TT 46: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Friday 10:15–12:45 Location: HSZ 301

TT 46.1 Fri 10:15 HSZ 301

Spatial Variation of Fano Resonances in the STM Tunneling Density of States due to Sub-Surface Kondo Impurities — •Henning Prüser, Martin Wenderoth, Alexander Weismann, and Rainer G. Ulbrich — IV. Physikalisches Institut; Georg-August Universität Göttingen, Germany

Single magnetic atoms buried in copper have been investigated using low temperature scanning tunneling spectroscopy (STS). Cu alloys with a small amount ($\leq 0.02\%$) of iron and cobalt were epitaxially grown on a Cu(100) substrate. The embedded Fe and Co impurities were identified in STM topographies at 6K by their fourfold symmetric topography patterns. From comparison with scattering theory in anisotropic media we obtain their individual depths, ranging from 3 to 9 ML. In the STS data both Fe and Co show the expected Kondo feature: a Fano resonance centered at E_F, and a width directly related to the Kondo temperature T_K. Our T_K values for Fe and Co corroborate parameters deduced from bulk measurements. The line shape of the LDOS spectrum around E_F depends strongly on (i) the lateral distance of the tip from the impurity and (ii) the impurity depth below the surface. As a function of these two lengths the line shape shows an oscillatory behavior. The path length period equals the Friedel wave length of copper as predicted by theory [1, 2]. Work supported by DFG SFB 602 TPA3.

[1] Újsághy et al., PRL 82, 2557, 2000
[2] Plihal et al., PRB 63, 085404, 2001

TT 46.2 Fri 10:30 HSZ 301

Superperturbation solver for quantum impurity models — •Sergey Brener[1], Alexander Lichtenstein[1], Hartmut Hafermann[1], Christoph Jung[1], Kelly Patton[1], Mikhail Katsnelson[2], and Alexei Rubtsov[3] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Deutschland — [2]Institute for molecules and materials, Radboud University of Nijmengen, The Netherlands — [3]Department of physics, Moscow State University, Russia

We present a very efficient solver for a general Anderson impurity model. It is based on a perturbation around a solution obtained from exact diagonalization using a small number of bath sites. Satisfactory agreement is found for a single bath site over a wide range of parameters. The method proves superior to QMC for a calculation of spectral properties for real energies by analytical continuation due to the absence of statistical noise. It can also be applied to calculating of two-particle correlators, which allows to investigate, for example, transport properties of nano-systems or spin correlations which are essential for description of a Kondo cloud.

TT 46.3 Fri 10:45 HSZ 301

Kondo effect in a mesoscopic interacting electron system — •Stefan Rotter[1], Hakan Türeci[2], Yoram Alhassid[3], and Douglas Stone[3] — [1]TU–Vienna, Austria — [2]ETH–Zürich, Switzerland — [3]Yale, USA

We study the problem of a quantum dot with finite level spacing which is coupled anti-ferromagnetically to a Kondo spin ("Kondo box"). In particular, we investigate the influence of a ferromagnetic exchange interaction among the dot electrons as described by the "Universal Hamiltonian". The problem is solved numerically by diagonalizing the system Hamiltonian in a good-spin basis and analytically in the weak and strong Kondo coupling limits [1]. We provide an analytical solution for the effective strong coupling Hamiltonian which contains new interaction terms unknown from the conventional Kondo problem. The interplay between Kondo and ferromagnetic exchange correlations affects the ground-state spin of the system and can be probed with experimentally tunable parameters.

[1] S. Rotter, H. E. Türeci, Y. Alhassid, A. D. Stone, Phys. Rev. Lett. 100, 166601 (2008).

TT 46.4 Fri 11:00 HSZ 301

Kondo physics in regular and chaotic mesoscopic systems — •Rainer Bedrich[1], Sebastien Burdin[2], and Martina Hentschel[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [2]Institute of Theoretical Physics, Cologne University

We study the Kondo effect induced by a magnetic impurity interacting with a small metallic grain. Here, in contrast with the Kondo effect occurring in a bulk material, the metallic host is characterised by a finite mean level spacing. This low energy scale can generate deviations from the universal behavior which would be expected for a bulk system. The physical properties of the system are computed within a mean-field approximation for the Kondo interaction. In particular, we study the local magnetic susceptibility, the conductance, and the local density of electronic states as a function of the temperature, the mean level spacing, the Kondo coupling, and the number of electrons on the dot. As a first step, we consider a constant distribution of the non-interacting energy levels. Our results are in agreement with the results obtained from different approaches, suggesting that the mean-field approximation is valid. A more realistic situation is then considered, for which the energy levels are distributed randomly. This is realised within the random matrix theory. Finally we compare between chaotic and regular (e.g. parabolic quantum dot) systems.

15 min. break

TT 46.5 Fri 11:30 HSZ 301

Kondo decoherence: finding the right spin model for iron impurities in gold and silver — •Theodoulos Costi[1], Lars Bergqvist[1], Andreas Weichselbaum[2], Jan von Delft[2], Phivos Mavropoulos[1], Peter Dederichs[1], Tobias Micklitz[3,5], Achim Rosch[3], Francois Mallet[4], Laurent Saminadayar[4], and Christopher Bäuerle[4] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience,Ludwig-Maximilians-Universität München, 80333 München, Germany — [3]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [4]Institut Néel - CNRS and Université Joseph Fourier, 38042 Grenoble Cedex 09, France — [5]Materials Science Division, Argonne National Laboratory, Argonne, Illinois 60439, USA

We exploit the decoherence of electrons due to magnetic impurities, studied via weak localization, to resolve a longstanding question concerning the classic Kondo systems of Fe impurities in the noble metals gold and silver: which Kondo-type model yields a realistic description of the relevant multiple bands, spin and orbital degrees of freedom? Previous studies suggest a fully screened spin S Kondo model, but the value of S remained ambiguous. We perform density functional theory calculations that suggest $S = 3/2$. We also compare previous and new measurements of both the resistivity and decoherence rate in quasi 1-dimensional wires to numerical renormalization group predictions for $S = 1/2, 1$ and $3/2$, finding excellent agreement for $S = 3/2$.

TT 46.6 Fri 11:45 HSZ 301

Flow Equation Analysis of a Kondo Dot in a Magnetic Field — •Peter Fritsch and Stefan Kehrein — Physics Department, ASC, and CeNS, Ludwig-Maximilians-Universität, Theresienstrasse 37, 80333 Munich, Germany

Using infinitesimal unitary transformations (flow equations) [1,2] we derive a consistent perturbative scaling picture of a Kondo dot in a magnetic field for both equilibrium and non-equilibrium (dc voltage bias) situations. We work out the spin dynamics and the T-Matrix as functions of magnetic field, voltage bias and temperature. In particular, we report on the behavior of both the static spin susceptibility [3] and the magnetization including leading logarithmic corrections. This work is a generalization of the previous flow equation analysis of the non-equilibrium Kondo model in zero magnetic field [1,2,3].

[1] S. Kehrein, The Flow Equation Approach to Many-Particle Systems, Springer Tracts in Modern Physics 217
[2] S. Kehrein, Phys. Rev. Lett. 95, 056602 (2005)
[3] P. Fritsch and S. Kehrein, arxiv:0811.0759

TT 46.7 Fri 12:00 HSZ 301

Real-time renormalization group in frequency space: A complete 2-loop analysis of the nonequilibrium anisotropic Kondo model at finite magnetic field — Herbert Schoeller[1,2] and •Frank Reininghaus[1,2] — [1]Institut für Theor. Physik A, RWTH Aachen University, Germany — [2]JARA-Fundamentals of Future Information Technology

We use a recently developed real-time renormalization group method

in frequency space (RTRG-FS) to describe nonequilibrium phenomena in generic fermionic quantum system coupled weakly to several reservoirs via spin and/or orbital fluctuations. Within a 2-loop analysis we derive analytic formulas for the nonlinear conductance and the kernel determining the time evolution of the reduced density matrix. We apply the general formalism to the nonequilibrium anisotropic Kondo model at finite magnetic field. Besides the nonlinear conductance and the magnetic susceptibility, we calculate for the first time the spin relaxation and dephasing rates and the renormalized g-factor beyond leading order. Furthermore, we show in all orders in the exchange coupling that the RG flow of the vertices is cut off by relaxation and dephasing rates.

TT 46.8 Fri 12:15 HSZ 301

Dynamical spin-spin correlation functions in the Kondo model out of equilibrium — •Dirk Schuricht and Herbert Schoeller — Institut fuer Theoretische Physik A, RWTH Aachen

We calculate the dynamical correlation function of a Kondo spin coupled to two noninteracting leads held at different chemical potentials. We use real-time renormalization group in frequency space up to 2-loop. The formalism includes the renormalization of the vertices and the Liouvillian determining the dynamics of the reduced density matrix of the local spin. As a result the cutoff by relaxation/dephasing rates, temperature, external frequency, Laplace variable of the time dynamics, and the voltage can be described on a microscopic level. We show show how nonequilibrium correlation function in real-frequency space can be calculated in Matsubara space without the need of any analytical continuation.

TT 46.9 Fri 12:30 HSZ 301

Using DMRG to Study Quantum Impurity Models with Time-Dependent Hamiltonians — •Cheng Guo[1], Andreas Weichselbaum[1], Stefan Kehrein[1], Tao Xiang[2], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience, Ludwig-Maximilians-Universität München, D-80333 München, Germany — [2]Institute of Physics, Chinese Academy of Sciences, P.O. Box 603, Beijing 100080, China

We use the adaptive time-dependent density matrix renormalization group method (t-DMRG) to study the nonequilibrium dynamics of a benchmark quantum impurity system which has a time-dependent Hamiltonian. This model is a resonant-level model, obtained by a mapping from a certain ohmic spin-boson model describing the dissipative Landau-Zener transition. Some techniques from the numerical renormalization group method (NRG) are borrowed to transform this model to a DMRG-friendly form. We compare t-DMRG results with exact results at zero temperature and find very good agreement. We also give a physical interpretation of the numerical results.