TT 15: Correlated Electrons: Quantum Impurities, Kondo Physics 1

Time: Monday 16:45–18:00 Location: BH 334

TT 15.1 Mon 16:45 BH 334

Two-electron transfer dynamics in a donor-acceptor system coupled to a dissipative bosonic bath — •Christian Kleine and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We model a donor-acceptor (DA) system coupled to a dissipative bosonic bath which is motivated by electron charge transfer within a DNA base pair. Using the time-dependent numerical renormalization-group (TD-NRG) we study the time-dependent electron dynamics in the DA system where two excess charges are initially localised on the donor. We consider the influence of the coupling strength of the DA system to the bosonic bath on the thermalisation. Additionally we introduce a finite bias between the donor and acceptor level and investigate the crossover between the two different regimes where the charge transfer is dominated by sequential or pairwise electron hopping.

TT 15.2 Mon 17:00 BH 334

Hybrid TD-NRG and tDMRG method — •Fabian Güttge and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

We present a non-equilibrium hybrid method which uses the numerical renormalization group (NRG) to generate an effective low energy Hamiltonian. This Hamiltonian is then solved with the density matrix renormalization group (DMRG) thereby reducing the major drawbacks of both methods: (i) discretization errors are minimized by not using a pure Wilson chain and (ii) long time scales can be simulated even for a very large bandwidth. The validity of this method is established by comparing the results to exact results for the resonant level model (RLM). We also apply this new NRG+DMRG hybrid method to the interacting RLM, which is not exactly solvable, and compare with analytic results in the limit $U \to \infty$.

TT 15.3 Mon 17:15 BH 334

NRG calculations of the magnetization of isotropic and anisotropic Kondo impurities — •Martin Höck and Jürgen Schnack — Universität Bielefeld, Fakultät für Physik, Bielefeld, Germany

The deposition of magnetic molecules on suitable substrates renders the addressing and thus manipulation of individual molecules possible and might facilitate their use for information storage or quantum computing purposes. However, the magnetic properties of the molecules, which are crucial for the proposed applications, will in general be influenced by the interaction with the substrate. Our goal is to better understand the form and extent of this effect by studying simplified model systems.

To this end, we perform Numerical Renormalization Group (NRG) calculations for single-impurity Kondo models with additional uniaxial anisotropy and a local or bulk magnetic field. The impurity part of the model might thus serve as a minimal representation of a magnetic molecule. We focus on the impurity magnetization, which has been measured in a number of experiments using XMCD and STM, and study its dependence on temperature and applied field for different anisotropy parameters. In case of a "hard axis" anisotropy, the magnetic field can lead to effective groundstate degeneracies and can therefore induce Kondo screening effects.

TT 15.4 Mon 17:30 BH 334

Numerical Renormalization Group for the Partially Broken SU(3) Kondo Model: 2-Channel Kondo Fixed Point. — •Evaristus Fuh Chuo, Laszlo Borda, and Johann Kroha — Physikalisches Institut der Universität Bonn, Germany

We use the numerical renormalization group (NRG) to investigate the partially broken two-channel SU(3) Kondo model with conserved conduction electron spin, comprised of a quantum impurity with a unique ground state and an excited doublet of the SU(2) subgroup of SU(3). The model was proposed earlier by Arnold et al. [1] to describe rotational impurities in a metal, like hydrogen ions in the interstitial space of a lattice, in order to explain the conductance anomalies (zero-bias anomaly and conductance spikes) found by Ralph and Buhrman [2] in point contact spectroscopy on ultrasmall Cu point contacts. We find a downward renormalization of the excited state energy by the Kondo correlations in the SU(2) doublet. In a wide range of parameter values this stabilizes the two-channel Kondo fixed point, in full agreement with the earlier perturbative RG results of Arnold et al. [1]. We map out the phase diagram of the model in the parameter space of excited-state level spacing and of the Kondo couplings within the excited state doublet and between the impurity ground and excited states, respectively. The robustness of the model with respect to dynamical screening as well as to coupling to higher impurity excitations is discussed.

[1] M. Arnold, T. Langenbruch, and J. Kroha, Phys. Rev. Lett. **99**, 186601 (2007).
[2] D. C. Ralph and R. A. Buhrman, Phys. Rev. Lett. **69**, 2118 (2007).

TT 15.5 Mon 17:45 BH 334

Finite-frequency noise of the anisotropic Kondo model at finite bias and magnetic field: a real-time renormalization group analysis — •Sarah Müller, Sabine Andergassen, Dirk Schuricht, Mikhail Pletyukhov, and Herbert Schoeller — Institut für Theorie der Statistischen Physik und JARA - Fundamentals of Future Information Nanotechnology, RWTH Aachen University

The non-equilibrium electron transport through mesoscopic systems dominated by spin fluctuations is affected by the relaxation and decoherence processes resulting from the coupling of the spin to its environment. The understanding of their origin and their impact on the transport properties is of fundamental importance. We here study the finite-frequency noise of a quantum dot in the Kondo regime in presence of a magnetic field by using the real-time renormalization group in frequency space [1]. Based on a systematic expansion in the reservoir-system coupling, we integrate out the reservoir degrees of freedom and provide an analytic solution of the resulting two-loop RG equations in the weak-coupling regime. In particular, the relaxation and decoherence rates characterizing the non-equilibrium transport of mesoscopic systems emerge during the RG flow. We extend the approach of Ref. [2] to derive analytic expressions for the finite-frequency noise in the stationary state. We discuss the results in relation to recent experiments [3].

[1] H. Schoeller, Eur. Phys. J. Special Topics 168, 179 (2009).
[2] D. Schuricht and H. Schoeller, Phys. Rev. B 80, 075120 (2009).
[3] J. Basset et al., arXiv:1110.1570.