TT 111: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Friday 9:30–12:15 Location: H 3005

TT 111.1 Fri 9:30 H 3005

Hybridization effects from the hydrogenation of the correlated impurity system Fe/Pt(111) — •Maria Valentyuk[1,3], A.A. Khajetoorians[1,2], M. Steinbrecher[1], T. Schlenk[1], A. Shick[4], I. Kolorenc[4], A. Lichtenstein[1], T.O. Wehling[5], R. Wiesendanger[1], and J. Wiebe[1] — [1]Department of Physics, Hamburg University, Germany — [2]Institute for Molecules and Materials, Radboud University, The Netherlands — [3]Department of Theoretical Physics and Applied Mathematics, Ural Federal University, Ekaterinburg, Russia — [4]Institute of Physics, ASCR, Na Slovance 2, Prague, Czech Republic — [5]Institute for Theoretical Physics, Bremen Center for Computational Material Science, University of Bremen, Germany

The presence of residual H_2 gas in ultra-high vacuum chambers is known to effect structural and transport properties of metallic samples. Scaling down to the level of one atomic impurity, this metal-hydrogen interaction brings new phenomena to the multi-orbital physics of d-shell metallic adatoms. Here, we show that in such a system with strong hybridization, i.e., iron adatoms on Pt(111), the hydrogenation serves as an additional complex parameter for the manipulation of the electronic interactions. We discuss the main electronic and magnetic features of the different iron-hydride complexes coupled to the Pt(111) substrate. By means of DFT calculations and by solving the multi-orbital Anderson impurity model (ED, CT-QMC) we found a significant qualitative change in the hybridization strength of different complexes and accordingly strong modifications of the correlated electronic behaviour.

TT 111.2 Fri 9:45 H 3005

Kondo temperature in the Anderson-Holstein Model with a displacement dependent hybridization. — •Andre Jovchev and Frithjof B. Anders — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund

Molecular junctions are potential candidates for future nano-electronic devices since they exhibit interesting phenomena such as nonlinear I-V curves and hysteresis effects attributed to conformational change in the molecule. Since the tunnel coupling depends exponentially on the distance, we have studied the influence of the vibrational couplings on the Kondo temperature in the Anderson-Holstein model(AHM) with a modified hybridisation term using the numerical renormalisation group (NRG). This includes a minimal model for the coupling of molecular vibrational modes to the electronic degree of freedom augmented with a vibrational dependent tunnelling term. Our investigation has been motivated by scanning tunnelling microscope experiments where the Kondo temperature in Co and Cu complexes on metallic surfaces has been reported to be mainly independent of the applied gate voltage which is in disagreement with the standard theory of the spin 1/2 Kondo effect.

TT 111.3 Fri 10:00 H 3005

Real-time dynamics induced by quenches across the quantum critical points in gapless Fermi systems with a magnetic impurity — •Christian Kleine[1], Julian Musshoff[2], and Frithjof B. Anders[1] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany — [2]Forschungszentrum Jülich GmbH, Institute for Advanced Simulation, 52425 Jülich, Germany

The energy-dependent scattering of fermions from a localized orbital at an energy-dependent rate $\Gamma(\epsilon) \propto |\epsilon|^r$ gives rise to quantum critical points (QCPs) in the pseudo-gap single impurity Anderson model separating a local moment phase with an unscreened spin moment from a strong-coupling phase which slightly deviates from the screened phase of standard Kondo problem. Using the time-dependent numerical renormalization group (TD-NRG) approach we show that local dynamic properties always equilibrate towards a steady-state value even for quenches across the QCP but with systematic deviations from the thermal equilibrium depending on the distance to the critical coupling. Local non-equilibrium properties are presented for interaction quenches and hybridization quenches. For interaction quenches within the screened phase we find an universal function for the time-dependent local double occupancy. We trace back the discrepancy between our results and the data obtained by a time-dependent Gutzwiller variational approach to restrictions of the wave-function ansatz in the Gutzwiller theory.

TT 111.4 Fri 10:15 H 3005

Transfering spin into an extended π-orbital of a large molecule – A comparison between NRG and experiment — •Benedikt Lechtenberg[1], Thorsten Deilmann[2], Taner Esat[3], Peter Krüger[2], Christian Wagner[3], Ruslan Temirov[3], Frithjof B. Anders[1], F. Stefan Tautz[3], and Michael Rohlfing[2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund — [2]Institut für Festkörpertheorie, WWU Münster, 48149 Münster — [3]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich

Recently, the adsorption of single Au atoms on a PTCDA monolayer physisorbed on a Au(111) surface has been investigated by means of low temperature scanning tunneling microscopy (STM) and spectroscopy (STS). The chemical reaction between the Au atom and PTCDA leads to the formation of a radical occupied with an unpaired spin. This radical formation can be observed as an additional zero bias differential conductance peak originating from the Kondo effect. An LDA calculation has identified the participating states of the Au-PTCDA complex, and the projected density of states from quasiparticle corrections provide all necessary first principle input parameter for the numerical renormalization group (NRG) calculation.
This talk focus on the NRG calculations and their results that are in excellent agreement with experiment: the calculated Kondo temperature matches very well the experimentally measured data.

TT 111.5 Fri 10:30 H 3005

One- and two-particle impurity Green's functions obtained using worm sampling — •Markus Wallerberger[1], Patrik Gunacker[1], Emanuel Gull[2], Giorgio Sangiovanni[3], and Karsten Held[1] — [1]TU Wien, Austria — [2]University of Michigan, Ann Arbor MI, USA — [3]Universität Würzburg, Germany

The single impurity Anderson model (SIAM) is one of the fundamental models of electronic correlation and lies at the computational core of dynamical mean field theory and diagrammatic extensions thereof. A state-of-the-art method for solving the SIAM is the continuous-time quantum Monte Carlo method in its hybridisation expansion (CT-HYB), because it is free of systematic bias and thus numerically exact.

In CT-HYB, one expands the partition function in terms of the hybridisation with the bath and stochastically sums the resulting diagrammatic series. The many-body propagators are usually obtained as a "by-product" of partition function sampling, as this allows for an easy implementation. We however show that this method leads to severe ergodicity problems for strong insulators and fails to yield spin-flip and pair-hopping terms of the vertex in high-symmetry cases.

Worm sampling avoids above complications by directly sampling the many-body propagators. We show that its use in CT-HYB significantly improves the quality and statistical uncertainties of the propagators. We also demonstrate how by using worm sampling for the impurity vertex, one can calculate frequency boxes of arbitrary sizes.

15 min. break.

TT 111.6 Fri 11:00 H 3005

Correlation effects in the extended Anderson model — •David Hämmerle[1], Lukas Merker[2], Theo A. Costi[2], and Sabine Andergassen[1,3] — [1]Universität Wien — [2]Forschungszentrum Jülich — [3]Universität Tübingen

We investigate the single-impurity Anderson model with an on-site Coulomb interaction U supplemented by $U'_{L/R}$ between the dot and the leads. Using the functional renormalization group in the static approximation we compute the linear conductance and the charge and spin susceptibilities at $T = 0$. The accuracy of our results is assessed by a comparison to NRG calculations. We analyze the physical behavior resulting from the competition between the Kondo effect and the characteristic power-laws of the interacting resonant level model. We find that for increasing $U'_{L/R}$ the effective on-site repulsion is reduced leading initially to an enhancement of the Kondo temperature. For sufficiently large $U'_{L/R}$, at particle-hole symmetry the low-energy properties resemble the ones of a charge Kondo effect as obtained for an attractive Coulomb interaction, while away from particle-hole asym-

metry a power-law behavior as for the interacting resonant level model is observed. For a more realistic modelling of a molecular quantum dot we include an additional local Coulomb interaction in the leads, which lead to novel signatures in the conductance line shape.

TT 111.7 Fri 11:15 H 3005

From the weak coupling regime to the Kondo crossover within the reduced density matrix framework — •Davide Mantelli and milena grifoni — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

When an Anderson quantum impurity is coupled to non interacting leads, many different regimes are accessible. In the weak coupling regime $\Gamma \ll k_{\rm B}T, U$ (with Γ the tunnelling coupling, T the temperature and U the charging energy), Coulomb blockade and co-tunnelling phenomena are well described within a perturbative approach in Γ. However, as the thermal energy approaches the coupling one, the perturbative method breaks down. By summing up a series of charge fluctuations events to all order in Γ we managed to reach the intermediate regime ($\Gamma \simeq k_{\rm B}T$) within the so-called "Dressed Second Order" (DSO)[1]. Considering its natural extension, the "Dressed-DSO", we achieved to describe the Kondo crossover where the thermal energy is comparable to the Kondo one ($T \simeq T_{\rm K}$). In this regime, equilibrium and non equilibrium fingerprints of the Kondo physics are carefully analysed.

[1] J. Kern and M. Grifoni, Eur. Phys. J. B **86**, 384 (2013)

TT 111.8 Fri 11:30 H 3005

Friedel oscillations at the Mott transition in fermionic systems — •Banhi Chatterjee, Jan Skolimowski, and Krzysztof Byczuk — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw , Warsaw,Poland

Friedel Oscillations (FO) in the Fermi liquid, Mott insulator, and at the Mott transition are studied within one and two dimensional Hubbard model. Electronic correlations are accounted for by solving the dynamical mean-field theory equations, using numerical renormalization group, for infinite homogeneous system. Next the obtained self-energy is transfered into a real-space Dyson equation with the impurity potential. The last problem is solved numerically by exact diagonalization. We observe that in the metallic phase the amplitudes of FO are damped with increasing the interactions while the period remains unchanged. FO almost disappear close to the Mott transition and completely on the insulating side. An additional bound state is observed in the spectral function at the impurity site which splits along with the sub-bands on increasing the interactions.

TT 111.9 Fri 11:45 H 3005

Kondo physics of multi-orbital Anderson models studied by distributional exact diagonalization — Sareh Motahari and •David Jacob — Max Planck Institute of Microstructure Physics

The Anderson impurity model (AIM) plays a central role in the understanding of one of the most intriguing many-body phenomena, the Kondo effect, and is at the heart of Dynamical Mean-Field Theory. But solving the AIM especially in the multi-orbital case still poses a challenge, although numerically exact solvers such as continuous time quantum Monte Carlo (CTQMC) method and the numerical renormalization group (NRG) exist. However, CTQMC produces data only on the Matsubara axis, so that numerical analytic continuation to the real axis is necessary in order to calculate dynamical quantities on the real axis which is problematic. On the other hand the NRG method is computationally too demanding to be applied to realistic systems with more than one or two impurity levels. Here, we use the novel distributional exact diagonalization (DED) [1] method in order to study Kondo physics in multi-orbital Anderson models. In DED we stochastically generate a distribution of finite Anderson models that are solved by exact diagonalization, and the self-energy is obtained from the sample average. First, we demonstrate the validity of the method by calculating the dynamical properties of the single-orbital AIM and comparing with available exact results. Then we explore different situations in multi-orbital Anderson models, in particular the underscreened, overscreened and fully screened Kondo effects.

[1] M. Granth and H. U. R. Strand, Phys. Rev. B 86, 115111 (2012).

TT 111.10 Fri 12:00 H 3005

Non-Fermi liquid behavior from dynamical effects of impurity scattering in correlated Fermi liquids — •Pramod Kumar[1] and N. S. Vidhyadhiraja[2] — [1]Institut für Theoretische Physik, Johann Wolfgang Goethe-Universität, Max-von-Laue-Str. 1, 60438 Frankfurt am Main, Germany — [2]Theoretical Sciences Unit, JNCASR, Jakkur, Bangalore, India 560094

In this work, we have investigated the effect of disorder due to chemical substitution on the dynamics and transport properties of correlated Fermi liquids. A low frequency analysis in the concentrated and dilute limits shows that the dynamical local potentials arising through disorder averaging generate a linear (in frequency) term in the scattering rate. Such non-Fermi liquid behavior (nFL) is investigated in detail for Kondo hole substitution in heavy fermions within dynamical mean field theory. We find closed form expressions for the dependence of the static and linear terms in the scattering rate on substitutional disorder and model parameters. A full numerical solution of the dynamical mean field theory equations reveals that the nFL term will show up significantly only in certain regimes, although it is present for any non-zero disorder concentration in principle. We highlight the dramatic changes that occur in the quasiparticle scattering rate in the proximity of p_c. Remarkably, we find that the nFL behavior due to dynamical effects of impurity scattering has features that are distinct from those arising through Griffiths singularities or distribution of Kondo scales. Relevance of our findings to experiments on alloyed correlated systems is pointed out.