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Kondo effect in single-molecule spintronic devices

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Abstract

We study the Kondo effect in a quantum dot or a single molecule coupled to ferromagnetic leads. Spin-dependent quantum charge fluctuations in the dot induce the lifting of the spin degeneracy of the dot. It leads to the dot's level spin splitting observed in the nonequilibrium transport as a splitting of a zero-bias anomaly in the differential conductance. We discuss basic properties of this effect and its temperature dependence using numerical renormalization group technique. Recent experimental results fit well to our theoretical consideration.

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Keywords: Kondo effect; Molecular spintronics; Quantum dot; Ferromagnetism; Spin-dependent transport

1. Introduction

Spintronics has recently become a mature branch of mesoscopic physics and nanotechnology. There is also significant progress in development of the molecular electronics. The intersection of these two fields namely molecular spintronics is just a rising topic. Here we discuss some first investigations in this direction and new experimental results obtained recently. We study a spin-dependent transport in a quantum dot or a single molecule attached to ferromagnetic leads. We investigate the low-temperature properties, where one can expect the many-body Kondo effect due to the presence of the strong correlations.

2. Model

We model a dot or single molecule, which is coupled to ferromagnetic leads by means of the Anderson model described by the Hamiltonian:

$$H = \sum_{rk\sigma} \varepsilon_{rk\sigma} a^{\dagger}_{rk\sigma} a_{rk\sigma} + \sum_{\sigma} \varepsilon_0 d^{\dagger}_{\sigma} d_{\sigma} + U d^{\dagger}_{\uparrow} d_{\uparrow} d^{\dagger}_{\downarrow} d_{\downarrow} + \sum_{rk\sigma} V_r d^{\dagger}_{\sigma} a_{rk\sigma} + \text{h.c.}, \quad (1)$$

where $a_{rk\sigma}$ (d_σ) are annihilation operators of electrons with spin-σ ($\sigma = \uparrow, \downarrow$) in the lead $r = \mathrm{L}, \mathrm{R}$ (dot). The energy of the single dot level ε_0 may be tuned by a gate voltage V_g, and U is the onsite Coulomb interaction. The ferromagnetism in the leads is accounted for by the spin-dependent dispersion $\varepsilon_{rk\sigma}$ and, hence, spin-dependent density of states $\nu_{r\sigma}(\varepsilon) = \sum_k \delta(\varepsilon - \varepsilon_{rk\sigma})$. The spin-dependent coupling strength between the dot and the leads is given by $\Gamma_{r\sigma} = 2\pi |V_r|^2 \nu_\sigma(\varepsilon)$.

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3. Nonequilibrium transport-resonant tunneling approximation

The main goal of our work is to investigate how ferromagnetic leads influence the Kondo effect. At the beginning, based on a poor man's scaling analysis we show that a splitting of the Kondo resonance similar to the usual magnetic-field-induced splitting will appear due to exchange interaction with leads [1]. The most important result is that this splitting can be fully compensated by an appropriately tuned external magnetic field and the strong coupling limit of the Kondo effect can be restored.

We analyze the nonlinear transport through the dot using a real-time diagrammatic technique that provides a systematic description of the nonequilibrium dynamics of a system with strong local electron correlations [1]. We develop a charge and spin conserving resonant tunneling approximation (in the limit $U \to \infty$) that accounts not only for Kondo correlations but also for the spin splitting and spin accumulation out of equilibrium.

4. Numerical renormalization group

Moreover, we adapt the numerical renormalization group (NRG) method to the case of a quantum dot coupled to ferromagnetic leads. We show that the Kondo effect in the presence of ferromagnetic leads has unique properties such as a strong spin polarization of the density of states (DOS) at the Fermi level [2]. In order to account the effect of a gate voltage on the spin splitting of an electronic level in the dot attached to ferromagnetic leads in the Kondo regime we have generalized the numerical renormalization group technique for an arbitrary DOS shape. We find that the V_g-dependence of the dot-level spin splitting strongly depends on the shape of the DOS shape. For one class of DOS shapes there is nearly no V_g-dependence; for another, V_g can be used to control the magnitude and sign of the spin splitting.

Using this approach we analyze a recent experiment of Nygård et al. [3] based on single wall carbon nanotubes contacted to non-magnetic Cr/Au electrodes, where an anomalous splitting of the zero-bias anomaly in the conductance in absence of a magnetic field was observed. The authors related the observed splitting of the Kondo resonance with the presence of a ferric iron nitrate nanoparticle, which, due to electronic tunnel coupling to the dot, introduces a spin-dependent hybridization. We model these results by means of a single-level dot tuned to the local moment regime $\varepsilon_0 = -U/2$. Since a splitting of the Kondo resonance was observed for $\varepsilon_0 = -U/2$, a particle-hole asymmetry must exist to achieve a splitting [3]. We try to model this effect by using flat band structure and by introducing the Stoner splitting $\Delta = 2.5U$. The presence of the nanoparticle introduces a spin-dependent hybridization which we parameterize via the leads spin polarization P.

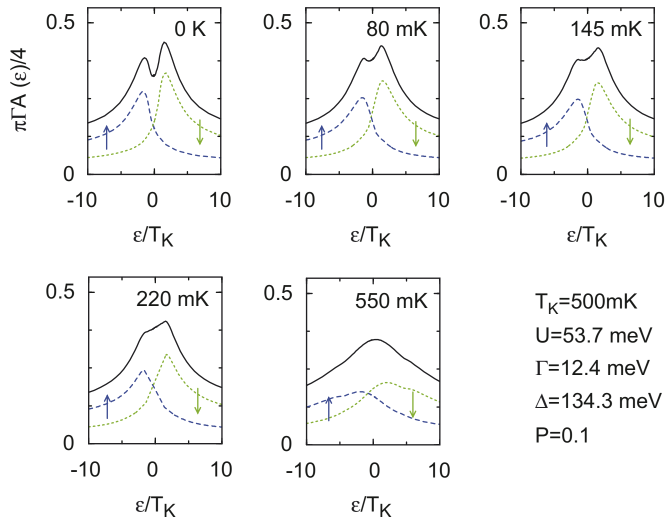

Fig. 1. Spin-resolved equilibrium spectral function $A_\sigma(\omega, T, V=0)$ obtained using parameters extracted from Ref. [3]. The dashed lines correspond to $A_\uparrow(\omega, T, V=0)$, the long dashed lines to $A_\downarrow(\omega, T, V=0)$, and the solid ones to the sum of both, $A(\omega, T, V=0)$. The temperature gradually increases as in Ref. [3]. Note that the splitting of the Kondo resonance disappears upon increasing temperature.

The comparison of the $\mathrm{d}I/\mathrm{d}V$ vs. V characteristics of Ref. [3] with the theoretical result turns out to be rather complicated as it involves the nonequilibrium spectral function $A(\omega, T, V)$ which itself is not known how to compute accurately. It is possible to compare qualitatively the splitting in the non-equilibrium conductance obtained in the experiment to the single particle spectral function. Due to the splitting in the particle spectral function for the dot, that is strongly related with the low-bias conductance measurements we find close similarity between both of them. When we approximate the experimental results of $\mathrm{d}I/\mathrm{d}V$ with $A(\omega, T, V=0)$ we achieve the best agreement between theory and experiment for $P = 0.1$. We compute the temperature dependent equilibrium spectral function $A(\omega, T, V=0)$ presented in Fig. 1, which qualitatively confirms the behavior found in the experiment of Nygård and collaborators, namely vanishing splitting in the $\mathrm{d}I/\mathrm{d}V$ curves upon with increasing temperature. A similar behavior was also observed for a single C_{60} molecule attached to nickel electrodes [4].

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