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Nonequilibrium Kondo Effect in a Single-Channel Quantum Dot Asymmetrically Coupled to Two Ferromagnetic Reservoirs

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Nonequilibrium Kondo effect in a quantum dot asymmetrically coupled to two ferromagnetic metallic leads is analyzed theoretically. The nonequilibrium Green function technique is used to calculate density of states and electric current. The lesser and retarded (advanced) Green functions are calculated by the equation of motion method within a consistent approximation scheme. The case where one electrode is half-metallic is analyzed numerically in details.

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1. Introduction

Kondo anomaly in electronic transport through quantum dots (QDs) strongly coupled to metallic leads was first predicted theoretically [1] and then observed experimentally [2]. The effect is of current interest from both experimental and theoretical points of view — mainly due to fundamental physics involved. Several theoretical techniques have been developed in the past decade to describe this phenomenon [3–6]. The description is simplified in the linear response regime, where the equilibrium methods can be employed. The Kondo peak in density of state (DOS) develops then at the Fermi level. However, the situation becomes more

complex in the nonlinear regime, when the bias voltage drives the system out of equilibrium. The Kondo peak becomes then split [6, 7]. Additional spin splitting of the Kondo peak occurs in an external magnetic field [8, 9].

One of the methods used in nonequilibrium situations is based on the nonequilibrium Green functions [3, 6]. The retarded Green function is generally calculated by the equation of motion method in the framework of some approximation schemes [3, 10]. On the other hand, the correlation Green function is usually calculated within approximations which are not consistent with those used for the retarded Green functions. Recently, we have developed a formalism in which both Green functions are calculated on equal footing, i.e., by applying the same approximation scheme to both cases [11]. Here, we apply this formalism to QDs coupled asymmetrically to external ferromagnetic metallic leads. Two kinds of asymmetry are taken into account: (i) asymmetry in the coupling of the dot to the two electrodes, and (ii) spin asymmetry in the coupling of the dot to each of the two electrodes. In particular, a large spin asymmetry of the coupling may occur in the case of half-metallic electrodes, where DOS at the Fermi level almost vanishes for one spin orientation. We show that when the electrodes are coupled asymmetrically, the splitting of the Kondo peak in equilibrium occurs in both parallel (P) and antiparallel (AP) magnetic configurations, contrary to the case of symmetric coupling studied recently, where splitting only in the parallel configuration was found [12, 13].

2. Model and method

We consider a single-level QD coupled to metallic leads (electron reservoirs). The whole system can be described by the Hamiltonian $H = H_{\rm L} + H_{\rm R} + H_{\rm D} + H_{\rm T}$, where the terms H_β (with $\beta = {\rm L}, {\rm R}$) describe the left and right electrodes in the non-interacting particle approximation, $H_{\rm D}$ describes the quantum dot, $H_{\rm D} = \sum_\sigma \varepsilon_{\rm d} d_\sigma^+ d_\sigma + U d_\uparrow^+ d_\uparrow d_\downarrow^+ d_\downarrow$ with $\varepsilon_{\rm d}$ denoting the energy of the discrete dot level and U the electron correlation parameter. The energy $\varepsilon_{\rm d}$ as well as the single electron energies of reservoirs include the electrostatic energy due to applied voltage [14]. The last term, $H_{\rm T}$, in the Hamiltonian describes tunnelling processes between the dot and electrodes, and is of the form $H_{\rm T} = \sum_{k\beta\sigma} V_{k\beta\sigma}^* c_{k\beta\sigma}^+ d_\sigma + {\rm h.c.}$, where $V_{k\beta\sigma}$ are the components of the tunnelling matrix. The spin asymmetry as well as the asymmetry in the coupling to the left and right electrodes is contained just in these parameters.

Electric current I flowing through the biased system is determined by the retarded (advanced) $G_\sigma^{\rm r(a)}$ and correlation (lesser) $G_\sigma^<$ Green functions [15]. To determine them on equal footing, we used the equation of motion method [16] and applied the same approximation scheme for both Green functions. The formula for electric current I_σ can be then written in the following form:

$$I_\sigma = \frac{\mathrm{i}e}{2\hbar}\int \frac{\mathrm{d}E}{2\pi}\frac{\Gamma_\sigma^{\mathrm{L}}\widetilde{\Gamma}_\sigma^{\mathrm{R}} + \Gamma_\sigma^{\mathrm{R}}\widetilde{\Gamma}_\sigma^{\mathrm{L}}}{\widetilde{\Gamma}_\sigma^{\mathrm{L}} + \widetilde{\Gamma}_\sigma^{\mathrm{R}}}(G_\sigma^{\mathrm{r}} - G_\sigma^{\mathrm{a}})(f_{\mathrm{L}} - f_{\mathrm{R}}), \tag{1}$$

where Γ_σ^β is defined as $\Gamma_\sigma^\beta = 2\pi\sum_k V_{k\beta\sigma}V_{k\beta\sigma}^*\delta(E - \varepsilon_{k\beta\sigma})$ (for $\beta = \mathrm{L}, \mathrm{R}$), f_β is the Fermi–Dirac distribution function, and $\widetilde{\Gamma}_\sigma^\beta$ are some effective coupling parameters which are determined by the appropriate self-energies [11]. In the following we assume Γ_σ^β constant within the electron band ($\widetilde{\Gamma}_\sigma^\beta$ remains energy dependent). To determine the Green functions we need occupation numbers, which are given by

$$n_\sigma = \mathrm{i}\int \frac{\mathrm{d}E}{2\pi}\frac{\widetilde{\Gamma}_\sigma^{\mathrm{L}} f_{\mathrm{L}} + \widetilde{\Gamma}_\sigma^{\mathrm{R}} f_{\mathrm{R}}}{\widetilde{\Gamma}_\sigma^{\mathrm{L}} + \widetilde{\Gamma}_\sigma^{\mathrm{R}}}(G_\sigma^{\mathrm{r}} - G_\sigma^{\mathrm{a}}). \tag{2}$$

When replacing $\widetilde{\Gamma}_\sigma^\beta$ by Γ_σ^β, the above formulae reduce to the corresponding ones commonly used in the literature. However, such a replacement is correct only in the equilibrium situation.

3. Numerical results

Let us consider the situation when the left electrode is made of a $3d$ ferromagnetic metal, whereas the right one is half-metallic. This is reflected in the spin asymmetry of the bare coupling constants, for which we assume $\Gamma_\uparrow^{\mathrm{L}} = 2.8$ and $\Gamma_\downarrow^{\mathrm{L}} = 1.2$ for the left electrode, and $\Gamma_\uparrow^{\mathrm{R}} = 0.4$ and $\Gamma_\downarrow^{\mathrm{R}} = 0.002$ for the right one. Apart from this, we limit considerations to the case of strong electron correlation on the dot by assuming $U = 500$. It should be pointed here that the energy is measured in dimensionless units, and as the unit we assume $W/50$, where W is the electron band width. Numerical calculations are performed for the thermal energy $k_BT = 0.01$ and for the energy of the bare discrete level $\epsilon_{\mathrm{d}}^0 = -4$.

An important point of our calculations is a self-consistent renormalization of the dot energy level due to spin dependent coupling between the dot and electrodes. This coupling leads to spin splitting of the renormalized dot level, which is crucial for the splitting of the equilibrium Kondo peak in DOS and also in conductance [12]. The spin splitting of the renormalized dot level also leads to spin dependence of the relaxation time of intermediate states [3]. In numerical calculations we used the low temperature limit of this relaxation time.

In Fig. 1 we show DOS in the parallel (left column) and antiparallel (right column) magnetic configurations, calculated for three different values of applied bias voltage. We define positive bias V as the one with the electrochemical potential of the right electrode equal to zero and of the left electrode shifted up by eV (for simplicity we disregard negative sign of the electron charge e assuming $e > 0$). Accordingly, electrons flow from left to right. The negative bias, in turn, is defined as the one with the electrochemical potential of the left electrode equal to zero and of the right electrode shifted up by $|eV|$. Thus, the electrons flow then from right to left.

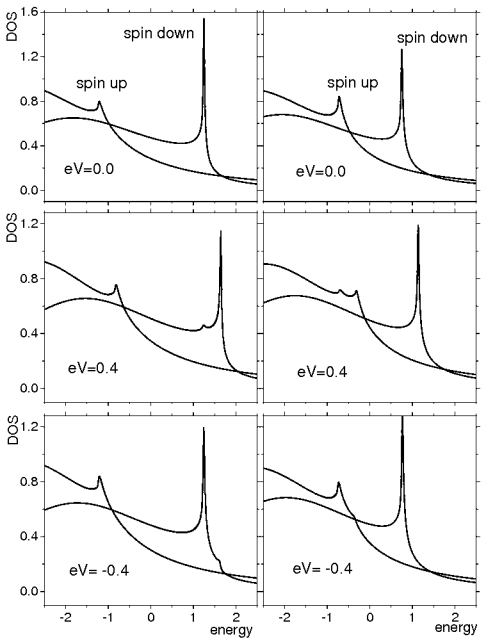

Fig. 1. Density of states (DOS) of the dot in the parallel (left column) and antiparallel (right column) magnetic configurations, calculated for indicated values of the bias voltage and for $\Gamma_{\uparrow}^{\mathrm{L}} = 2.8$, $\Gamma_{\downarrow}^{\mathrm{L}} = 1.2$, $\Gamma_{\uparrow}^{\mathrm{R}} = 0.4$, $\Gamma_{\downarrow}^{\mathrm{R}} = 0.002$, $U = 500$, $\varepsilon_{\mathrm{d}}^{0} = -4$, and $kT = 0.01$.

Let us consider first the parallel configuration. At $V = 0$ the Kondo peak in DOS is spin-split. The intensity of the spin-down peak is relatively large, whereas that of the spin-up peak is much smaller. The asymmetry in peak height is a consequence of the spin asymmetry in the coupling of the dot to the metallic electrodes (this coupling is larger for spin-up electrons and determines the height of the Kondo peak for spin-down electrons).

When a bias voltage is applied, each of the two Kondo peaks generally becomes additionally split into two components. One of them (the one associated with the coupling to the source electrode) should move up in energy, whereas position of the second one (the one associated with the drain electrode) should be unchanged. This is because the electrochemical potential of the drain electrode is independent of the voltage according to our definition. For positive bias, $eV > 0$, the splitting of the large-intensity peak is clearly visible, although one component of the double peak is relatively small. This is just the component which is associated with the coupling of the dot to the right electrode in the spin-up channel. Since this coupling is relatively small, the intensity is small, too. On the other hand, the second component is much larger because it is associated with the spin-up coupling to the left electrode, which is the largest coupling in the system

considered. The splitting of the low-intensity peak in DOS is not resolved. This is a consequence of the fact that the intensity of the component associated with the coupling to the right electrode in the spin-down channel practically vanishes because this coupling is very small.

For negative bias the situation is changed. Now the electrochemical potential of the left electrode is independent of the bias. Consequently, intensity of the components whose position is independent of energy is much larger than intensity of the components that shift up in energy (the ones associated with the right electrode). As before, the component associated with the coupling to the right electrode in the spin-down channel is not visible.

In the AP configuration, the magnetic moment of the right electrode is reversed. Thus, the coupling parameters to the right electrode are now $\Gamma^{\mathrm{R}}_{\downarrow} = 0.4$ and $\Gamma^{\mathrm{R}}_{\uparrow} = 0.002$, whereas the coupling parameters to the left electrode remain unchanged. As in the P configuration, the Kondo peak at equilibrium is spin-split, contrary to the case of symmetric coupling to two magnetic electrodes, where the spin splitting occurs only in the P configuration [12]. Apart from this, the situation is qualitatively similar to the one for P configuration. The main difference is that now the splitting of the high-intensity peak is not resolved, whereas the splitting of the low-intensity peak is resolved. This difference follows from the reversed spin asymmetry of the coupling to the right electrode, which in turn is due to reversed magnetization of the right electrode.

The Kondo peaks in DOS give rise to anomalous behavior of the transport characteristics. The differential conductance in the Kondo regime is shown in Fig. 2 for both magnetic configurations. In the P configuration the Kondo peak in the total conductance occurs for both positive and negative bias voltages. On the other hand, in the AP configuration the Kondo anomaly occurs only for negative bias.

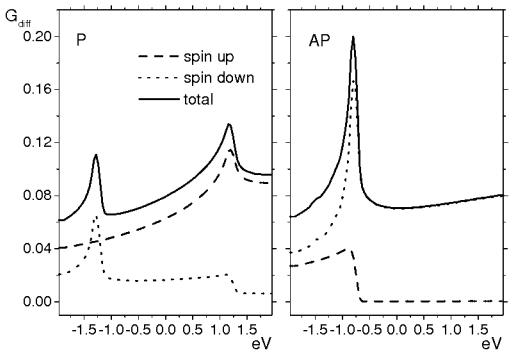

Fig. 2. Differential conductance G_{diff} of the system in the parallel (P) and antiparallel (AP) configurations. The other parameters are as in Fig. 1.

The absence of the Kondo peak in differential conductance $G_{\rm diff}$ for positive bias can be accounted for by taking into account behavior of the Kondo peaks shown in Fig. 1 for the AP configuration. When the bias voltage increases, the spin-down Kondo peak in DOS shifts up and does not enter the "tunnelling window". On the other hand, one of the two components of the spin-up Kondo peak can enter the tunnelling window, but the corresponding contribution is negligible due to vanishingly small coupling of the spin-up electrons to the right electrode in the AP configuration. Consequently, there is no Kondo peak in the conductance for positive bias in the AP configuration.

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