Kondo effect in quantum dots coupled to ferromagnetic leads with noncollinear magnetizations

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Non-equilibrium Green’s function technique has been used to calculate spin-dependent electronic transport through a quantum dot in the Kondo regime. The dot is described by the Anderson Hamiltonian and is coupled either symmetrically or asymmetrically to ferromagnetic leads, whose magnetic moments are noncollinear. It is shown that the splitting of the zero bias Kondo anomaly in differential conductance decreases monotonically with increasing angle between magnetizations, and for antiparallel configuration it vanishes in the symmetrical case while remains finite in the asymmetrical one.

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Introduction  Electronic transport through quantum dots attached to nonmagnetic leads was studied extensively in the past decade - both theoretically and experimentally. Quantum dots, particularly those including only a few or few tens of electrons offer a unique opportunity to study single-electron charging effects and electron-electron correlations. In particular, the many-body Kondo phenomenon was predicted [1] and then observed experimentally at low temperatures [2, 3]. The phenomenon is understood rather well [4, 5, 6, 7, 8, 9, 10, 11], although some of its features are still a subject of some discussion in the literature – for instance, the magnitude of the magnetic-field-induced splitting of the Kondo peak in differential conductance decreases monotonically with increasing angle between magnetic moments, whereas no such a splitting occurs for antiparallel alignment (in symmetrical situations the overall coupling of the dot to the leads is independent of the spin orientation), and for antiparallel configuration it vanishes in the symmetrical case while remains finite in the asymmetrical one.

It has been shown recently that the Kondo anomaly in electronic transport through a quantum dot attached symmetrically to ferromagnetic leads becomes suppressed in the parallel configuration [12, 13, 14, 15, 16], while in the antiparallel configuration it has features similar to those in the case of quantum dots attached to nonmagnetic leads. This behavior has also been observed experimentally [14]. The partial or total suppression of the anomaly is a consequence of an effective exchange field originating from the coupling of the dot to ferromagnetic electrodes. The exchange field gives rise to a nonzero spin-splitting of the equilibrium Kondo peak in the density-of-states (DOS) in the parallel configuration, whereas no such a splitting occurs for antiparallel alignment (in symmetrical situations the overall coupling of the dot to the leads is independent of the spin orientation for antiparallel alignment).

The splitting and suppression of the Kondo anomaly in electronic transport through quantum dots attached to ferromagnetic leads was studied up to now only for collinear magnetic configurations (parallel and antiparallel). The noncollinear configuration was considered in Ref. [20]. However, the approximations used to derive the appropriate Green functions do not take into account the exchange-induced splitting of the anomaly. Therefore, in this letter we address the problem of angular variation of the zero bias anomaly, i.e., variation of the Kondo peak with the angle between magnetic moments of the leads. We consider two situations: a symmetrical one – like that described above – and a nonsymmetrical case corresponding to different strengths and spin asymmetries of the coupling to the two electrodes.

We show that the the Kondo peak in differential conductance is suppressed already at small deviations from the antiparallel configuration. For larger deviations the anomaly varies rather slowly with the angle between magnetic moments.

Model and method  We consider a single-level quantum dot described by a Hamiltonian of the general form

\[ H = H_L + H_R + H_D + H_T. \]

The terms \( H_\beta \) describe the left (\( \beta = L \)) and right (\( \beta = R \)) electrodes in the non-interacting quasi-particle approximation. The term \( H_D \) stands for the dot Hamiltonian and is of the form,

\[ H_D = \sum_\sigma \epsilon_\sigma d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow, \]

where \( \epsilon_\sigma \) is the energy of the dot level (we assume that the energy level \( \epsilon_\uparrow \) corresponds to the spin-up electron, \( \epsilon_\downarrow \) to the spin-down electron), and \( U \) is the Hubbard-type electron correlation parameter. The tunneling part, \( H_T \), of the Hamiltonian describes electron transitions between the dot and electrodes, and is written in the form [21]

\[
H_T = \sum_{k\beta} \sum_{\sigma\sigma'} W_{k\beta}^{\sigma\sigma'} c_{k\beta\sigma}^\dagger d_{\sigma'} + \text{h.c.,}
\]  

(1)

where \( c_{k\beta\sigma}^\dagger \) is the creation operator of an electron with the wave vector \( k \) and spin \( s \) (\( s = + \) for majority electrons and \( s = - \) for minority ones) in the lead \( \beta \), \( d_{\sigma} \) annihilates an electron on the dot with spin \( \sigma \) (\( \sigma = \uparrow, \downarrow \) along the quantization axis of the dot), and \( W_{k\beta}^{\sigma\sigma'} \) is the corresponding matrix element. The matrix \( W_{k\beta}^{\sigma\sigma'} \) can be...
where $\phi_\beta$ is the angle between the local spin quantization axis in the lead \( \beta \) and the quantization axis on the dot, and \( T_{k\beta s} \) are the matrix elements for electron tunneling from the dot to the spin majority \((s=+\)) and spin minority \((s=-\)) electron bands in the lead \( \beta \) when \( \phi_\beta = 0 \). As the quantization axis for the dot we assume orientation of the exchange field created by the ferromagnetic electrodes. For a symmetrical and unbiased system one can assume \( \phi_R = -\phi_L = \theta/2 \), where \( \theta \) is the angle between magnetic moments of the leads.

Electric current \( I \) has been calculated from a formula derived by Meir et al.\(^2\) for nonequilibrium situation. This formula has been extended to noncollinear magnetic configurations. It includes retarded (advanced) and correlation Green functions of the dot in the presence of bias voltage applied to the leads (nonequilibrium situation).

To calculate the retarded Green functions we used the equation of motion method and restricted calculations to the large \( U \) limit. The higher order Green functions have been decoupled according to the procedure described by Meir.\(^2\) Such an approach gives reasonable results for temperatures comparable to the Kondo temperature \( T_K \). However, we go beyond this approximation by calculating the Green functions, renormalized dot level, and occupation numbers self-consistently. Strictly speaking, the bare (spin-degenerate) dot level \( \epsilon_0 \) in the self energy \( \Sigma_1 \) was replaced by the corresponding level spin-split by the effective exchange field \( \Sigma_1 \)

\[
\mathbf{B}_{\text{exch}} = (1/g_{\mu_B}) \sum_\beta n_\beta \Re \int \frac{d\epsilon}{2\pi} (\Gamma^\beta_+ - \Gamma^\beta_-) \frac{f_\beta(\epsilon)}{\epsilon - \epsilon_0 - i\hbar/\tau_0},
\]

where \( n_\beta \) is a unit vector along the magnetic moment of the \( \beta \)-th electrode, \( \tau_0 \) is a relevant relaxation time \( \mathbf{3} \), \( f_\beta \) is the Fermi distribution functions for the electrode \( \beta \), and \( \Gamma^\beta_+ = 2\pi \sum_k T_{k\beta s}^\beta \delta(E - \epsilon_k) \) for \( s = +, - \). In the following \( \Gamma^\beta_s \) are assumed to be independent of energy within the electron band and zero otherwise; \( \Gamma^\beta_s = \Gamma^\beta_s (1 + sp_\beta) \), where \( p_\beta \) is the spin polarization of the lead \( \beta \).\(^15\)

The renormalization of the dot level plays an important role in transport through quantum dots attached to ferromagnetic electrodes, and leads to the spin splitting and suppression of the Kondo anomaly in differential conductance.\(^14\)\(^16\)\(^17\)\(^18\). The approach based on the equation of motion with the renormalization procedure including the exchange field gives results which are fully consistent with those obtained for collinear configurations by the perturbational real-time diagrammatic approach.\(^2\)

For \( U \rightarrow \infty \), the equation of motion for the Green function \( G \) leads to the Dyson equation \((1 - g_0 \Sigma) G = g_0 \), where \( g_0 = \delta_{\sigma\sigma'}(E - \epsilon_0)^{-1} \) and \( \Sigma = g_0^{-1} - n^{-1} g_0^{-1} - \Sigma \). Here, \( n_{\sigma\sigma} = 1 - n_{\sigma\sigma} \) and \( \tilde{n}_{\sigma\sigma} = n_{\sigma\sigma} \), where \( \sigma = -\sigma \) and \( n_{\sigma\sigma'} = (d^+_{\sigma'} d_{\sigma}) \). The self-energy \( \Sigma \) is defined as \( \Sigma = \Sigma_0 + \Sigma_1 \), where \( \Sigma_0 = (i/2) \sum_\beta \Gamma_{\sigma\sigma}^\beta \) with \( \Gamma_{\sigma\sigma}^\beta = \Gamma^\beta_+ \cos^2(\phi_\beta/2) + \Gamma^\beta_- \sin^2(\phi_\beta/2), \Gamma^\beta_+ = \Gamma^\beta_+ - \Gamma^\beta_- \sin^2(\phi_\beta/2) + \Gamma^\beta_+ \cos^2(\phi_\beta/2), \Gamma^\beta_+ = (1/2)(\Gamma^\beta_+ - \Gamma^\beta_-) \sin(\phi_\beta) \). In turn, \( \Sigma_1 \) is given by

\[
\Sigma_{1\sigma\sigma} = \sum_\beta \int \frac{d\epsilon}{2\pi} \frac{\Gamma_{\sigma\sigma}^\beta f_\beta(\epsilon)}{E - \epsilon_0 - i\hbar/\tau_0},
\]

\[
\Sigma_{1\sigma\sigma} = -\sum_\beta \int \frac{d\epsilon}{2\pi} \frac{\Gamma_{\sigma\sigma}^\beta f_\beta(\epsilon)}{E - \epsilon_0 - i\hbar/\tau_0}.
\]

The corresponding lesser Green function \( G^< \) has been calculated from the Keldysh equation \( G^< = G^r \Sigma G^a \) with the self energy \( \Sigma^< \) calculated from the Ng ansatz. Writing \( \Sigma^r - \Sigma^a = -i\Sigma^\text{eff} \) and \( \Sigma^r - \Sigma^a = -i\Sigma = -i(\Gamma^L + \Gamma^R) \), the formula for electric current takes the form

\[
I = \frac{e}{2h} \int \frac{d\epsilon}{2\pi} \Gamma^L \bar{G}^r \bar{T}^R G^a + \Gamma^R \bar{G}^r \bar{T}^L G^a)(f_L - f_R),
\]

where \( \bar{G}^\beta = \Gamma^\beta \bar{T}^{-1} \Sigma^\text{eff} \), and \( e \) is the electron charge.

**Numerical results** Let us write \( \Gamma^\beta_0 = \alpha \Gamma^\beta_0 \) = \( \alpha \tilde{G}_0 \). Numerical calculations have been performed for \( \epsilon_0 = -0.35 \), \( kT = 0.001 \), and \( \Gamma_0 = 0.1 \) (energy is measured in the units of \( D/50 \), where \( D \) is the width of electron band extending from \(-D/2 \) to \( D/2 \)). Consider first the symmetrical situation: \( \alpha = 1 \) and \( p_L = p_R = p \). In Fig.1 we show the corresponding DOS for unbiased (a) and biased (b) system for parallel \( (\theta = 0) \), antiparallel \((\theta = \pi) \), and perpendicular \((\theta = \pi/2) \) magnetic configurations. In the unbiased system, the spin splitting of the Kondo peak in DOS is maximal in the parallel configuration and decreases with increasing angle between the magnetic moments, vanishing exactly for the antiparallel configuration. This splitting is a direct consequence of the exchange field exerted on the dot by ferromagnetic electrodes. The largest exchange field occurs in the parallel configuration, so the corresponding splitting of the anomaly is also maximal in this configuration. In the antiparallel configuration the exchange fields from the two electrodes cancel each other so the splitting vanishes (see Fig.1(a)). A further consequence of the spin splitting of DOS is a suppression of the zero bias anomaly in the differential conductance, as will be discussed below.

In the biased system, the Kondo peak in DOS becomes split due to different electrochemical potentials of the two electrodes. Such a splitting exists also in nonmagnetic situations. The exchange field in parallel and noncollinear configurations introduces further splitting, as shown in Fig.1(b), similarly as an external magnetic field does in the case of quantum dots attached to nonmagnetic leads.\(^12\)

Numerical results for the corresponding differential conductance and tunnel magnetoresistance (TMR) vs bias voltage are shown in Fig.2 for several values of the
angle $\theta$ between magnetic moments of the leads, and for two values of the spin polarization factor $p$. In the antiparallel configuration ($\theta = \pi$) there is a well defined zero bias anomaly due to the Kondo correlations. When the angle between magnetic moments decreases, the conductance peak becomes split and its intensity becomes suppressed. The splitting as well as the suppression of the intensity grow with decreasing $\theta$. Finally, in the parallel configuration only low-intensity peaks occur at nonzero positive and negative bias. The results are consistent with the limiting situations of collinear configurations, $\theta = 0$ and $\theta = \pi$, considered in Refs \[15, 17, 18, 23\]. It is interesting to note a fast decrease of the peak intensity already at small deviations from the antiparallel configuration, as follows from Fig.2(a) and (b). Variation of the peak intensity with $\theta$ is rather small for $\theta < \pi/2$. Comparison of Fig.2(a) and (b) also shows that the splitting increases with increasing spin polarization of the leads, while the peak intensity decreases with increasing $p$.

The associated TMR ratio, defined by the system resistance $R(\theta)$ as $[R(\theta) - R(\theta = 0)]/R(\theta = 0)$, shows a peculiar behavior displayed in Fig.2 (c) and (d) for two values of $p$. For $\theta = \pi$ the TMR has a dip in the zero bias regime and is negative. The negative sign is a consequence of the suppression of the Kondo peak in the parallel configuration, which makes the system more conducting in the antiparallel configuration (inverse TMR effect). The dip at zero bias disappears when the initial configuration departs from the antiparallel one, and instead of a minimum there is a local maximum of TMR at $V = 0$. Two side local minima of TMR occur then at some nonzero voltages. The maximum at $V = 0$ increases and becomes more flat when the angle between magnetic moments decreases from $\theta = \pi$ to $\theta = 0$.

In the situation described above the quantum dot was coupled symmetrically (in the parallel configuration) to the leads. When the coupling is not symmetrical, then a certain splitting and suppression of the zero bias anomaly exist also in the antiparallel configuration \[23, 24\]. This is because the exchange fields from the two leads do not compensate each other as they did when the dot was coupled symmetrically. Accordingly, the splitting of the Kondo anomaly may be observed also when only one of the leads is ferromagnetic while the other one is nonmagnetic \[24\].

Let us consider now angular variation of the Kondo anomaly in a strongly asymmetric system; $\alpha = 0.1$, $p_L = 0.4$, $p_R = 0.8$. The corresponding DOS is shown in Fig.1(c) and (d) respectively for the unbiased and biased system, and for parallel, antiparallel and perpendicular magnetic configurations. At $V = 0$ the Kondo peak in DOS is spin-split in the antiparallel configuration and the splitting increases when the configuration varies from antiparallel to parallel. In the biased system the peaks are additionally split due to different electrochemical potentials of the two leads, but intensity of one of the two components of the peak is relatively small and only weakly resolved in Fig.1(d). The asymmetry in peak intensities

FIG. 1: Density of states in the Kondo regime in (a,b) symmetrical ($\alpha = 1$, $p = 0.2$) and (c,d) asymmetrical ($\alpha = 0.1$, $p_L = 0.4$, $p_R = 0.8$) systems for three indicated values of the angle between magnetic moments and for unbiased (a,c) and biased (b,d) systems. The other parameters as described in the text.

FIG. 2: Bias dependence of the Kondo anomaly in differential conductance (a,b) and of the TMR effect (c,d), calculated for indicated values of the angle $\theta$ between magnetic moments of the leads and for two different polarization factors $p$. The other parameters as in Fig.1.
is a consequence of the spin asymmetry in the coupling of the dot to metallic electrodes, and a difference in spin polarizations, \( p_L \neq p_R \). The differential conductance and TMR are shown in Fig.3 (a) and (b), respectively. In the parallel configuration the dominant Kondo anomaly occurs in the spin–up channel and for \( eV > 0 \) (electrons flow from left to right). The corresponding peak at \( eV < 0 \) is significantly weaker. In the antiparallel configuration, on the other hand, the Kondo peak in differential conductance occurs for \( eV < 0 \) only. This behavior can be accounted for by taking into account behavior of the Kondo peaks in DOS and spin asymmetry in the coupling to electrodes [24].

The corresponding TMR is shown in Fig.3(b). It is interesting to note that TMR is highly asymmetric with respect to the bias reversal. It becomes positive for \( eV \) exceeding a certain positive value, and negative below this voltage. This is a consequence of the fact that for positive \( eV \) the Kondo peak in differential conductance is clearly visible in the parallel configuration, whereas for \( eV < 0 \) the Kondo peak occurs in the antiparallel configuration. Such a behavior of the conductance and TMR may be interesting from the point of view of applications in mesoscopic devices like diodes, for instance.

In summary, we have analyzed the Kondo phenomenon in a quantum dot attached to ferromagnetic leads with noncollinear magnetizations. Our results show a monotonic dependence of the Kondo peak suppression with the angle between magnetic moments of the leads. A fast decrease of the Kondo peak takes place already at small deviations from the antiparallel configuration.

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