] and Fabian H. L. Essler[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen — [2]JARA-Fundamentals of Future Information Technology — [3]The Rudolf Peierls Centre for Theoretical Physics, University of Oxford

We study the real-time dynamics of the magnetization $\langle\sigma^z(t)\rangle$ in the Ising field theory after a quench in the fermion mass, which corresponds to a quench in the transverse field of the corresponding transverse-field Ising chain. The long-time behavior is obtained analytically by a resummation of the leading divergent terms in a form-factor expansion for $\langle\sigma^z(t)\rangle$. We determine the dominant exponential relaxation and the corresponding relaxation rate and show that the leading corrections behave as $\sim 1/(Mt)$ and $\sim \cos(2Mt - \pi/4)/(Mt)^{3/2}$.

TT 10.6 Mon 16:15 H 3010

Bosonization in arbitrary dimensions and its applications to Quantum Monte Carlo simulations — •Ervand Kandelaki and Konstantin Efetov — Theoretische Physik III, Ruhr-Universität-Bochum

The applicability of Quantum Monte Carlo simulations for fermionic models using the Auxiliary Field method is often limited if the measure is not strictly positive. We investigate to what extent the recently suggested bosonization scheme for fermionic systems in an arbitrary dimension allows for simulations with positive weights. Choosing a proper regularization of the dynamical equation for the bosonic field, we derive an expression for the action which is purely real. We relate the partition function obtained after bosonization to the common fermionic one and present some first numerical results.

[1] R. Blankenbecler, D. J. Scalapino, and R. L. Sugar, Phys. Rev. D 24, 2278 (1981)

[2] K. B. Efetov, C. Pépin, and H. Meier, Phys. Rev. Lett. 103, 186403 (2009)

[3] K. B. Efetov, C. Pépin, and H. Meier, Phys. Rev. B 82, 235120 (2010)

15 min. break.

TT 10.7 Mon 16:45 H 3010

Continued Fractions and Bath-Parametrizations for Quantum Cluster Methods — •Monica Bugeanu and Erik Koch — German Research School for Simulation Sciences, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich

The Lanczos method is an ideal solver for dynamical mean-field approaches. Calculations are performed for the ground-state and extensions to finite temperature are straightforward. Dynamical quantities are obtained directly on the real axis without need for analytic continuations. The main limitation, however, is that calculations can only be done for finite baths. The rapidly growing size of the many-body Hilbert space limits actual calculations to quite small bath-sizes. It is therefore crucial to be able to treat as large baths as possible and to choose the bath parameters in an optimal way. We show how this

can be achieved using continued fraction representations of the Green function.

TT 10.8 Mon 17:00 H 3010

Orbital and magnetic order in the infinite-dimensional two-band Hubbard model — •Ernst von Oelsen, Götz Seibold, and Jörg Bünemann — Lehrstuhl Computational Physics, BTU Cottbus, Postfach 101344, 03013 Cottbus

Based on the time-dependent Gutzwiller approximation (GA), generalized to the case of multiple bands [1,2], we investigate the stability of magnetic and orbital order in the infinite dimensional two-band Hubbard model. Contrary to the Hartree-Fock plus random-phase approximation, the incorporation of the local multiplet-structure within our approach leads to a much larger sensitivity of ferromagnetism on the the ratio between Hund coupling and intra-orbital repulsion J/U. Besides, we find that the Brinkman-Rice localization transition, which in the paramagnetic GA appears at integer doping is always masked by an antiferromagnetic (for two particles per site) or an orbitally ordered (for one particle per site) ground state. In addition, at larger values of J/U a quantum Lifshitz point is found where ferro-, para- and incommensurate magnetic phases meet.

[1] E. von Oelsen, G. Seibold, and J. Bünemann, New J. Phys. **13**, 113031 (2011).
[2] E. v. Oelsen, G. Seibold, and J. Bünemann, Phys. Rev. Lett. **107**, 076402 (2011).

TT 10.9 Mon 17:15 H 3010

Momentum-dependent pseudogaps in the half-filled 2d Hubbard model — •Daniel Rost[1], Elena Gorelik[1], Fakher Assaad[2], and Nils Blümer[1] — [1]Institute of Physics, Johannes Gutenberg-University, Mainz, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Würzburg, Germany

A peculiar feature of (underdoped) high-T_c superconductors is the occurrence of pseudogaps in the normal state, i.e. a suppression of the density of states at the Fermi energy. It has been unclear for a long time whether and in which parameter regimes this phenomenon is captured by the two-dimensional Hubbard model: spectra obtained from determinantal quantum Monte Carlo (DQMC) simulations suffer from large finite-size (as well as Trotter and statistical) errors; partial conclusions for the thermodynamic limit were only possible by complementing DQMC data with cluster extensions of the dynamical mean-field theory (DMFT) and with the dynamical vertex approximation.

We present a method for extrapolating DQMC Green functions to the limit of infinite cluster size $L \to \infty$ and vanishing Trotter discretization $\Delta\tau \to 0$. Thus, we obtain, via the maximum entropy method, the first unbiased spectra in the thermodynamic limit. Our results establish that a pseudogap opens in the $2d$ Hubbard model at weak coupling below a characteristic temperature $T_{\rm pg}$ which (for $U = 4t$) agrees with DMFT Néel temperature. It opens first at $\mathbf{k}a = (\pi, 0)$, i.e. shows d wave type anisotropy at $T \lesssim T_{\rm pg}$ even at half filling; this momentum dependence (an effect not captured by DMFT) decays towards larger interactions.

TT 10.10 Mon 17:30 H 3010

Pomeranchuk and pairing instabilities in two-dimensional Hubbard models — •Jörg Bünemann[1], Tobias Schickling[2], and Florian Gebhard[2] — [1]Institut für Physik, BTU Cottbus, D-03013 Cottbus, Germany — [2]Fachbereich Physik, Philipps Universität Marburg, D-35032 Marburg, Germany

We have developed a diagrammatic method which permits the analytical evaluation of Gutzwiller wave functions in finite dimensions [1]. Unlike numerical schemes for the evaluation of such wave functions, our approach does not suffer from significant finite-size limitations and it can be readily generalised for the study of multi-band models. In our presentation we will introduce the main ideas of our approach and show results on single-band Hubbard models in two dimensions. In particular, we shall discuss the correlation-induced deformation of Fermi surfaces and the stability of phases with broken symmetry ("Pomeranchuk instabilities" and superconducting order).

[1] J. Bünemann, T. Schickling, F. Gebhard, arXiv:1108.4284

TT 10.11 Mon 17:45 H 3010

Superconductivity and the Pseudogap in the 2d Hubbard model — •Emanuel Gull[1], Olivier Parcollet[2], and Andrew J. Millis[1] — [1]Columbia University, New York, NY — [2]Institut de Physique Théorique (IPhT), CEA, France

Using a numerically exact continuous-time quantum Monte Carlo impurity solver and the DCA cluster dynamical mean field method with cluster sizes up to 16, we have been able to access the superconducting phase of the two dimensional Hubbard model for parameters believed to be relevant to high temperature copper oxide superconductivity. We present results for the phase diagram, the gap to transition temperature ratio, and the interplay of the pseudogap and the superconducting gap. The gap results are obtained by direct inference from imaginary frequency data and analytically continued spectral functions.

TT 10.12 Mon 18:00 H 3010

Heavy fermion properties in the Kondo lattice model — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, Institute for Theoretical Solid State Physics, P.O. Box 270116, D-01171 Dresden, Germany — [2]Technische Universität Dresden, Institut für Theoretische Physik, D-01062 Dresden, Germany

The Kondo lattice model is believed to describe the low-energy physics of heavy-fermion systems. It includes a band of conduction electrons, interacting via an exchange with a regular array of immobile spins $\mathbf{S}_i$. No exact results are known for this model in any spatial dimension. We have studied the model using the quite novel projective renormalization method (PRM). Using this analytical technique we obtain a solvable effective Hamiltonian $\tilde{\mathcal{H}}$ which consists of conduction electrons with renormalized dispersion $\tilde{\varepsilon}_{\mathbf{k}}$ and an RKKY interaction term which is generated naturally within the renormalization procedure. The present approach allows us to evaluate static and dynamical properties such as the specific heat, the density of states or the electrical resistivity. For low enough temperatures we find an additional dispersionless excitation around the Fermi surface due to the formation of a singlet state. Simultaneously, a large γ-coefficient develops in the specific heat which is usually traced back to the huge effective mass of heavy fermion quasiparticles.