TT 8: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Monday 10:15–13:00 Location: H21

TT 8.1 Mon 10:15 H21

Discovery of a new phase with magnetic short range correlations and its possible relevance for the hidden order in URu_2Si_2 — •Steffen Sykora[1] and Klaus W. Becker[2] — [1]IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — [2]Technische Universität Dresden, D-01062 Dresden, Germany

In this paper we discuss a new phase of the Kondo lattice model which arises from the competition of Kondo and RKKY energy scales. Normally the Kondo lattice model is used to capture the low-energy physics of heavy fermion systems. However, according to the so-called Doniach picture the Kondo state will be replaced by an antiferromagnetic state for the case that the Kondo energy scale becomes smaller than the magnetic interaction between magnetic ions. In the present study we start instead from a modified electronic one-particle dispersion which avoids nesting of particle-hole excitations. Thus the magnetic ordered state should be suppressed which provides an opportunity for the inset of a new low-energy state with competing Kondo and magnetic energies. As will be shown, this new state avoids magnetic symmetry breaking but leads to a number of physical properties which are relevant for the understanding of the hidden order state in URu_2Si_2.

TT 8.2 Mon 10:30 H21

Effect of a magnetic moment on quantum spin Hall edge transport — •Florian Geissler[1], Jukka Väyrynen[2], and Leonid Glazman[2] — [1]Universität Würzburg, Würzburg, Germany — [2]Yale University, New Haven, USA

A local magnetic moment coupled to one dimensional helical transport channels, such as the edge states of a 2D quantum spin Hall insulator, can be a source of time-reversal invariant backscattering. We study the resulting correction to the conductance as a function of temperature T, dc bias voltage V and the repulsive electron-electron interactions characterized by the Luttinger liquid parameter $K < 1$. Such corrections display a characteristic power law dependence on V or T, with distinct scaling in the two regimes above and below the Kondo temperature, corresponding to the mechanisms of elastic and inelastic single-particle backscattering, respectively.

At energies above the Kondo temperature, the coupling to the magnetic moment can be considered weak. In this regime, if interactions are very small, $K \approx 1$, the correction to the conductance remains almost insensitive to V/T, even at high values of V/T. If electron interactions are more effective, $3/4 < K < 1$, this leads to corrections with small power law exponents below 1/2. Our findings agree with the experimental observation of a weak temperature dependence of the conductance in presumably weakly interacting QSH systems like HgTe and may further provide an alternative explanation for the recent experiment in more strongly correlated InAs/GaSb samples [1].

[1] Li et al., PRL **115**, 136804 (2015)).

TT 8.3 Mon 10:45 H21

The numerical renormalization group and symmetric multi-orbital models — •Andreas Weichselbaum[1], Katharina Stadler[1], Jan von Delft[1], Zhiping Yin[2], Gabriel Kotliar[2], and Andrew Mitchell[3] — [1]Ludwig Maximilians University, Munich, Germany — [2]Rutgers University, New Jersey, USA — [3]Utrecht University, The Netherlands

The numerical renormalization group (NRG) is a highly versatile and accurate method for the simulation of (effective) fermionic impurity models. Despite that the cost of NRG is exponential in the number of orbitals, by now, symmetric three-band calculations have become available on a routine level. [1] Here we present a recent detailed study on the spin-orbital separation in a three-band Hund metal with relevance for iron-pnictides via the dynamical mean field theory (DMFT). [2] In cases, finally, where the orbital symmetry is broken, we demonstrate that interleaved NRG [3] still offers an accurate alternative approach within the NRG with dramatically improved numerical efficiency at comparable accuracy relative to conventional NRG.

[1] A. Weichselbaum, Annals of Physics **327**, 2972 (2012)
[2] K. Stadler et al., PRL **115**, 136401 (2015)
[3] A. Mitchell et al., PRB **89**, 121105(R) (2014)

TT 8.4 Mon 11:00 H21

The path Integral formulation of the Schrieffer-Wolff transformation — •Farzaneh Zamani[1], Pedro Ribeiro[2], and Stefan Kirchner[3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]CeFEMA, Instituto Superior Tecnico, Universidade de Lisboa Avenida Rovisco Pais — [3]Center for Correlated Matter, Zhejiang University

The equivalence between the low-energy sector of the Anderson model in the so-called Kondo regime and the spin-isotropic Kondo model is usually established via a canonical transformation performed on the Hamiltonian, followed by a projection. Here, we present a path integral version of this important canonical transformation which relates the functional integral form of the partition function of the Anderson model to that of its effective low-energy model. The resulting functional integral assumes the form of a spin path integral and includes a geometric phase factor, i.e. a Berry phase. Our approach stresses the underlying symmetries of the model and allows for a straightforward generalization of the transformation to more involved models. It thus offers a systematic route of obtaining effective low-energy models and higher order corrections. We demonstrate the effectiveness of our approach by considering the charge Kondo model, and a quantum dot attached to magnetic leads.

TT 8.5 Mon 11:15 H21

Tailoring the magnetic ground state of a two-molecule Kondo system by chemical interactions — •Benedikt Lechtenberg[1], Taner Esat[3], Thorsten Deilmann[2], Christian Wagner[3], Peter Krüger[2], Ruslan Temirov[3], Michael Rohlfing[2], F. Stefan Tautz[3], and Frithjof B. Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund — [2]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich — [3]Institut für Festkörpertheorie, WWU Münster, 48149 Münster

We propose a novel approach for tailoring the magnetic properties of a nanostructure that relies on the ubiquitous non-magnetic chemical interaction between the constituents of the nanostructure instead of a magnetic exchange interaction. This is demonstrated in a dimer of metal-molecule complexes on the Au(111) surface: Changing the tunneling between both complexes, we tune the coupled dimer through a quantum phase transition from an underscreened Kondo doublet to a singlet ground state. In this talk, we explain the nature of the competing ground states and the role of parity breaking for the understanding of the STM spectra. Employing the results of a LDA calculation as a first principle input for a numerical renormalization group calculation, we are able to reproduce the experiment with excellent agreement.

15 min. break

TT 8.6 Mon 11:45 H21

Kondo effect in a carbon nanotube with spin-orbit interaction and valley mixing: A DM-NRG study — •Davide Mantelli[1], Catalin Pascu Moca[2,3], Gergely Zarand[2], and Milena Grifoni[1] — [1]Iunstitut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland — [2]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, HU-1521 Budapest, Hungary — [3]Department of Physics, University of Oradea, 410087 Oradea, Romania

We investigate the effects of spin-orbit interaction (SOI) and valley mixing on the transport and dynamical properties of a carbon nanotube (CNT) quantum dot in the Kondo regime. As these perturbations break the pseudo-spin symmetry in the CNT spectrum but preserve time-reversal symmetry, they induce a finite splitting Δ between formerly degenerate Kramers pairs. Correspondingly, a crossover from the SU(4) to the SU(2)-Kondo effect occurs as the strength of these symmetry breaking parameters is varied. Clear signatures of the crossover are discussed both at the level of the spectral function as well as of the conductance. In particular, we demonstrate numerically and support with scaling arguments that the Kondo temperature scales inversely with the splitting Δ in the crossover regime. In presence of a finite magnetic field, time reversal symmetry is also broken. We investigate the effects of both parallel and perpendicular fields (with respect to the tube's axis) and discuss the conditions under which Kondo revivals may be achieved.

TT 8.7 Mon 12:00 H21

Magnetic anisotropy in Shiba bound states across a quantum phase transition — •Nino Hatter[1], Benjamin W. Heinrich[1], Michael Ruby[1], José I. Pascual[2], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]CIC nanoGUNE and Ikerbasque, Basque Foundation for Science, Tolosa Hiribidea 78, Donostia-San Sebastian 20018, Spain

Magnetic adsorbates on a superconductor create a scattering potential for the quasi-particles of the superconductor. This leads to so-called Yu-Shiba-Rusinov (Shiba) states inside the superconducting gap and a Kondo resonance outside the gap.

We performed scanning tunneling microscopy and spectroscopy on paramagnetic manganese phthalocyanine molecules adsorbed on the type-I superconductor Pb. At 1.2 K we resolve triplets of Shiba resonances. A multitude of different adsorption sites provides access to a large range of magnetic coupling strengths with the substrate, which we use to identify the origin of the multiplets. We resolve the splitting of the Shiba states throughout the quantum phase transition from the "Kondo screened" to the "free spin" ground state and can link the splitting to the presence of magnetic anisotropy in the molecule-substrate system. Furthermore, the change in intensities of the Shiba resonances allows the unambiguous determination of the many-body ground and excited states.

TT 8.8 Mon 12:15 H21

Lindblad-Driven Discretized Leads for Non-Equilibrium Steady-State Transport in Quantum Impurity Models — •Frauke Schwarz[1], Moshe Goldstein[2], Andreas Weichselbaum[1], and Jan von Delft[1] — [1]Physics Department, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich — [2]Raymond and Beverly Sackler School of Physics and Astronomy, Tel Aviv University, Tel Aviv 6997801, Israel

The description of interacting quantum impurity models in steady-state non-equilibrium is an open challenge for computational many-particle methods: the numerical requirement of using a finite number of lead levels and the physical requirement of describing a truly open quantum system are seemingly incompatible. One possibility to bridge this gap is the use of additional continuous reservoirs coupled to the lead levels and represented by Lindblad terms in the Liouville equation [1]. Based on a simple scheme for the evaluation of Green's functions in quadratic Lindblad models, we discuss some important properties of this Lindblad approach. Moreover, we present first results on the single-impurity Anderson model out of equilibrium obtained within a matrix product state framework.

[1] A.A. Dzhioev, D. S. Kosov, J. Chem. Phys. **134**, 044121 (2011).

TT 8.9 Mon 12:30 H21

Tunneling processes into localized subgap states in superconductors — •Michael Ruby[1], Falko Pientka[1,2], Yang Peng[1,2], Benjamin W. Heinrich[1], Felix v. Oppen[1,2], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The Yu-Shiba-Rusinov states bound by magnetic impurities in conventional s-wave superconductors are a simple model system for probing the competition between superconducting and magnetic correlations. Shiba states can be observed in scanning tunneling spectroscopy (STS) as a pair of resonances at positive and negative bias voltages in the superconducting gap. These resonances have been interpreted in terms of single-electron tunneling into the localized sub-gap states. This requires relaxation mechanisms that depopulate the state after an initial tunneling event. Recently, theory suggests that the current can also be carried by Andreev processes which resonantly transfer a Cooper pair into the superconductor.

We performed high-resolution STS experiments on single adatom Shiba states on the superconductor Pb, and provide evidence for the existence of two transport regimes. The single-electron processes dominate at large tip-sample distances and small tunneling currents, whereas Andreev processes become important at stronger tunneling. Our conclusions are based on a careful comparison of experiment and theory.

TT 8.10 Mon 12:45 H21

Terahertz Spectroscopy of Kondo-Lattice Systems — •Christoph Wetli[1], Johann Kroha[2], Cornelius Krellner[3], Kristin Kliemt[3], Oliver Stockert[4], Hilbert v. Loehneysen[5], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich — [2]Institute of Physics, Bonn University — [3]Institute of Physics, Goethe University Frankfurt — [4]MPI for Chemical Physics of Solids, Dresden — [5]Institute of Solid State Physics, KIT

Quantum phase transitions are boosting the interest in the field of Kondo-lattice systems. Experimental insights have been mainly obtained by measuring the specific heat or the magnetic susceptibility and relating them to the increase of the quasiparticle effective mass. Lately, it has been demonstrated that ARPES experiments allow direct access to the electrons contributing to the Kondo-lattice effect. We show that THz radiation is a powerful and highly accurate alternative for investigating the approach to the coherent Kondo state of heavy-fermion systems. Photons in the THz range directly couple to the electronic heavy quasiparticles arising from the Kondo effect. This technique allows to study Kondo-lattice dynamics on the picosecond time scale. We report lifetime measurements of excited Kondo singlets for two crystalline rare earth heavy-fermion systems $CeCu_6$ and $YbRh_2Si_2$ and find that the lifetimes scale inversely with the Kondo temperature. THz spectroscopy thus gives a very different perspective towards the Kondo-lattice effect, with the unique ability to combine temporal resolution and possible measurements in magnetic field.