

TT 30: Correlated Electrons: Quantum Impurities, Kondo Physics

Time: Tuesday 14:00–16:00

Location: HSZ 03

TT 30.1 Tue 14:00 HSZ 03

Renormalized Perturbation Theory as a General Solver for Quantum Impurities — ●SIMON JAHNS and GERTRUD ZWICKNAGL — Institut für Mathematische Physik, TU Braunschweig, Germany

In systems with magnetic impurities conduction electrons are scattered by low energy spin fluctuations leading to the Kondo effect. Due to the strong local electron interactions the low energy scales can not be accessed perturbatively. However, here we are demonstrating the efficiency and flexibility of the RPT [1] as a general impurity solving technique, with which this problem is circumvented.

The central idea is to first determine the renormalized quasiparticle characteristics and to subsequently calculate the Green's functions from a perturbation expansion in terms of the quasiparticle propagators and effective interactions.

The fully renormalized quasiparticle parameters are derived from flow equations connecting a (sometimes hypothetical) weak-coupling regime to the physically relevant strong-coupling regime. Typical examples for the flow variable are an external magnetic field or the chemical potential. Results for the single impurity Anderson model (SIAM) have been found in excellent agreement with exact solutions [2].

We discuss the extension of the scheme to more general quantum impurity models accounting to e.g. for Hund's rule correlations.

[1] K. Edwards, A. C. Hewson, J. Phys.: Condens. Matter 23 (2011)

[2] K. Edwards, A. C. Hewson, V. Pandis, Phys. Rev. B 87 (2013)

TT 30.2 Tue 14:15 HSZ 03

Numerical Renormalization Group study of Gate Induced Kondo Screening in Graphene — ●DANIEL MAY¹, JINHA MAO², YUHANG JIANG², PO-WEI LO^{3,4}, GUOHONG LI², GUANG-YU GUO^{3,4}, FRITHJOF ANDERS¹, and EVA Y. ANDREI² — ¹Technische Universität Dortmund, Lehrstuhl für Theoretische Physik 2, Germany — ²Rutgers University, Department of Physics and Astronomy, USA — ³National Taiwan University, Department of Physics, Taiwan — ⁴National Center for Theoretical Sciences, Physics Division, Taiwan

Graphene in its pristine form has transformed our understanding of 2D electron systems leading to fundamental discoveries. When graphene's honeycomb lattice is disrupted by single atom vacancies, new phenomena, namely a re-entrance Kondo effect, may emerge. We present numerical renormalization group (NRG) calculations for a two-orbital model consisting of a local σ orbital and a localized π state induced by the vacancy. Guided by ab-initio calculations for the parameters we determine two regimes. The re-entrance regime (i) is characterized by a conventional Kondo effect (p doping), a breakdown of the Kondo peak for vanishing chemical potential $|\mu| \rightarrow 0$, and an underscreened Kondo (n doped) where the π conduction band is screening the magnetic moment of the σ orbital. Increasing the hybridization between the σ orbital and the π conduction band further drives the system into the second regime (ii) where the π state is depopulated and a conventional Kondo effect is present (p doped).

TT 30.3 Tue 14:30 HSZ 03

Interplay of Superconductivity and Magnetism in the 2D Kondo Lattice Model: A Variational Cluster Approach — ●BENJAMIN LENZ, RICCARDO GEZZI, and SALVATORE R. MANMANA — Institute for Theoretical Physics, Georg-August-Universität Göttingen

We present results for the interplay of d-wave superconductivity and antiferromagnetism in the Kondo lattice model using the variational cluster approximation (VCA). Both the paramagnetic and the antiferromagnetic phase of the model are investigated and regions with different Fermi surface topology are found in the latter. The transition between these two different antiferromagnetic phases is investigated close to and off half-filling. VCA is used to probe the system for s-wave and d-wave superconductivity for all coupling regions. It is shown that only by treating antiferromagnetism and superconductivity on equal footing artificial superconducting solutions at half-filling can be avoided. No true s-wave superconducting solutions due to correlation effects are found, but d-wave pairing proves to be robust for various coupling strengths off half-filling. Its interplay with antiferromagnetism is analyzed at weak coupling.

TT 30.4 Tue 14:45 HSZ 03

Nonequilibrium Kondo effect in a magnetic field: Auxiliary master equation approach — ●DELIA FUGGER¹, FRAUKE SCHWARZ², ANTONIUS DORDA¹, JAN VON DELFT², WOLFGANG VON DER LINDEN¹, and ENRICO ARRIGONI¹ — ¹Institute of Theoretical and Computational Physics, TU Graz, Austria — ²Faculty of Physics, LMU Munich, Germany

We solve the single-impurity Anderson model in a magnetic field and out of equilibrium with an auxiliary master equation approach [1,2]. Employing Matrix Product States techniques to solve the many-body Lindblad equation allows us to generate highly accurate results, especially for the spectral functions. In equilibrium we find a remarkable agreement with spectral functions obtained with NRG, cf. [2].

The application of a bias voltage V and a magnetic field B both individually result in a splitting of the Kondo resonance around the Kondo temperature. With our method we can resolve a four-peak structure in the spectral function for nonzero B and V , due to both effects. This four-peak structure manifests itself in the differential conductance, which is very well accessible by experiments.

We investigate the stationary properties of the system as well as its dynamics after a quantum quench. We finally compare our results to recent experiments [3] and draw conclusions about the underlying spectral functions. We find that our results nicely agree with experimental data also outside the Kondo regime.

[1] E. Arrigoni et al., PRL 110, 086403 (2013)

[2] A. Dorda et al., PRB 92, 125145 (2015)

[3] A. V. Kretinin et al., PRB 84, 245316 (2011)

TT 30.5 Tue 15:00 HSZ 03

Topological protected quantum critical point in 1D Two Impurity Models — ●FABIAN EICKHOFF, BENEDIKT LECHTENBERG, and FRITHJOF ANDERS — Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44227 Dortmund

The two impurity Anderson model exhibit an additional quantum critical point at infinitely many specific distances between both impurities for an inversion symmetric 1D dispersion. Unlike the quantum critical point previously established by Jones and Varma, it is robust against particle-hole or parity symmetry breaking. The quantum critical point separates a spin doublet from a spin singlet ground state and is, therefore, topologically protected. A finite single particle tunneling t or an applied uniform gate voltages will drive the system across the quantum critical point. The discriminative magnetic properties of the different phases cause a jump in the spectral functions at low temperature which might be useful for future spintronics devices. A local parity conservation will prevent the spin-spin correlation function to decay to its equilibrium value after spin-manipulations.

TT 30.6 Tue 15:15 HSZ 03

AFM mechanical dissipation due to onset of Kondo impurity screening — ●PIER PAOLO BARUSELLI, MICHELE FABRIZIO, and ERIO TOSATTI — SISSA, Via Bonomea 265 34136 Trieste (Italy)

In nanomechanical systems such as STM tips approaching magnetic sites on a surfaces, some cases have been reported where the tip may cause the switching of the impurity spin from zero or one, to a spin $1/2$ showing up as a Kondo conductance peak. Since at the same time one can in principle measure the tip mechanical dissipation, it is relevant to investigate theoretically what contribution will the onset of a Kondo state make to that dissipation. As a starting point we model the Kondo state as a non-interacting resonant level, showing that the dissipation, proportional to the Kondo energy, diverges roughly as the logarithm of the temperature. We then discuss extensions of our approach using an Anderson model solved by numerical renormalization group, which accounts for many-particle effects. We finally speculate about the role of a finite driving frequency.

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TT 30.7 Tue 15:30 HSZ 03

The spinless Anderson-Holstein impurity model — ●ANDISHEH KHEDRI^{1,2}, VOLKER MEDEN^{1,2}, and THEO COSTI² — ¹RWTH Aachen University — ²Forschungszentrum Jülich

We consider a spinless resonant level in a wide conduction band which is coupled to a phonon mode. This coupling induces an effective retarded and attractive electron-electron interaction which leads to a

suppression of the tunneling rate from the local level to the conduction sea. Conventional perturbation theory in the coupling strength does neither capture the underlying polaron physics nor the power-law like renormalization as known from the purely fermionic interacting resonant level model (anti-adiabatic limit). We use the functional renormalization group to study the renormalization of the tunneling rate for arbitrary bare rate and phonon frequency in the limit of small to intermediate electron-phonon coupling. We compare to results obtained by the numerical renormalization group.

TT 30.8 Tue 15:45 HSZ 03

A modified Anderson impurity model in a continuum limit

of the Hubbard model — ●YAHYA ÖZ and ANDREAS KLÜMPER —
Bergische Universität Wuppertal

Starting from the integrable Hubbard model by use of the R -matrix a new model with impurity and modified dispersion relation is obtained. We consider the thermodynamical approach based on the well-known finite set of non-linear integral equations (NLIE) of convolution type for obtaining the integrable modification of the energy-momentum dispersion for the derivation of the thermodynamic equations of this new model. This integrable lattice model can be used for obtaining the Anderson impurity model in the continuum with a modified dispersion relation.