TT 15: Dual-Method Approaches to Quantum Many-Body Systems I

To make an impact on possible applications, theoretical approaches for correlated many-body systems must allow for studying more realistic models and lead to more accurate predictions as compared to what is achievable nowadays. This requires, on the one hand, the development of specialized tools which are mathematically and/or algorithmically demanding. On the other hand, an emergent promising approach to make significant progress beyond toy-model understanding of many-body physics is the combined use of two or more complementary methods. The demand for such type of approaches is growing. The two session of contributed talks will provide an overview of recent successes in such dual-(multi-)method approaches involving analytical as well as numerical tools, and will indicate prospects for future directions.

Compilation: Volker Meden, RWTH Aachen; Stefan Wessel, RWTH Aachen

Time: Monday 15:00–18:45 Location: H 0104

TT 15.1 Mon 15:00 H 0104

Combining diagrammatic Monte-Carlo with large-N field theory — •Gunnar Möller — School of Physical Sciences, University of Kent, Canterbury, UK

We explore a new avenue for quantitative investigations of strongly interacting systems by combining large-N fermionic theories with stochastic sampling of high order Feynman graphs.

Our work focuses on the unitary Fermi gas as a blueprint example for a strongly interacting system of fermions without a small expansion parameter in the Hamiltonian. The unitary Fermi gas is realised experimentally in cold atomic gases of two-species fermions interacting via a Feshbach resonance [1]. Previous work has established a diagrammatic Monte-Carlo (diagMC) approach [2] but it has left uncertainties about the convergence properties of the interaction expansion [3,4]. Here, we re-examine the problem by introducing a small parameter via a large-N generalisation [5,6], to which we then apply diagMC. Formally, this yields an expansion around the mean-field superconducting theory, whose properties are recovered in the $N \to \infty$ limit. We benchmark the approach by examining density distributions and the contact parameter against prior approaches.

[1] W. Zwerger, Springer (2012).
[2] Van Houcke, K. et al., Nat Phys 8, 366 (2012); and arXiv:1305.3901 (2013).
[3] Kozik, E., Ferrero & Georges, PRL 114, 156402 (2015)
[4] Rossi, R., Werner, F., Prokof'ev, N. V. & Svistunov, B., Phys. Rev. B 93, 161102 (2016).
[5] Veillette, M. Y., Sheehy, D. E. & Radzihovsky, L. Phys. Rev. A 75, 043614 (2007).
[6] Nikolić, P. & Sachdev, S. Phys. Rev. A 75, 033608 (2007).

TT 15.2 Mon 15:15 H 0104

Parquet equations for the 2D Hubbard model using channel decomposition — •Christian Eckhardt[1], Giulio Schober[1], and Carsten Honerkamp[1,2] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany — [2]JARA-FIT, Jülich Aachen Research Alliance - Fundamentals of Future Information Technology, Germany

The parquet equations are a set of self consistent equations for the effective interaction vertex of an interacting many-fermion system. The application of the parquet equations in bulk models is, however, complicated by the complex emergent momentum and frequency structure of the vertex. Here we show how techniques for the treatment of the momentum dependence, that were developed in the context of the functional renormalization group, can be applied to the parquet equations. We present solutions using this technique for the half-filled Hubbard model on the square lattice and discuss ways to include the frequency dependence of the vertices.

TT 15.3 Mon 15:30 H 0104

New approach towards conceptual and numerical extensions of cluster dynamical mean-field theory — •Marcel Klett, Sabine Andergassen, and Philipp Hansmann — Institut für Theoretische Physik, Universität Tübingen, 72076 Tübingen

The dynamical mean-field theory (DMFT) provides the exact solution of a quantum many-body Hamiltonian in the limit of infinite spatial dimensions. The accurate (and non-perturbative) description of all local correlations allows to describe the Mott-Hubbard metal-to-insulator transition in three-dimensional bulk systems. At the same time, the mean-field nature with respect to the spatial degrees of freedom implies that all non-local spatial correlation effects are neglected in DMFT. These can be included in cluster extensions which have been introduced both in real and momentum space [1,2]. Here we propose an idea to improve upon typical re-periodization problems of real space cluster DMFT and discuss the transformation of the Hubbard model between lattice orbital and so-called ligand orbital basis sets.

[1] Parcollet et al., Phys. Rev. Lett **92**, 226402 (2004)
[2] Kotliar et al., Phys. Rev. Lett **101**, 186403 (2008)

TT 15.4 Mon 15:45 H 0104

Functional RG investigation of the antiferromagnetic phase diagram of the three dimensional Hubbard model — •Jannis Ehrlich[1,2], Carsten Honerkamp[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institut für Theoretische Festkörperphysik, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen, Germany

The phase diagram of the three dimensional Hubbard model shows a phase transition to an antiferromagnetic ground state for repulsive interactions. While the Néel temperature can be obtained by Hartree Fock and the Heisenberg model for the limit of weak and strong interactions respectively, the intermediate range of interactions is subject of recent investigations.

We use the recently developed truncated unity functional renormalization group (TUfRG) approach, which has been used successfully to study the phase diagram of the extended 2D Hubbard model. This approach enables us to study this model on a fine momentum grid in an unbiased form, i.e. including the particle-particle and both particle-hole channels. We compare the resulting Néel temperature curve to those from previous studies using DΓA, DCA, QMC and dual fermion approaches.

TT 15.5 Mon 16:00 H 0104

A nonequilibrium DMFT+FLEX formalism for dynamics of d-wave superconductivity — •Sharareh Sayyad[1], Naoto Tsuji[2], Abolhassan Vaezi[3], Massimo Capone[4,5], Martin Eckstein[6], and Hideo Aoki[7,8,9] — [1]Institute for Solid State Physics, University of Tokyo, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan — [2]RIKEN Center for Emergent Matter Science (CEMS), Wako, 351-0198, Japan — [3]Department of Physics, Stanford University, Stanford, CA 94305, USA — [4]International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy — [5]CNR-IOM Democritos, Via Bonomea 265, I-34136 Trieste, Italy — [6]Department of Physics, University of Erlangen-Nürnberg, 91058 Erlangen, Germany — [7]Department of Physics, ETH Zürich, 8093 Zürich, Switzerland — [8]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, 305-8568, Japan — [9]Department of Physics, University of Tokyo, Tokyo 113-0033,Japan

For studying nonequilibrium dynamics of d-wave superconductors, we have constructed a nonequilibrium DMFT+FLEX method with a novel full-SU(2) slave-boson impurity-solver. An advantage of the method is that it can treat multiple phases on an equal footing for the Hubbard model on bipartite lattices. With the method, we expect to deal with the competition between antiferromagnetic and superconducting phases and to shed some light on the pseudogap physics with a slave-particle decomposition.

TT 15.6 Mon 16:15 H 0104

Lattice susceptibility calculations via a generalized CT-Hyb

QMC DMFT solver — •Julian Musshoff[1,2], Amin Kiani[1], and Eva Pavarini[1,3] — [1]Forschungszentrum Juelich GmbH, Institute for Advanced Simulation, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany — [3]JARA-HPC, RWTH Aachen University, Aachen, Germany

Linear-response functions are essential for comparing theory to experiments, and yet for strongly correlated systems their calculation is very challenging. The state-of-the-art technique for real materials is based on the dynamical mean-field (DMFT) approach and the local-vertex approximation. The bottleneck of this method is the calculation of local susceptibilities. Here we present an efficient scheme based on the massively-parallel general implementation of the continuous-time quantum Monte Carlo impurity solver of Ref. [1]. We use both the Legendre polynomial representation and a recently proposed numerical basis [2], and compare efficiency. To calculate lattice susceptibilities we solve the Bethe-Salpeter equation. We present results for the static and dynamical response functions of representative systems: $La_{2-x}Sr_xCuO_4$ and several orbitally ordered materials.

[1] A. Flesch, E. Gorelov, E. Koch, E. Pavarini, Phys. Rev. B **87**, (2013) 195141
[2] H. Shinaoka, J. Otsuki, M. Ohzeki, K. Yoshimi, Phys. Rev. B **96**, (2017) 035147

TT 15.7 Mon 16:30 H 0104

Effective models for correlated systems: effects of basis orthogonalization — •Qian Zhang and Erik Koch — Institute for Advanced Simulation, Forschungszentrum Jülich, 52428 Jülich, Germany

Setting up a many-body Hamiltonian requires choosing an orbital basis. Starting from atomic orbitals we have to deal with the non-orthogonality of the basis functions on different sites. We demonstrate the effects arising from orthogonalization on the example of the Hubbard dimer. First we study the change in hopping matrix elements with the bond length for the hydrogen molecule ion. Then we analyze the change in Coulomb matrix elements for the hydrogen molecule. In particular, we investigate how orthogonalization changes the on-site interaction as well as the direct and the exchange contributions to the long-range Coulomb terms. Finally, we discuss how the Coulomb tensor transforms under general (i.e. non-unitary) basis changes.

15 min. break.

TT 15.8 Mon 17:00 H 0104

Non-equilibrium dynamics of correlated materials: perturbation theory approach. — •Viktor Valmispild[1,2], Evgeny Gorelov[3], Nagamalleswara Dasari[4], Martin Eckstein[4], and Alexander Lichtenstein[1,2] — [1]Institute of Theoretical Physics, University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]European XFEL GmbH, Holzkoppel 4, 22869 Schenefeld, Germany — [4]Department of Physics, University of Erlangen-Nurnberg, 91058 Erlangen, Germany

We study the single-band Hubbard model on a infnite-dimensional and finite 2D square lattices in the presence of a large spatially uniform electric field. We study the model out of equilibrium using the Keldysh formalism and perturbation theory in the Coulomb interaction U. *Thus using time dependent dynamical mean-field theory and different impurity solvers: second order perturbation theory (SOPT) and fluctuation exchange approximation (FLEX) we investigate the behavior of the total energy of the system, double occupancy and spectral function as a function of time, strength of an external electric field and on-site Coulomb repulsion U.

TT 15.9 Mon 17:15 H 0104

Logarithmic corrections to the dynamical correlation functions of one-dimensional fermion systems with impurities — •Polina Matveeva[1], Dominik Strassel[1,2], Sebastian Eggert[1], and Imke Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [2]Competence Center for High Performance Computing, Fraunhofer ITWM, 67663 Kaiserslautern, Germany

Dynamical correlation functions are central objects in neutron scattering and photoemission spectroscopy experiments. They provide us with important information about the interactions and the spectrum of elementary excitations in strongly correlated systems. In one-dimensional gapless systems the correlation functions decay like power laws, with multiplicative logarithmic corrections from marginal operators. We study this corrections for general one-dimensional electron systems and the Heisenberg spin chain in the presence of impurities using bosonization. We obtain different multiplicative logarithmic corrections for the correlation functions in the boundary and bulk limits. Our results are supplemented by numerical Quantum Monte Carlo data. Finally, we discuss implications on the local density of states in the 1D-Hubbard model where previous numerical results revealed unexpectedly strong finite size corrections due to the marginal operator in the spin channel.

TT 15.10 Mon 17:30 H 0104

The dynamic structure factor in impurity-doped spin chains — •Kevin Jägering[1], Annabelle Bohrdt[2], Sebastian Eggert[1], and Imke Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern — [2]Department of physics and Institute for Advanced Study, Technische Universität München, 85748 Garching, Germany

The effects of impurities in spin-1/2 Heisenberg chains are recently experiencing a renewed interest due to experimental realizations in solid state systems and ultra-cold gases. The impurities effectively cut the chains into finite segments with a discrete spectrum and characteristic correlations, which have a distinct effect on the dynamic structure factor. Using bosonization and the numerical Density Matrix Renormalization Group we provide detailed quantitative predictions for the momentum and energy resolved structure factor in doped systems. Due to the impurities, spectral weight is shifted away from the antiferromagnetic wave-vector $k = \pi$ into regions which normally have no spectral weight in the thermodynamic limit. The effect can be quantitatively described in terms of scaling functions, which are derived from a recurrence relation based on bosonization. We present length-averaged and kintegrated results in terms of the doping concentration.

TT 15.11 Mon 17:45 H 0104

Influence of phonon-assisted tunneling on the thermoelectric transport through molecular quantum dots — •Andisheh Khedri[1,2], Theo Costi[2], and Volker Meden[1] — [1]Institut für Theorie der Statistischen Physik, RWTH Aachen University and JARA–Fundamentals of Future Information Technology, 52056 Aachen, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Research Center Jülich, 52425 Jülich, Germany

We investigate the effect of vibrational degrees of freedom on the thermoelectric transport through a single level quantum dot described by the spinless Anderson-Holstein impurity model. To study the effects of strong electron-phonon coupling in the linear response regime, we use the nonperturbative numerical renormalization group approach. We also compare our results, at weak to intermediate coupling, with those obtained by employing the functional renormalization group method, finding good agreement in this parameter regime. When applying a gate voltage at finite temperatures, the inelastic scattering processes, induced by phonon-assisted tunneling, result in an interesting interplay between electrical and thermal transport. We explore different parameter regimes and identify situations for which the thermoelectric power as well as the dimensionless figure of merit are significantly enhanced. By applying the functional renormalization group on the Keldysh contour, we further study the nonlinear thermoelectric transport in scenarios, in which the vibrating molecule is coupled to reservoirs held at different temperatures and chemical potentials.

TT 15.12 Mon 18:00 H 0104

Functional Renormalization Group Approach to Transport through a Kondo Quantum Dot — •Jan Diekmann and Severin G. Jakobs — Institute for Theory of Statistical Physics, RWTH Aachen University, 52056 Aachen, Germany

We study nonequilibrium properties of the Kondo model. For this we use the 1PI functional renormalization group (fRG), and work in Keldysh formalism. We choose a drone-fermion representation for the impurity spin.

As a first step we reproduce the leading logarithmic approximation in the weak-coupling regime ($T \gg T_K$) known as Poor Man's Scaling (PMS), which is an equilibrium result. Within fRG the employed approximation scheme emerges in a very natural way, and a clear interpretation of the flowing quantities is given as amplitudes of the renormalized 1PI vertex functions.

We devise a more sophisticated fRG approximation scheme as a direct extension of the one used to reproduce the PMS result. In particular we take frequency dependence and the self energy of the spin back

into account. With this we seek to describe the nonequilibrium case and to check whether the approach is suitable to describe the crossover to the strong-coupling regime.

A long term goal is to investigate the relation between different RG approaches to the nonequilibrium Kondo problem.

TT 15.13 Mon 18:15 H 0104

New hierarchical quantum master equation approach based on an interaction expansion: A first implementation for an Anderson impurity — •Jakob Bätge[1,2] and Rainer Härtle[1,2] — [1]Institut für theoretische Physik, Georg-August-Universität Göttingen — [2]Institute of Physics, University of Freiburg

The description of transport through open quantum systems is important for the quantum information processing or molecular electronics. Physical systems of interest are, for example, several coupled qubits or the voltage profile along a molecule. As the amount of possible states of quantum systems increases exponentially with the number of degrees of freedom, the numerical effort for exact techniques typically increases exponentially with system size. The exact treatment of large systems might open the view on new physical effects. The numerically exact hierarchical quantum master equation approach (HQME)[1-3] is based on a systematically improvable hybridization expansion and predicts the time-evolution of the quantum system. Due to its time-local formulation stationary state properties can be studied. Here we present an extension of the HQME, which includes an additional expansion in the many-body interaction. The new approach focuses on the low-particle reduced density matrices and hence shows a power law dependence on system size. The newly extended HQME is still a numerically exact approach. A first implementation for the well studied Anderson impurity model shows the usefulness of the new method.

[1] J. Jin *et al.*, JCP **128**, 234703 (2008)
[2] R. Härtle *et al.*, PRB **88**, 235426 (2013)
[3] R. Härtle *et al.*, PRB **92**, 085430 (2015)

TT 15.14 Mon 18:30 H 0104

Auxiliary master equation approach within stochastic wave functions — •Delia Fugger, Max Sorantin, Antonius Dorda, Wolfgang von der Linden, and Enrico Arrigoni — Institute of Theoretical and Computational Physics, Graz University of Technology, Austria

The auxiliary master equation approach AMEA [1,2] allows us to assess the time evolution and, in particular, the steady state properties of quantum impurities and small molecules in as well as out of equilibrium. It is based on a mapping of the physical system to an auxiliary open quantum system, whose dynamics is determined by a Lindblad master equation. In this talk I will present results obtained from a scheme to address the resulting Lindblad equation based on the stochastic evolution of the wave function [3-6]. A set of wave functions sampling the density operator is propagated by piecewise deterministic time evolutions, which are interrupted by stochastic jump processes [6]. This implementation aims at extending the capabilities of the AMEA approach as well as making it more efficient.

[1] E. Arrigoni *etal.*, PRL **110**, 086403 (2013)
[2] A. Dorda *etal.*, PRB **89**, 165105 (2014) + PRB **92**, 125145 (2015)
[3] J. Dalibard *etal.*, PRL **68**, 580 (1992)
[4] K. Mølmer *etal.*, J. Opt. Soc. Am. B **10**, 524 (1993)
[5] H.-P. Breuer *etal.*, PRA **56**, 2334 (1997)
[6] B. Kappler, PhD thesis, University of Freiburg (1998)