TT 18: Correlated Electrons: Quantum Impurities, Kondo Physics 2

Time: Tuesday 9:30–12:45 Location: H 3005

TT 18.1 Tue 9:30 H 3005

Dynamical Mean-Field Theory of Indirect Magnetic Exchange — •Irakli Titvinidze, Andrej Schwabe, Niklas Rother, and Michael Potthoff — I. Institut für Theoretische Physik Universität Hamburg Jungiusstraße 9 20355 Hamburg Germany

Two magnetic impurities on a metallic substrate surface experience the Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction. This indirect non-local magnetic exchange competes with the local Kondo effect. While the latter is described in principle exactly within single-site dynamical mean-field theory, the effects of the RKKY coupling are taken into account approximately only. Here, this is demonstrated by comparing the DMFT results with numerically exact data obtained by the density-matrix renormalization group for a one-dimensional model with two Anderson impurities. With the two-site DMFT, we also benchmark a simplified DMFT variant. Varying the inter-impurity distance d and the local exchange coupling $J \sim -V^2/U$, different parameter regimes with dominating Kondo physics or with dominating RKKY interaction are studied. The reliability of DMFT for magnetic nanostructures on metallic surfaces is shown to crucially depend on the respective parameter regime as well as on geometrical and finite-size effects. The prospects of DMFT (and two-site DMFT) as a reliable approach to study nanomagnetism of more complex RKKY-interacting systems are discussed.

TT 18.2 Tue 9:45 H 3005

DFT++ Method for Vacuum States — •Michael Karolak, Tim O. Wehling, and Alexander I. Lichtenstein — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany

The theoretical description of scanning probe experiments, like scanning sunneling microscopy (STM), still poses a challenge. Since these methods probe electronic states in the vacuum a few angstrom above the actual sample a theory focussing exclusively on electronic states of the bulk must be necessarily incomplete.

To bridge this gap we have extended our DFT++ methodology [1] to incorporate vacuum states. We are thus able to investigate the effects of strong electronic correlations on states in the vacuum above the sample. In this way we can provide a true *ab initio* description of an STM experiment including electronic correlations. As an application we investigate the recently reported Two-Site Kondo Effect in $CoCu_nCo$ clusters on Cu(111) [2].

[1] M. Karolak *et al.*, J. Phys.: Condens. Matter **23**, 085601 (2011).
[2] N. Néel *et al.*, Phys. Rev. Lett. **107**, 106804 (2011).

TT 18.3 Tue 10:00 H 3005

Distributional exact diagonalization formalism for quantum impurity models — •Mats Granath and Hugo Strand — Department of Physics, University of Gothenburg, Gothenburg, Sweden

We develop a method for calculating the self energy of a general quantum impurity problem using a distribution of finite size Anderson models. When used in the context of dynamical mean field theory it provides an extension of the exact diagonalization formalism which gives a continuous real frequency self energy without the need for analytic continuation from imaginary frequencies.

TT 18.4 Tue 10:15 H 3005

Complex charge ordering in CeRuSn — •Ralf Feyerherm[1], Esther Dudzik[1], Sergio Valencia[1], John A. Mydosh[2,3], Wilfried Hermes[4], and Rainer Pöttgen[4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin — [2]MPI-CPFS, 01187 Dresden — [3]Kamerlingh Onnes Laboratory, Leiden University, 2300RA Leiden, The Netherlands — [4]Institut für Anorganische und Analytische Chemie, Universität Münster, 48149 Münster

At room temperature (RT), CeRuSn exhibits coexistence of trivalent Ce^{3+} and intermediate valent $Ce^{(4-\delta)+}$ in a metallic environment. Charge ordering produces a doubling of the unit cell along the c-axis with respect to the basic CeCoAl type structure. Below RT, a phase transition with broad hysteresis has been observed in various bulk properties. The present x-ray diffraction results show that at low temperatures the doubling of the CeCoAl type structure is replaced by an ill-defined modulated ground state in which at least three modulation periods compete. The dominant mode is close to a tripling of the basic cell. XANES data suggest that the average Ce valence remains constant. We propose a qualitative structure model with modified stacking sequences of Ce^{3+} and $Ce^{(4-\delta)+}$ layers in the various modulated phases. Surprisingly, far below 100 K the modulated state is sensitive to synchrotron x-ray irradiation. With a photon flux $\approx 10^{12}$ s^{-1}, the modulated ground state is destroyed on a timescale of minutes and the doubling of the CeCoAl cell observed at room temperature is recovered. The final state is metastable at 10 K. Heating the sample above 60 K again leads to a recovery of the modulated state.

TT 18.5 Tue 10:30 H 3005

Non-equilibrium transport through a multichannel Kondo dot at finite magnetic field — •Christoph B. M. Hörig and Dirk Schuricht — RWTH Aachen, Germany

Motivated by a recent work [1] on non-equilibrium transport through a multichannel Kondo model, we study a spin-1/2 quantum dot in a finite magnetic field using the real-time renormalization group (RG) method [2].

The quantum dot is coupled to K independent reservoirs via spin exchange interaction, which leads to the overscreened Kondo effect. Based on a systematic expansion in the exchange coupling we integrate out the reservoir degrees of freedom and solve the resulting two-loop RG equations in the weak-coupling regime $K >> 1$. We derive the scaling functions of the coupling constants towards the K-channel fix point and investigate the influence of decoherence during this flow.

Furthermore, we determine the effect of channel-dependent bias voltages on the magnetization and the differential conductance via inelastic cotunneling processes, and discuss our results in the context of previous experiments [3].

[1] A. Mitra and A. Rosch, Phys. Rev. Lett. 106, 106402 (2011).
[2] H. Schoeller and F. Reininghaus, Phys. Rev. B 80, 045117 (2009).
[3] R. M. Potok et al., Nature 446, 167 (2007).

TT 18.6 Tue 10:45 H 3005

Non-Fermi liquid physics in two-channel Kondo models — •Andrew Mitchell — Institut für Theoretische Physik, Universität zu Köln, Germany

The two-channel Kondo (2CK) model possesses a non-Fermi liquid (NFL) quantum critical point, arising when two conduction channels compete to Kondo-screen a single spin-$\frac{1}{2}$ impurity. The two-impurity Kondo (2IK) model also has a NFL critical point. We establish an exact connection between the models, showing that the 2IK critical fixed point is identical to that of a 2CK model with potential scattering. Furthermore, we demonstrate that the same critical physics arises in chains of impurities, and the spin-S generalization of the 2IK model. But conductance lineshapes measurable in experiment encode the full RG flow. We study the onset of NFL physics, showing that distinctive signatures arise as a function of device asymmetry; and the ultimate recovery of standard Fermi liquid behavior resulting from symmetry-breaking perturbations.

[1] Mitchell, Sela, Logan, `arXiv:1111.6503v1` (2011)
[2] Mitchell, Logan, Krishnamurthy, Phys. Rev. B **84**, 035119 (2011)
[3] Sela, Mitchell, Fritz, Phys. Rev. Lett. **106**, 147202 (2011)

15 min. break.

TT 18.7 Tue 11:15 H 3005

Nonequilibrium Kondo model: the RG flow from weak to strong coupling — •Mikhail Pletyukhov and Herbert Schoeller — Institut für Theorie der statistischen Physik, RWTH Aachen, Physikzentrum, D - 52074 Aachen

A renormalization group flow of the nonequilibrium Kondo model from high energies (weak coupling) to low energies (strong coupling) is discussed. A new flowing scheme (E-flow) within the Real Time Renormalization Group (RTRG) approach which uses the Laplace variable E as a flow parameter is introduced. The accuracy of this scheme in equilibrium is checked via the comparison against the benchmark NRG calculation of the linear conductance at finite temperatures. In nonequilibrium, the new results for the voltage dependence of the differential conductance are presented.

Another remarkable feature of the E-flow scheme is that it provides an access to the full time dynamics of a system, once the correspond-

ing flow equations have been integrated. An application of the E-flow scheme to the study of time evolution of the Kondo model in the strong coupling regime is discussed.

TT 18.8 Tue 11:30 H 3005

Non-abelian symmetries and the numerical renormalization group — •Markus Hanl, Andreas Weichselbaum, and Jan von Delft — Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, Munich, Germany

We present a numerical study of the magneto-conductance $G(B,T)$ of the fully symmetric three-channel Anderson-like model, which has been suggested recently as the microscopic model for Fe-impurities in gold or silver [1]. For this, we use the numerical renormalization group method (NRG) which allows us to calculate the magneto-conductance $G(B,T)$ for the relevant parameter space of both, the magnetic field B as well as the temperature T. We use an implementation of the NRG which allows to explicitly exploit any set of non-abelian symmetries. In the given case, this includes the SU(3) channel symmetry. This increases the efficiency by orders of magnitude compared to plain abelian NRG, which thus renders the simulation feasible. We show that our results are well converged, and, though the calculations are numerically very involving, the remaining error is small and controllable.
[1] T. Costi et al., Phys. Rev. Lett. **102**, 056802 (2009)

TT 18.9 Tue 11:45 H 3005

Kondo correlations in a disordered medium — •Michael Becker, Andrew Mitchell, and Ralf Bulla — Institut für theoretische Physik, Universität zu Köln

The Kondo effect is a classic paradigm, describing the formation of a many-body spin-singlet state between a local magnetic impurity and delocalized conduction electrons at low temperatures. However, in disordered systems, localization physics plays a key role. Here we consider the subtle interplay between Kondo physics and Anderson localization in disordered 1D and quasi 2D and 3D systems which contain a single correlated impurity site. Equations of motion and exact diagonalization are used to calculate hybridization functions for the non-interacting system, which constitute the input for NRG calculations in the interacting case. Real-space quantities are then extracted for the full system, and provide information on the Kondo screening length and localization length, whose relative magnitudes dictate the underlying physics.

TT 18.10 Tue 12:00 H 3005

Discarded weight and entanglement spectra in the numerical renormalization group — •Andreas Weichselbaum — Ludwig Maximilians University, Munich

A quantitative criterion to prove and analyze convergence within the numerical renormalization group (NRG) is introduced. By tracing out a few further NRG shells, the resulting reduced density matrices carry relevant information on numerical accuracy as well as entanglement. Their spectra can be analyzed twofold. The smallest eigenvalues provide a sensitive estimate of how much weight is discarded in the low-energy description of later iterations. As such, the discarded weight indicates in a site-specific manner whether sufficiently many states have been kept within a single NRG run. The largest eigenvalues of the reduced density matrices, on the other hand, lend themselves to a straightforward analysis in terms of entanglement spectra, which can be combined into entanglement flow diagrams. The latter show strong similarities with the well-known standard energy flow diagram of the NRG, supporting the prevalent usage of entanglement spectra to characterize different physical regimes [1].
[1] Phys. Rev B **84**, 125130 (2011)

TT 18.11 Tue 12:15 H 3005

Universal out-of-equilibrium transport in Kondo-correlated quantum dots: a renormalized superperturbation theory on the Keldysh contour — •Stefan Kirchner[1,2], Enrique Munoz[3], and Carlos Bolech[4] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute for Chemical Physics of Solids — [3]Pontificia Universidad Catolica de Valparaiso, Chile — [4]University of Cincinnati, US

The non-linear conductance of semiconductor heterostructures and single molecule devices exhibiting Kondo physics has recently attracted attention[1,2]. We address the observed sample-dependence across various systems by considering additional electronic contributions present in the effective low-energy model underlying these experiments. To this end we develop a novel version of the superperturbation theory [3] in terms of dual fermions on the Keldysh contour. We analyze the role of particle hole asymmetry on the transport coefficients. Our approach systematically extends the work of Yamada and Yosida and others to the particle-hole asymmetric Anderson model and reproduce the exactly solvable resonant level model and the special case considered in [4]. It correctly describes the strong coupling physics and is free of internal inconsistencies that would lead to a breakdown of current conservation.
[1] M. Grobis et al., Phys. Rev. Lett. 100, 246601 (2008).
[2] G. D. Scott et al., Phys. Rev. B 79, 165413 (2009).
[3] H. Hafermann et al., EPL 85, 27007 (2009).
[4] K. Yamada, Prog. Theo. Phys. 62, 354 (1979).

TT 18.12 Tue 12:30 H 3005

Indirect magnetic exchange and Kondo screening in one-dimensional metals with few magnetic impurities — •Andrej Schwabe and Michael Potthoff — University Hamburg, Hamburg, Germany

The Kondo effect of one impurity coupled to a metallic substrate by an exchange interaction J is known as an impressive many-body effect which is regarded as well understood. Adding another impurity may cause two separate Kondo effects, but can also introduce a new inter impurity RKKY coupling. The competition between both interactions gives rise to different parameter regimes: In the large J or large distance limit both impurities are separately screened while in the weak J or small distance limit they form a non-local spin which itself can be screened by the substrate.
We apply our variational matrix-product states code (VMPS) which is based on the implementation of the corrected one-site algorithm and exploits $U(1)$ symmetries. Calculations are presented for three impurities coupled to a nano chain within an Anderson model. We discuss its manifold properties by referring to results for the single and two impurity model. We focus explicitly on a substrate of finite size and discuss the consequences of finite-size gaps and symmetry.
The transition from the diluted case with few impurities to the dense lattice with one impurity on every substrate site, leads to further, even richer physics, including the exhaustion problem and magnetic long-range order. General trends considering the transition to dense chains are given.