TT 30: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Tuesday 9:30–13:00 Location: H21

TT 30.1 Tue 9:30 H21

Kondo effect on the surface of 3D topological insulators: Signatures in scanning tunneling spectroscopy — •Lars Fritz[1], Andrew Mitchell[1,2], Dirk Schuricht[3], and Matthias Vojta[4] — [1]Universität zu Köln, Institut für Theoretische Physik — [2]Department of Chemistry, Physical and Theoretical Chemistry, Oxford University, UK — [3]Institute for Theory of Statistical Physics and JARA-Fundamentals of Future Information Technology, RWTH Aachen University — [4]nstitut für Theoretische Physik, Technische Universität Dresden

We investigate the scattering off dilute magnetic impurities placed on the surface of three- dimensional topological insulators. In the low-temperature limit, the impurity moments are Kondo- screened by the surface-state electrons, despite their exotic locking of spin and momentum. We determine signatures of the Kondo effect appearing in quasiparticle interference (QPI) patterns as recorded by scanning tunneling spectroscopy, taking into account the full energy dependence of the T matrix as well as the hexagonal warping of the surface Dirac cones. We identify a universal energy dependence of the QPI signal at low scanning energies as fingerprint of Kondo physics, markedly different from the signal due to non-magnetic or static magnetic impurities. Finally, we discuss our results in the context of recent experimental data.

TT 30.2 Tue 9:45 H21

Solution of the Anderson impurity model via the functional renormalization group — Simon Streib, •Aldo Isidori, and Peter Kopietz — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Strasse 1, 60438 Frankfurt, Germany

We show that the functional renormalization group is a numerically cheap method to obtain the low-energy behavior of the Anderson impurity model describing a localized interacting electron coupled to a bath of conduction electrons. Our approach uses an external magnetic field as flow parameter, partial bosonization of the transverse spin fluctuations, and frequency-independent interaction vertices which are fixed by Ward identities. We calculate the quasi-particle residue and the spin susceptibility in the particle-hole symmetric case and obtain excellent agreement with the Bethe ansatz results for arbitrary strengths of the interaction.

TT 30.3 Tue 10:00 H21

Kondo effect and magnetic frustration in a system of magnetic trimer on a metal surface — •Hoa Nghiem — Forschungszentrum Jülich, PGI-2/IAS-3, Jülich, Germany

We use quantum Monte Carlo simulation to clarify the competition between Kondo screening and magnetic frustration in a system of three magnetic adatoms on a metal surface [1]. We observe the feature of spectral density depending on the geometric configuration of three magnetic adatoms on the surface [2, 3]. In the isosceles configuration, the spectral density exhibits a significant peak near the Fermi level, which we attribute to the Yosida-Kondo resonance. In the equilateral configuration, no peak is observed near the Fermi level. This observation suggests the two separate regimes; the Yosida-Kondo dominant regime with the singlet ground state, and the magnetic frustration dominant regime with the degenerate ground state, - changing from one regime to another is realized as we gradually switch the geometric configuration from the isosceles triangle to equilateral one. By calculating the spectral density and the magnetic susceptibility in a wide range of temperatures, we prove the existence of the two separate regimes and suggest the critical crossover between them.

[1] N. T. M. Hoa, W. A. Diño, and H. Kasai: J. Phys. Soc. Jpn. 81 (2012) 023706
[2] T . Jamneala, V. Madhavan, and M. F. Crommie: Phys. Rev. Lett 87 (2001) 256804
[3] N. T. M. Hoa, W. A. Diño, and H. Kasai: J. Phys. Soc. Jpn. 79 (2010) 113706

TT 30.4 Tue 10:15 H21

Magnetic exchange coupling mediated by Kondo singlets — •Andrej Schwabe, Irakli Titvinidze, and Michael Potthoff — University Hamburg, Hamburg, Germany

When a magnetic impurity is antiferromagnetically exchange coupled to a metallic bath its spin degree of freedom may be quenched due to the Kondo effect. For several impurities, this competes with the RKKY indirect magnetic exchange. In a finite quantum box and for a weak coupling, this competition may encounter drastic modifications due to the presence of a finite size gap [1,2].
Here we extend our previous studies to the strong-coupling regime where almost local Kondo singlets are formed. In the ideal situation of a one-dimensional nano chain and large coupling, the bath is effectively cut into several pieces, which are magnetically coupled by a new type of indirect exchange that is mediated by virtual excitations of the local Kondo singlets. We derive an effective low-energy Hamiltonian for this strong-coupling regime. Its main contributions stem from an "inverse indirect magnetic exchange" between substrate pieces connected by local Kondo singlets. Different magnetic states depending on the number and the position of the impurities are analysed and compared with numerical calculations performed with a variational matrix-product states code. These can be understood by the adiabatic connection between the weak and the strong-coupling regime.

[1] A. Schwabe, D. Gütersloh, M. Potthoff, arXiv:1208.2209 (2012)
[2] W. B. Timm, J. Kroha, J. von Delft, PRL **82**, 2143 (1999)

TT 30.5 Tue 10:30 H21

Identifying Kondo orbitals through spatially resolved STS — •Andrey Antipov[1,2], Pedro Ribeiro[2], Johann Kroha[3], and Stefan Kirchner[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [3]Physikalisches Institut and Bethe Center for Theoretical Physics, Universitat Bonn, Nussallee 12, 53115 Bonn, Germany

In this contribution we study the influence of angular degrees of freedom of magnetic adatoms on metallic surfaces onto scanning tunneling spectra. Kondo scattering of conduction electrons off the adatom changes the local density of states near the Fermi level. The spatial dependence of this correction is set by the orbital structure of the local moment localized on the adatom. By considering a multilevel Anderson model with non-degenerate orbitals of differing orbital structure, using the multi orbital extension of the slave-boson mean field theory [1] we demonstrate that the spatial dependence of the scanning tunneling spectrum contains sufficient information to infer the orbital degrees of freedom of the magnetic adatom [2].

[1] P. Coleman, Phys. Rev. B 29, 3035-3044 (1984); J. Kroha et al., Physica E 18, 69 (2003)
[2] A. E. Antipov, P. Ribeiro, J. Kroha, S. Kirchner, to be published

TT 30.6 Tue 10:45 H21

Hydrogen-induced Kondo effect for single Co atoms adsorbed on Pt(111) — Quentin Dubout, Fabian Calleja, Markus Etzkorn, •Fabio Donati, Laurent Claude, Anne Lehnert, Pietro Gambardella, and Harald Brune — Institute of Condensed Matter Physics (ICMP),Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland.

We report on 0.4 K STM measurements revealing the H-induced Kondo effect for single Co atoms on a Pt(111) surface. Clean Co/Pt(111) has $S = 1$ and out-of-plane anisotropy [1], its ground state is $m = \pm 1$ and therefore cannot exhibit a first order Kondo effect [2]. Upon H_2 adsorption, or upon exposing the sample to the residual gas of the UHV chamber, we find two hydrogenated species, CoH and CoH_2. Both complexes show a number of differential conductance steps, some shift upon isotope substitution, revealing their vibrational origin. The most interesting feature is that CoH_2 presents a large conductance peak at the Fermi level. It shows the thermal broadening and magnetic field splitting identifying its origin as the Kondo effect. The CoH_2 complex has $S = 3/2$ and in-plane hard axis. To our knowledge, this is the first observation of adsorbate induced Kondo effect. In our case, the adsorbate changes the spin and the magnetic anisotropy energy.

[1] P. Gambardella et al., Science **300**, 1130 (2003).
[2] A. F. Otte et al., Nat. Phys. **4**, 847 (2008).

15 min. break

TT 30.7 Tue 11:15 H21

Single magnetic impurities in the Kane-Mele model — •Florian Goth, David J. Luitz, and Fakher F. Assaad — Institut für theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The realization of the spin-Hall effect in quantum wells has led to a plethora of studies regarding the properties of the edge states of a 2D topological insulator. These edge states constitute a class of one-dimensional liquids, called the helical liquid, where an electron's spin direction is coupled to its direction of movement. In contrast to one dimensional conductors, magnetic impurities — below the Kondo temperature — cannot block transport and one expects the current to circumvent the impurity. To study this phenomenon, we consider the single impurity Anderson model embedded into an edge of a Kane-Mele ribbon with up to 512×80 sites and use numerically exact continuous time QMC methods to study the Kondo effect. We present results on the temperature dependence of the spectral properties of the impurity and the bulk system that show the behaviour of the system in the various regimes of the Anderson model. Furthermore we show results on the spatial behaviour of the spin-spin correlation functions.

TT 30.8 Tue 11:30 H21

2-channel Kondo fixed point without fine tuning in a 3-level SU(3) quantum impurity: NRG results — •Evaristus Fuh Chuo, Katinka Ballmann, Laszlo Borda, and Johann Kroha — Physikalisches Institut, Universität Bonn

The 2-channel Kondo (2CK) effect with its exotic ground state properties has remained difficult to realize in physical systems. At low energies, a quantum impurity with orbital degree of freedom, like a proton bound in an interstitial lattice space, comprises a 3-level system with a unique ground state and (at least) doubly degenerate rotational excitations with excitation energy Δ. When immersed in a metal, electronic angular momentum scattering induces transitions between any two of these levels (couplings J), while the electron spin is conserved. We show by extensive NRG calculations that without fine-tuning of parameters this system exhibits a 2CK fixed point, due to Kondo correlations in the excited-state doublet whose degeneracy is stabilized by the the host lattice parity, while the channel symmetry (electron spin) is guaranteed by time reversal symmetry. We find a pronounced plateau in the entropy at $S(T_K < T < \Delta) = k_B \ln 2$ between the high-T value, $S(T \gg \Delta) = k_B \ln 3$, and the 2CK ground state value, $S(0) = k_B \ln \sqrt{2}$. This indicates a down-renormalization of the doublet *below* the non-interacting ground state, thus realizing the 2CK fixed point, in agreement with earlier conjectures [1]. We map out the phase diagram in the J–Δ plane and compare with analytical results. T_K shows non-monotonic J-dependence, characteristic for 2CK systems.

[1] M. Arnold, T. Langenbruch, J. Kroha, PRL **99**, 186601 (2007)

TT 30.9 Tue 11:45 H21

Out-of-equilibrium steady-states near quantum critical points - A dynamical large-N study of the Bose-Fermi Kondo model — •Pedro Ribeiro[1] and Stefan Kirchner[1,2] — [1]Max Planck Institute for the Physics of Complex Systems - Nothnitzer Str. 38, , D-01187 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids - Nothnitzer Str. 40, D-01187 Dresden, Germany

We study the out-of-equilibrium steady state properties of the Bose-Fermi-Kondo model, describing a local magnetic moment coupled to two ferromagnetic leads that support bosonic (magnons) and fermionic (Stoner continuum electrons) low energy excitations. In equilibrium, this model describes the destruction of the Kondo effect as the coupling to the bosons is increased, its phase diagram comprises three non-trivial fixed points. Using a dynamical large-N approach on the Keldysh contour, we study two different non-equilibrium setups: (a) a finite bias voltage and (b) a finite temperature gradient, imposed across the leads. The scaling behavior of the charge and energy currents is identified and characterized for the different fixed points. We report the existence of an effective temperature, defined based on the fluctuation dissipation relations of the local spin-susceptibility, that permits to recover the equilibrium scaling behavior of both dynamical and static spin susceptibilities in all the studied cases.

TT 30.10 Tue 12:00 H21

Inverse indirect magnetic exchange in one and higher dimensions — •Irakli Titvinidze, Andrej Schwabe, Anke Braun, and Michael Potthoff — I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Deutschland

It is well known that magnetic adatoms on a metallic substrate surface experience the Ruderman-Kittel-Kasuya-Yosida (RKKY) indirect magnetic exchange. Here we consider the limit of a strong antiferromagnetic Kondo coupling J which for certain geometries can lead to a quantum confinement of conduction electrons and the formation of local magnetic moments at substrate sites. It is argued that these local moments may couple magnetically via almost completely localized Kondo singlets that are formed for strong J. This novel inverse indirect magnetic exchange (IIME) is investigated numerically by means of the density-matrix renormalization group for one-dimensional multi-impurity Kondo models and for diluted Kondo lattices with "adatoms" present at every second "substrate" site. For the latter, our calculations show that as a function of J there is a crossover from ferromagnetic order driven by the RKKY interaction at weak J to ferromagnetism induced by the IIME interaction for strong J. We find excellent agreement with the results of corresponding calculations obtained by real-space dynamical mean-field theory (R-DMFT). R-DMFT is then used to study different adatom nanostructures on top of a two-dimensional substrate. We analyze the conditions under which the IIME interaction and ferromagnetic order induced by IIME also persists in two- and higher-dimensional systems.

TT 30.11 Tue 12:15 H21

Correlations outside the light cone — •Mariya Medvedyeva and Stephan Kehrein — Goerg-August University, Goettingen

We consider a Kondo impurity which couples to the conduction band electrons at some moment t=0. The commutator of the spin of the impurity and the spin of the conduction band electron vanishes outside the light cone determined by the speed of the propagation of the quasiparticles from the conduction band, as a consequence of the relativistic nature of the latter. While the correlation of the spin of the impurity and the spin of the conduction is non-zero outside the effective lightcone and follows a power law/exponential decay at zero/non-zero temperature. Non-zero correlation reveals the initial entanglement of the ground state of the conduction band electrons.

TT 30.12 Tue 12:30 H21

Possible non-Fermi liquid behavior in transport through Co doped Au chains — •Andreas Weichselbaum[1], Solange Di Napoli[2], Pablo Roura-Bas[2], Armando A. Aligia[3], Yuriy Mokrousov[4], and Stefan Blügel[4] — [1]Ludwig-Maximilians-Universität, München, Germany — [2]Departamento de Física de la Materia Condensada, Buenos Aires, Argentina — [3]Centro Atómico Bariloche and Instituto Balseiro, Bariloche, Argentina — [4]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

We calculate the conductance as a function of temperature G(T) through monoatomic Au chains, which contain one Co atom as a magnetic impurity and are connected to two conducting leads with a 4-fold symmetry axis. Using the information derived from ab initio calculations, we construct an effective model Hamiltonian H_{eff} that hybridizes a $3d^7$ quadruplet at the Co site with two $3d^8$ triplets through the hopping of $5d_{xz}$ and $5d_{yz}$ electrons of Au. The quadruplet is split by a term $DS^2_{z,\text{Co}}$ due to spin-orbit coupling at the Co site. Solving H_{eff} with the numerical renormalization group (NRG), we find at low temperatures $G(T) = a - b\sqrt{T}$ together with a ground state impurity entropy of $\ln(2)/2$, a behavior similar to the two-channel Kondo model. Stretching the chain one expects a quantum phase transition to a non-Kondo phase, with the physics of the underscreened Kondo model at the quantum critical point.

TT 30.13 Tue 12:45 H21

Interaction-driven transition between topological states in a Kondo insulator — •Jan Werner and Fakher Assaad — Theoretische Physik 1, Universität Würzburg, Deutschland

Heavy fermion materials naturally combine strong spin-orbit interactions and electronic correlations. When there is precisely one conduction electron per impurity spin, the coherent heavy fermion state is insulating. This Kondo insulating state has recently been argued to belong to the class of quantum spin Hall states [1]. Motivated by this conjecture and a very recent experimental realisation of this state[2], we investigate a model for Kondo insulators with spin-orbit coupling. Using DMFT, we observe an interaction-driven transition between two distinct topological states, indicated by a closing of the bulk gap and a simultaneous change of the Z_2 topological invariant. Upon reopening of the bulk gap the system remains a topological insulator, however with a zero energy edge mode now at the X-point instead of the Gamma-point.

[1] M. Dzero, K. Sun, P. Coleman, and V. Galitski, Phys. Rev. B 85, 045130 (2012)

[2] S. Wolgast et. al., arXiv:1211.5104 (2012)