TT 4: CE: Quantum Impurities, Kondo Physics

Time: Monday 10:15–12:45 Location: H21

TT 4.1 Mon 10:15 H21

Kondo physics in chaotic and regular mesoscopic systems — •Rainer Bedrich[1], Sebastien Burdin[2], and Martina Hentschel[1] — [1]Max Planck Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Condensed Matter Theory Group, CPMOH, UMR 5798, Université de Bordeaux I, 33405 Talence, France

We study the mesoscopic Kondo box, consisting of a quantum spin 1/2 interacting with an electronic bath as can be realized by a magnetic impurity coupled to electrons on a quantum dot using a mean-field approach for the Kondo interaction. Its numerical efficiency allows us to analyze the Kondo temperature, the local magnetic susceptibility, and the conductance statistics for a large number of samples as a function of the temperature, the Kondo coupling, and the number of electrons on the dot. Here, in contrast to the Kondo effect occurring in a bulk material, the metallic host is characterized by a finite mean level spacing, generating deviations from the universal behavior. We contrast the behavior of chaotic systems, described within the random matrix theory, to that of regular systems, e.g. rectangular quantum dots. Besides the system geometry we find that the boundary of the dot affects the physical properties in a significant way.

TT 4.2 Mon 10:30 H21

Lattice density-functional theory of the single-impurity Anderson model — •Waldemar Töws and Gustavo Pastor — Institut für Theoretische Physik, Universität Kassel, Germany

A lattice density-functional theory of the single-impurity Anderson model is presented. In this approach the basic variable is the single-particle density matrix $\gamma_{ij\sigma}$ with respect to the lattice sites. The central interaction-energy functional $W[\gamma]$ is shown to be invariant under unitary transformations of orbitals in the conduction band. This property is exploited to find a unitary transformation such that the localized impurity orbital experiences charge fluctuations only to a particular single-particle state of the conduction band. A simple analytical approximation to $W[\gamma]$ is then derived from the solution of the resulting two-level problem. This so-called two-level approximation can be shown to be exact in the limit of a totally degenerated conduction band as well as in the limit of widely separated discrete conduction-band levels. The minimization of the total energy functional $E[\gamma]$ with respect to $\gamma_{ij\sigma}$ yields the ground-state properties such as the kinetic, interaction and total energy, as well as the occupation and spin polarization of the impurity orbital. The results obtained with the two-level-approximation for finite rings having $N \leq 12$ sites are in agreement with exact Lanczos diagonalizations in all interaction regimes, from weak to strong correlations. In particular the singlet-triplet gap, which determines the Kondo temperature, is correctly described. This constitutes a remarkable qualitative improvement over mean-field approximations. Advantages and limitations of this approach are discussed.

TT 4.3 Mon 10:45 H21

A weak coupling CTQMC study of the single impurity and periodic Anderson models with s-wave superconducting baths — •David J. Luitz and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, Deutschland

We apply the unbiased weak-coupling continuous time quantum Monte Carlo (CTQMC) method to review the physics of a single magnetic impurity coupled to s-wave superconducting leads described by the BCS reduced Hamiltonian. As a function of the superconducting gap Δ, we study the first order transition between the singlet and doublet (local moment) states by examining the crossing of the Andreev bound states in the single particle spectral function. Within DMFT, this impurity problem provides a link to the periodic Anderson model with superconducting conduction electrons (BCS-PAM). The first order transition observed in the impurity model is reproduced in the BCS-PAM and is signalized by the crossing of the low energy excitations in the local density of states. The momentum resolved single particle spectral function in the singlet state reveals the coherent, Bloch-like, superposition of Andreev bound states. In the doublet or local moment phase the single particle spectral function is characterized by incoherent quasiparticle excitations.

TT 4.4 Mon 11:00 H21

Spectral function of the Anderson impurity model at finite temperatures — •Aldo Isidori[1], Hermann Freire[2], and Peter Kopietz[1] — [1]Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany — [2]Instituto de Física, Universidade Federal de Goiás, 74.001-970, Goiânia-GO, Brasil

Using the functional renormalization group (FRG) and the numerical renormalization group (NRG), we calculate the spectral function of the Anderson impurity model at zero and finite temperatures. In our FRG scheme spin fluctuations are treated non-perturbatively via a suitable Hubbard-Stratonovich field, but vertex corrections are neglected. Although at zero temperature this FRG scheme does not quantitatively reproduce the known exponential narrowing of the Kondo resonance for large values of the interaction, a comparison with the numerically exact NRG results shows that the FRG gives a reasonable description of the spectral line-shape both at high energies and for temperatures larger than the Kondo scale.

15 min. break

TT 4.5 Mon 11:30 H21

The Kondo exciton: a quantum quench towards strong spin-reservoir correlations — Hakan E. Türeci[1], •Markus Hanl[2], Martin Claassen[1], Andreas Weichselbaum[2], Theresa Hecht[2], Bernd Braunecker[3], Alexander Govorov[4], Leonid Glazman[5], Jan von Delft[2], and Atac Imamoglu[1] — [1]ETH-Zürich — [2]Ludwig-Maximilians-Universität München — [3]University of Basel — [4]Ohio University — [5]Yale University

We consider a semiconductor quantum dot coupled to a Fermionic reservoir, and study the dynamics after a quantum quench induced by the sudden creation of an exciton via optical absorption of an incident photon of definite frequency [1]. The subsequent emergence of correlations between the spin degrees of freedom of the dot and reservoir, ultimately leading to the Kondo effect, can be probed via a simple optical absorption experiment. The resulting lineshape is found to unveil three very different dynamical regimes, corresponding to short, intermediate and long times after the initial excitation, which are in turn described by the three fixed points of the single-impurity Anderson Hamiltonian. At low temperatures and just beyond the absorption threshold, the lineshape is dominated by a power-law singularity, with an exponent that is a universal function of magnetic field and gate voltage. Analytical results obtained by fixed-point perturbation theory are in excellent agreement with numerical renormalization group results.

[1] arXiv:0907.3854v1 [cond-mat.str-el]

TT 4.6 Mon 11:45 H21

Non-equilibrium Scaling Properties of a Double Quantum Dot System: Comparison between Perturbative Renormalization Group and Flow Equation Approach — •Verena Koerting[1], Peter Fritsch[2], and Stefan Kehrein[2] — [1]Niels Bohr Institute, Universitetsparken 5, DK-2100 København Ø, Denmark — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

Since the discovery of Kondo physics in quantum dots, its far-from-equilibrium properties have generated considerable theoretical interest. By now several new theoretical methods have analyzed the interesting interplay of non-equilibrium physics and correlation effects in this model.

In this talk the differences and commons between the flow equation method out of equilibrium [1] and the frequency-dependent poor man's scaling approach [2] will be presented. We will focus on the non-equilibrium properties of a double quantum dot system, which will turn out to be a particularly suitable testing ground while being experimentally interesting in its own right.

[1] S. Kehrein, PRL 95, 056602 (2007).
[2] A. Rosch, J. Paaske, J. Kroha, and P. Wölfle, PRL 90, 076804 (2003).

TT 4.7 Mon 12:00 H21

Relaxation vs decoherence: Spin and current dynamics in the

anisotropic Kondo model at finite bias and magnetic field — •Mikhail Pletyukhov, Dirk Schuricht, and Herbert Schoeller — Institut für theoretische Physik A, RWTH Aachen, Germany

Using a nonequilibrium renormalization group method we study the real-time evolution of spin and current in the anisotropic Kondo model (both antiferromagnetic and ferromagnetic) at finite magnetic field h_0 and bias voltage V. We derive analytic expressions for all times in the weak-coupling regime $\max\{V, h_0, 1/t\} \gg T_c$ (T_c = strong coupling scale). We find that all observables decay both with the spin relaxation and decoherence rates $\Gamma_{1/2}$. Various V-dependent logarithmic, oscillatory, and power-law contributions are predicted. The low-energy cutoff of logarithmic terms is generically identified by the difference of transport decay rates. For small times $t \ll \max\{V, h_0\}^{-1}$, we obtain universal dynamics for spin and current.

TT 4.8 Mon 12:15 H21

Discretization artifacts in the TD-NRG — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

One approach to study the nonequilibrium dynamics of quantum impurity systems is the time-dependent numerical renormalization-group (TD-NRG). Like the conventional NRG the TD-NRG relies on a logarithmic discretization of the bath continuum by mapping the bath onto a Wilson chain. We demonstrate in the real-time dynamics of a toy model, the resonant level model, that the group velocity of the wave propagation along the Wilson Chain is strongly position dependent. The induced reflection of waves corrupt the calculation of the time-dependent impurity occupation. The time period for which the occupation number is calculated reliably can be extended by using a hybrid approach combining different discretizations of the bath continuum.

TT 4.9 Mon 12:30 H21

Nonequilibrium functional RG with frequency dependent vertex function – a study of the single impurity Anderson model — •Severin Jakobs[1,2], Mikhail Pletyukhov[1,2], and Herbert Schoeller[1,2] — [1]Institut für Theoretische Physik A, RWTH Aachen University, D-52056 Aachen, Germany — [2]JARA – Fundamentals of Future Information Technologies, Germany

We investigate nonequilibrium properties of the single impurity Anderson model by means of the functional renormalization group (fRG) within Keldysh formalism. We present how the level broadening $\Gamma/2$ can be used as flow parameter for the fRG. This choice preserves important aspects of the Fermi liquid behaviour that the model exhibits in case of particle-hole symmetry. An approximation scheme for the Keldysh fRG is developed which accounts for the frequency dependence of the two-particle vertex in a way similar but not equivalent to a recently published approximation to the equilibrium Matsubara fRG. Our method turns out to be a rather flexible tool for the study of weak to intermediate on-site interactions $U \lesssim 3\Gamma$. In equilibrium we find excellent agreement with NRG results for the linear conductance at finite gate voltage, magnetic field, and temperature. In nonequilibrium, our results for the current agree well with TD-DMRG. For the nonlinear conductance as function of the bias voltage, we propose reliable results at finite magnetic field and finite temperature. Furthermore, we demonstrate the exponentially small scale of the Kondo temperature to appear in the second order derivative of the self-energy.