TT 70: Correlated Electrons: General Theory 2

Time: Friday 9:30–11:00 Location: H24

TT 70.1 Fri 9:30 H24

Prethermalization and thermalization of weakly interacting quantum systems — •Marcus Kollar and Michael Stark — Theoretical Physics III, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg

When a quantum many-body system is suddenly forced out of equilibrium, it is expected to relax to the thermal state predicted by statistical mechanics, which depends only on energy and particle number. However, integrable systems usually relax instead to a nonthermal state, because a detailed memory on the initial conditions persists due to the many constants of motion. A special situation arises for weakly interacting systems: because of the nearby integrable, noninteracting Hamiltonian they are first trapped in a so-called prethermalized state, and can thermalize only at a later stage [1]. This prethermalization plateau is again due to a large number of – now only approximate – constants of motion and can be represented by a generalized Gibbs ensemble [2]. As the time evolution continues, we can describe the decay of this quasistationary state and the crossover to the thermal state by a kinetic integro-differential equation, with good quantitative agreement for quenches to small Hubbard interaction [3]. This approach provides a controlled and conceptually straightforward description of the thermalization dynamics and establishes that thermalization can occur even in the perturbative regime.

[1] M. Moeckel and S. Kehrein, PRL **100**, 175702 (2008).
[2] M. Kollar, F. A. Wolf, and M. Eckstein, PRB **84**, 054304 (2011).
[3] M. Eckstein, M. Kollar, and P. Werner, PRL **103**, 056403 (2009).

TT 70.2 Fri 9:45 H24

Steady-State Nonequilibrium Dynamical Mean Field Theory: an auxiliary Master Equation approach — •Enrico Arrigoni, Michael Knap, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics TU Graz, 8045 Graz, Austria

We present an approach to deal with nonequilibrium steady state properties of strongly correlated quantum many-body systems based on dynamical mean-field theory (DMFT). The impurity solver is based on the exact solution of an auxiliary system consisting of a finite number of bath sites coupled to the interacting impurity and to two Markovian reservoirs. The method can be seen as the extension of the DMFT impurity solver for the nonequilibrium case based on exact diagonalisation. We apply the method to study nonlinear quantum transport across correlated heterostructures.

TT 70.3 Fri 10:00 H24

A variational cluster approach to strongly correlated quantum systems out of equilibrium — •Martin Nuss, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology, Petersgasse 16 8010 Graz , Austria

The theoretical understanding of the non-equilibrium behaviour of strongly correlated quantum many-body systems is a long standing challenge, which has become increasingly relevant with the progress made in the fields of molecular-and nano- electronics, spintronics, spectroscopy or quantum optics and simulation. We report on the development of non-equilibrium cluster perturbation theory, and its variational improvement, the non-equilibrium variational cluster approach for steady-state situations. Both methods are based on the Keldysh Green's function technique which allows accessing single particle dynamic quantities. These flexible and versatile techniques can in principle be applied to any fermionic / bosonic lattice Hamiltonian, including multi-band and multi-impurity systems. We present results for the steady-state of molecular / nanoscopic devices under bias including the effects of electron-electron interactions and magnetic fields.

TT 70.4 Fri 10:15 H24

Dynamics in model systems of strongly interacting electrons — •Malte Behrmann[1], Michele Fabrizio[2], and Frank Lechermann[1] — [1]I. Institut für Theoretische Physik, Jungiusstr. 9, 20355 Hamburg — [2]SISSA, via Bonomea 265, 34136 Trieste

Explicit time-dependent phenomena in strongly interacting quantum systems have recently become of great interest, especially in view of novel challenging experiments with time-dependent probing. Understanding the dynamic evolution of electronic correlations is a key issue in describing the non-equilibrium physics taking place in concrete material systems, e.g. after photo-excitation. This talk discusses work performed on the dynamics of strongly correlated model systems by means of a time-dependent slave-boson mean-field theory that allows for full rotational invariance in spin and orbital space. Therewith a generic time-dependent Mott scenario is accessible and the dynamics of quasiparticle and multiplet degrees of freedom may be monitored. Our approach is closely related to the time-dependent Gutzwiller framework by Fabrizio and coworkers [1].

[1] M. Schiró and M. Fabrizio, Phys. Rev. Lett. 105, 076401 (2010)

TT 70.5 Fri 10:30 H24

Calculations of resonant x-ray emission spectra in compounds with localized f-electrons — •Jindrich Kolorenc[1], Alexander B. Shick[1,2], and Roberto Caciuffo[2] — [1]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic — [2]European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe, Germany

We discuss a theoretical description of the resonant x-ray emission spectroscopy (RXES) that is based on the Anderson impurity model. The theory builds on the ideas from [1-3] and extends them to take into account the f-electron multiplets. The parameters of the impurity model are taken from the LDA+DMFT calculations, and the coherent second-order optical process is calculated using the Lanczos method. The theory is applicable across the whole f series, not only in the limits of nearly empty (La, Ce) or nearly full (Yb) f shell. We illustrate the method on selected f-electron systems.

[1] O. Gunnarsson and K. Schönhammer, Phys. Rev. B **28**, 4315 (1983)
[2] S. Tanaka, H. Ogasawara, Y. Kayanuma, and A. Kotani, J. Phys. Soc. Jpn. **58**, 1087 (1989)
[3] M. Nakazawa, S. Tanaka, T. Uozumi, and A. Kotani, J. Phys. Soc. Jpn. **65**, 2303 (1996)

TT 70.6 Fri 10:45 H24

Continuous Estimators for CT-HYB — •Pavel Augustinský — University of Augsburg

We present an improved algorithm for measurement of the Green's function in the hybridization-expansion quantum Monte Carlo. The method is based on using continuous rather then discrete delta-function estimators. It fixes drawbacks of the standard approach at low perturbation orders and it can produce high-accuracy data for numerical analytical continuation of the selfenergy.