TT 74: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Wednesday 15:00–18:45 Location: BEY 81

TT 74.1 Wed 15:00 BEY 81

The Kondo model in nonequilibrium: Interplay between voltage and temperature and crossover from weak to strong coupling — Frank Reininghaus, Mikhail Pletyukhov, and •Herbert Schoeller — Institut für Theorie der Statistischen Physik, RWTH Aachen

We analyze the 1-channel spin-1/2 nonequilibrium Kondo model at finite voltage and temperature by using a new formulation of real-time renormalization group with the Laplace variable E as flow parameter [1,3]. If the effective Liouvillian in Laplace space is analytic around E=0 (corresponding to the stationary state), we present convincing arguments that the method is capable of describing reliably the crossover from weak to strong coupling for the stationary conductance as function of voltage and temperature. Besides universal line shapes, we propose an elegant way to determine the Kondo temperature from the voltage dependence of the conductance. Furthermore, for a fixed finite voltage, we find that the temperature-dependence of the differential conductance exhibits non-monotonic behavior. We compare our results with recent experiments and find good agreement [2,3]. For the N-channel Kondo model with N¿¿1, we calculate the transient dynamics and find a pure power-law decay typical for non-Fermi liquid behaviour.
[1] M. Pletyukhov and H. Schoeller, Phys. Rev. Lett. 108, 260601 (2012)
[2] A.V. Kretinin, H. Shtrikman, and D. Mahalu, Phys. Rev. B 85, 201301(R) (2012)
[3] O. Klochan et al., Phys. Rev. B 87, 201104(R) (2013)

TT 74.2 Wed 15:15 BEY 81

Transport properties of fully screened Kondo models — •Christoph B. M. Hörig[1,3], Christophe Mora[2], and Dirk Schuricht[3] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University and JARA-Fundamentals of Future Information Technology, Germany — [2]Laboratoire Pierre Aigrain, École Normale Supérieure, France — [3]Institute for Theoretical Physics, Utrecht University, The Netherlands

We study the crossover from strong to weak coupling in two fully screened Kondo quantum dots, the spin-1/2 and the spin-1 model coupled to one or two screening channels respectively. The quantum dots are subject to either a finite bias voltage or a finite temperature. Using a real-time renormalisation group method we calculate the static susceptibility, dynamical spin-spin correlation functions, and the differential conductance. We extract the various Kondo scales and Fermi liquid coefficients at low energies and compare with exact known and newly derived Fermi liquid results.

TT 74.3 Wed 15:30 BEY 81

Spatial and temporal propagation of Kondo correlations — •Benedikt Lechtenberg and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

While the equilibrium properties of the Kondo problem are theoretically well understood, its non-equilibrium properties are subject to recent research. To set the stage, we present the spatial correlation function $\langle \vec{S}_{\rm imp}\vec{s}(r)\rangle$ between the impurity spin $\vec{S}_{\rm imp}$ and the spin density of the conduction electrons in thermodynamic equilibrium using the numerical renormalization group (NRG). Then, we will address the key question, how this spatial correlation function builds up as function of time starting from an initially decoupled impurity spin. We will show that the spatial and temporal Kondo correlations propagate along a light-cone determined by the Fermi-velocity. Surprisingly, we find that $\langle \vec{S}_{\rm imp}\vec{s}(r)\rangle(t)$ contains significant non-exponential contributions outside of the light-cone. Augmenting our time-dependent NRG calculation with perturbative expansion of the density operator we can explicitly trace the origin of these correlations to the intrinsic spin-density correlations of the initial Fermi see. Contributions outside of the light-cone only vanish in a true linear response function.

TT 74.4 Wed 15:45 BEY 81

Spin-noise in the anisotropic central spin model — •Johannes Hackmann and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

We have investigated the spin noise in an ensemble of semiconductor quantum dots (QDs) using the anisotropic central spin model. This model describes the dynamics of both electron and/or hole doped QDs. First, we have computed the spectral correlation function $\langle S^z(\omega)S^z\rangle$ for a single QD to reveal the influence of the external magnetic field and the anisotropy factor on the spin dynamics. Second, we have performed an ensemble average to compare our results to recent experiments. We will show that the measurement of spin noise on an ensemble of hole doped QDs reveals more about the distribution function of the QD parameters than on the dynamics of a single QD spin.

TT 74.5 Wed 16:00 BEY 81

Finite-Temperature Studies of Inverse Indirect Magnetic Exchange — •Maximilian Aulbach, Irakli Titvinidze, Andrej Schwabe, and Michael Potthoff — Universität Hamburg, Hamburg, Deutschland

The standard Ruderman-Kittel-Kasuya-Yosida (RKKY) exchange interaction emerges as an effective low-energy coupling in systems where the magnetic moments of impurities are coupled via a weak local exchange J to the spins of a system of itinerant conduction electrons. Contrary, in the case of antiferromagnetic and strong J, the impurity spins are screened individually by the formation of almost local Kondo singlets. In confined magnetic nanostructures, this results in a localization of conduction electrons and a corresponding formation of local magnetic moments which are indirectly coupled via virtual excitations of the Kondo singlets. This new "inverse" indirect magnetic exchange (IIME) [1] can also be studied in Anderson-lattice models with diluted impurities and results in a ferromagnetic ground state.

Here we focus on the finite-temperature properties. Using dynamical mean-field theory and a continuous-time quantum Monte-Carlo impurity solver, we calculate the temperature-dependent magnetization at the different inequivalent sites as well as the Curie temperature. The QMC results are compared with the predictions of static mean-field theory applied to an effective low-energy spin-only Hamiltonian that is derived in fourth-order strong-coupling perturbation theory.
[1] A. Schwabe, I. Titvinidze and M. Potthoff, Phys. Rev. B 88, 121107(R) (2013)

TT 74.6 Wed 16:15 BEY 81

Continuous-time Quantum Monte Carlo approach for quantum impurity problems in Tomonaga-Luttinger liquids — •Kazumasa Hattori[1,2] and Achim Rosch[1] — [1]Institute for Theoretical Physics, University of Cologne, Germany — [2]Institute for Solid State Physics, University of Tokyo, Japan

We have developed a continuous-time quantum monte carlo method [1] for single-impurity problems in Tomonaga-Luttinger (TL) liquid in one-dimension. The method is negative-sign free and applicable to varieties of models. In this contribution, we will show results for a potential barrier problem in one-channel TL liquid [2] as a benchmark and also discuss an anisotropic Kondo problem in a helical TL liquid on the edge of two-dimensional topological insulator. Various correlation functions are calculated and we discuss the crossover functions from high- to very low-temperature fixed points and their critical behaviors.
[1] E. Gull, et al., Rev. Mod. Phys. 83, 349 (2011)
[2] C. L. Kane and M. P. A. Fisher, Phys. Rev. Lett. 68, 1220 (1992)

TT 74.7 Wed 16:30 BEY 81

Time Evolution of a Quantum Impurity System following a Quantum Quench at Finite Temperatures - a td-NRG Study — •Hoa Nghiem and Theodoulos A. Costi — Peter Grünberg Institut and Institute for Advanced Simulation, Research Centre Jülich, 52425 Jülich, Germany

To study the time evolution of an observable of a quantum impurity system after a sudden quench at an arbitrary temperature, we apply the recently developed time-dependent numerical renormalization group approach (td-NRG) to the Anderson model [1]. The quenches studied include switching from mixed valence to Kondo regime or vice versa, and from a uncorrelated to a correlated system or vice versa. We quantify the results in the short and long time limits by comparing them to the thermodynamic values in the initial and final states. We also present the time evolution due to general continuous pulses, acting in a finite time interval. The study is based on the general-

ization of td-NRG to a general pulse [1], where we consider the pulse as a sequence of smaller quenches, and formulate the time evolution following an arbitrary number of quenches.
[1] H. Nghiem and T. A. Costi, Preprint (2013).

15 min. break.

TT 74.8 Wed 17:00 BEY 81

The Kondo effect in atomic chains — •Deung-Jang Choi[1,2], Shichao Yan[1,2], Jacob Burgess[1,2], Steffen Rolf-Pissarczyk[1,2], and Sebastian Loth[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

We can construct atomic model structures to engineer Spin Hamiltonians using a sub-Kelvin scanning tunneling microscope (STM). For that, different kinds of transition metal atoms were manipulated and construction of atomic chains was performed. The chains composed of transition metal atoms form a highly correlated spin singlet ground state exhibiting a Kondo resonance. We studied temperature and magnetic field dependence to confirm the Kondo effect in this composite magnetic system. It is revealed that the occurrence of the Kondo resonance sensitively depends on the length of the atomic chain and the spin anisotropy energy of each atom. We build chains with different elemental composition and obtain various spin ground states. In this way, we can tailor the singlet ground state on and off. Such composite magnetic chains present a fruitful experimental model spin system and make it possible to engineer prototypical correlated spin states at atomic dimensions.

TT 74.9 Wed 17:15 BEY 81

Nonequilibrium evolution of the Kondo screening cloud — •Martin Nuss, Martin Ganahl, Hans Gerd Evertz, Enrico Arrigoni, and Wolfgang von der Linden — Institute of Theoretical and Computational Physics, Graz University of Technology

Quantum impurity models feature nonperturbative physics at low temperatures, manifest in the Kondo effect. In equilibrium, the Kondo effect is accompanied by a diverging length scale for increasing interaction strength. While elusive in experiment this "Kondo length" has been observed in the spin-spin correlation functions in theoretical work. We extend these studies to the nonequilibrium regime by studying the interacting single impurity Anderson model after a quantum quench. Making use of Density Matrix Renormalization Group techniques, we present high accuracy numerical results for time dependent correlation functions and discuss the spatio-temporal evolution of the Kondo cloud. We furthermore present results for a system under bias, its temporal evolution as well as steady state characteristics [1].
[1] Phys. Rev. B 88, 045132 (2013)

TT 74.10 Wed 17:30 BEY 81

Local susceptibility and Kondo scaling — Markus Hanl and •Andreas Weichselbaum — Ludwig Maximilians University, Munich

The Kondo scale T_K for quantum impurity systems is typically assumed to guarantee universal scaling of physical quantities. In practice, however, not every definition of T_K necessarily supports this notion away from the strict scaling limit for finite bandwidth D. Various theoretical definitions of T_K are analyzed based on the inverse magnetic impurity susceptibility at zero temperature. While conventional definitions in that respect quickly fail to ensure universal Kondo scaling for all D, an altered definition of T_K^{sc} is presented which allows universal scaling of dynamical or thermal quantities for a given fixed Hamiltonian. If the scaling is performed with respect to an external parameter which directly enters the Hamiltonian, such as magnetic field, the corresponding $T_K^{\mathrm{sc,B}}$ for universal scaling may differ, yet becomes equivalent to T_K^{sc} in the scaling limit. The only requirement for universal scaling in the full Kondo parameter regime with a residual error of less than 1% is a well-defined isolated Kondo feature with $T_K \leq 0.01\,D$. In particular, by varying D over a wide range relative to the bare energies of the impurity, this allows a smooth transition from the Anderson to the Kondo model.

TT 74.11 Wed 17:45 BEY 81

π Fluxes near the Edge of a Topological Insulator: Kondo Screening of a Soliton — •Manuel Weber, Martin Hohenadler, and Fakher F. Assaad — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The insertion of a π flux into a quantum spin Hall insulator creates four spin-charge separated states: the two chargeons with $Q = \pm 1$ and the two spinons with $S_z = \pm 1/2$. In the presence of repulsive Coulomb interactions the charged states are gapped out and a local moment is formed. For both free and interacting systems the fluxons lead to a characteristic Curie law in the magnetic susceptibility. We consider the Kane-Mele-Hubbard model on a ribbon with zigzag edges to show that the spinon can be screened by the edge states of a quantum spin Hall insulator. At $U = 0$ their hybridization is dominated by the extent of the edge states, which becomes larger with increasing spin-orbit coupling λ. As the fluxons are exponentially localized, it is sufficient to include Hubbard interactions only at lattice sites directly around the π flux. We have extended the CTQMC method by global susceptibility measurements that reproduce the Curie law of a free π flux even for this reduced interacting system. When the spinon is screened by the edge states, we observe deviations from the Curie law for different U and λ that follow the universal behavior obtained from a data collapse. Moreover, at low temperatures a Kondo resonance arises in the spectral function between two low-lying Hubbard peaks.

TT 74.12 Wed 18:00 BEY 81

Kondo effect in Transition Metal Phthalocyanine Molecules on metal surfaces — •Michael Karolak and Giorgio Sangiovanni — Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany

We study the impact of strong electronic correlations on the electronic structure of Phthalocyanine (PC) molecules with 3d transition metal centers, adsorbed on different surfaces. Specifically, we investigate MnPC and CuPC adsorberd on Au(111), Ag(100), as well as Cu(100) surfaces. To this end we employ a first principles DFT++ method (density functional theory combined with an impurity solver) for calculating the electronic structure, explicitly taking into account the dynamic correlations arising from the strongly interacting 3d shell of the transition metal center. We compare our calculations with new scanning tunnelling microscopy experiments. Depending on the chemical valence of the transition metal center and the geometry of the molecule in contact with the different surfaces very different spectra are observed in the experiment. Our first principles calculations provide explanations of the observed data in terms of multi-orbital Kondo physics.

TT 74.13 Wed 18:15 BEY 81

Double Kondo effect induced by combining two non-Kondo systems: Fe atoms and polyphenyl molecules on Cu(111) — •Giulia Pacchioni, Marina Pivetta, Luca Gragnaniello, Fabio Donati, Stefano Rusponi, and Harald Brune — Institute of Condensed Matter Physics, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We use scanning tunneling spectroscopy and X-ray magnetic circular dichroism to investigate the Kondo effect for a system formed by individual Fe atoms adsorbed under polyphenyl-dicarbonitrile molecules on Cu(111).

Neither the molecules nor the Fe atoms adsorbed on the substrate display the Kondo effect. Combining them by burying the Fe adatoms below a phenyl ring of the organic molecules induces a Kondo effect in the Fe atoms as well as in the molecules. For the molecules this is inferred from scanning tunneling spectroscopy showing an intense Kondo peak above the phenyl ring. A Fano dip with twice the Kondo temperature is detected above the buried Fe atoms. X-ray magnetic circular dichroism reveals the screening of the magnetic moment for the buried Fe atoms, confirming the Kondo effect also for Fe.

TT 74.14 Wed 18:30 BEY 81

Irregular $4f^1$ spin-orbit splitting in collapsed α-cerium — •Jürgen Röhler — Universität zu Köln, 50937 Köln

The $J_{5/2} - J_{7/2}$ spin-orbit splitting of the $4f^1$ groundstate manifold in solid cerium systems is generally close to the value of free ions, $\Delta_{\mathrm{SO}} \simeq 3100$ K. Inelastic neutron scattering confirmed this for elemental γ-Ce, but not for the collapsed α-phase with strongly increased $\Delta_{\mathrm{SO}} \simeq 5300$ K [1]. Also α-type Ce-compounds exhibit significantly increased Δ_{SO}. Renormalization of Δ_{SO} in strongly correlated $4f$-systems is usually attributed to $4f$-c.e. hybridization increasing slightly the mean orbital expectation value $< r_{4f} >$, hence decreasing Δ_{SO}. In fact in most Kondo-type and mixed valent systems Δ_{SO} is decreased by $\simeq -10\%$, but not in collapsed α-type Ce systems. The apparent deficiency of the Kondo volume collapse model will be adressed. In particular we discuss the significance of $4f^n$ occupation numbers in the framework of a Mott transition within the $4f$ configuration.
[1] A.P. Murani et al., Phys. Rev. B**48**, 13981 (1993).