Kondo correlation and spin-flip scattering in spin-dependent transport through a quantum dot coupled to ferromagnetic leads

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We investigate the linear and nonlinear dc transport through an interacting quantum dot connected to two ferromagnetic electrodes around Kondo regime with spin-flip scattering in the dot. Using a slave-boson mean field approach for the Anderson Hamiltonian having finite on-site Coulomb repulsion, we find that a spin-flip scattering always depresses the Kondo correlation at arbitrary polarization strength in both parallel and antiparallel alignment of the lead magnetization and that it effectively reinforces the tunneling related conductance in the antiparallel configuration. For systems deep in the Kondo regime, the zero-bias single Kondo peak in the differential conductance is split into two peaks by the intradot spin-flip scattering; while for systems somewhat further from the Kondo center, the spin-flip process in the dot may turn the zero-bias anomaly into a three-peak structure.

Spin-dependent electron transport through systems consisting of two ferromagnetic layers (FM) sandwiched by a quantum-dot (QD) has recently become one of the major focuses of the rapidly developing spin-electronics.1 Different from other nonmagnetic sandwiches, a quantum dot features its small size and the strong many-body correlation among electrons in it such that, not only the Coulomb blockade can dominate its electronic transport, but particularly, a significant Kondo effect may arise. Very rich behavior has been disclosed when varying the strength and/or the relative orientation of the spin polarizations of two magnetic electrodes, the dot energy level and the on-site Coulomb correlation in the dot.2–10

Effect of spin-flip scatterings in the QD has also been explored very recently. By means of the equation of motion method11 and the Ng ansatz12, Zhang et. al.9 predicted that, in a FM/QD/FM system having infinite on-site Coulomb repulsion, the presence of the spin-flip process in the dot may split the original single Kondo resonance in the density of states into two or three well-defined peaks. Utilizing a slave boson mean field (SBMF) technique for infinite-U systems,13,14 López and Sáchez15 found a splitting of the zero-bias peak of the nonlinear differential conductance when the spin-flip scattering amplitude is of the order of the Kondo temperature. However, the failure of detecting the Kondo peak splitting induced by lead magnetization in the parallel configuration and the unphysical prediction of complete quenching of the zero-bias anomaly and vanishing widths of the nonzero-bias peaks at large spin-flip scattering,10 indicate the limitation of the infinite-U SBMF approach to FM/QD/FM systems.

In this Letter we investigate effects of intradot spin-flip scatterings on the dc conductance through a FM/QD/FM system using the finite-U SBMF approach of Kotляр and Ruckenstein.15–17 With the help of four slave boson parameters, this SBMF approach not only allows to deal with finite on-site Coulomb repulsion but also to take account of charge fluctuations to certain degree. For a FM/QD/FM system without spin-flip scattering8 it derives a clear splitting of the Kondo peak in differential conductance due to lead magnetization in the parallel configuration in agreement with other techniques,6,7 and predicts the physically reasonable peak widths and heights.

We consider a quantum dot (QD) of single bare level εd having a finite on-site Coulomb repulsion U and a spin-flip scattering amplitude R, is coupled to two ferromagnetic leads through tunneling Vk,α (α = L, R). Both the left and the right leads are magnetized along the z axis but may be in parallel (P) or antiparallel (AP) alignments (configurations) and the electrons in the leads are described by wavevector k and spin index σ with energy εk,σ (σ = ±1 or ↑↓).

In terms of the finite-U slave-boson approach,15 we introduce four auxiliary boson operators e, pσ and d, which are associated respectively with the empty, singly occupied and doubly occupied electron states of the QD, to describe the above physical problem without interparticle coupling in an enlarged space with constraints. Within the mean-field scheme one can start with the following effective Hamiltonian:

\[ H_{\text{eff}} = \sum_{k,\sigma} \epsilon_{k,\sigma} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{\sigma} \epsilon_d c_{d,\sigma}^{\dagger} c_{d,\sigma} + Ud^\dagger d + R(c_{d,\uparrow}^{\dagger} c_{d,\downarrow} + \text{H.c.}) + \sum_{k,\sigma} [V_{k,\sigma} c_{k,\sigma}^{\dagger} c_{d,\sigma} + \text{H.c.}] + \lambda^{(1)} \left( \sum_{\sigma} p_{\sigma}^{\dagger} p_{\sigma} + e^{\dagger} e + d^{\dagger} d - 1 \right) + \sum_{\sigma} \lambda^{(2)}_{\sigma} \left( c_{d,\sigma}^{\dagger} c_{d,\sigma} - p_{\sigma}^{\dagger} p_{\sigma} - d^{\dagger} d \right), \]  

(1)

where \( c_{d,\sigma}^{\dagger} (c_{d,\sigma}) \) and \( c_{k,\sigma}^{\dagger} (c_{k,\sigma}) \) are the creation (annihilation) operators of electrons in the dot and in the electrodes, the three Lagrange multipliers \( \lambda^{(1)} \) and \( \lambda^{(2)}_{\sigma} \) take account of the constraints, and in the hopping term
the fermion operator $c^\dagger_{ds}$ and $c_{ds}$ are replaced by $z_{ds}^\dagger c^\dagger_{ds}$ and $z_{ds} c_{ds}$ to consider the many body effect on tunneling. $z_{ds}$ embodies the physical process with which an electron with spin $\sigma$ in the dot is annihilated: $z_{ds} = (1 - d_{\sigma}^d d_{\sigma}^\dagger - p_{\sigma}^d p_{\sigma}^\dagger) - 1/2$. The Heisenberg equations of motion for the four slave-boson operators derived from the effective Hamiltonian together with the three constraints, form the basic equations. Then we use the mean-field approximation in the statistical expectations of these equations, in which all the boson operators are replaced by their expectation values which serve as the instrumental parameters in the mean-field scheme. In the wide-band limit the final equations are:

$$
\sum_{\sigma} \frac{\partial z_{ds}}{\partial t} K_{ds} + 2\lambda^{(1)}_{ds} = 0, \quad (2)
$$

$$
\sum_{\sigma} \frac{\partial z_{ds}}{\partial p_{\sigma'}} K_{ds} + 2\lambda^{(1)}_{ds} - \lambda^{(2)}_{ds} = 0, \quad \sigma' = \pm 1, \quad (3)
$$

$$
\sum_{\sigma} \frac{\partial z_{ds}}{\partial d} K_{ds} + 2(U + \lambda^{(1)}_{ds} - \lambda^{(2)}_{ds}) = 0, \quad (4)
$$

$$
\sum_{\sigma} |p_{\sigma}|^2 + |d|^2 = 1, \quad (5)
$$

$$
\frac{1}{2\pi i} \int d\omega G_{ds}^\sigma(\omega) = |p_{\sigma}|^2 + |d|^2, \quad \sigma = \pm 1. \quad (6)
$$

Here

$$
K_{ds} = \frac{1}{\pi} \int d\omega \{ z_{ds} \text{Re}(G_{d\sigma}^\sigma(\omega)) [f_L(\omega)\Gamma_{L\sigma} + f_R(\omega)\Gamma_{R\sigma}] \}, \quad (7)
$$

where $f_\sigma(\omega) = 1/(e^{\beta(\omega - \mu_\sigma)} + 1)$ is the Fermi function and $\mu_\sigma$ is the chemical potential of the $\sigma$th lead, which is assumed in an equilibrium state at temperature $1/\beta$, and $\Gamma_{d\sigma}(\omega) = 2\pi \sum_{k_{\sigma}} |V_{k_{\sigma}}|^2 \delta(\omega - \epsilon_{k_{\sigma}})$ is the coupling strength function between the QD and the lead $\alpha$. $G_{d\sigma}^\sigma(\omega)$ and $G_{d\sigma}^{-\sigma}(\omega)$ are the elements of the 2x2 retarded (advanced) and correlation Green’s function matrices $G_{d\sigma}^\sigma(\omega)$ and $G_{d\sigma}^{-\sigma}(\omega)$ in the spin space of the QD. In the SBMF scheme, the strong correlating problem of the dot electrons with finite Coulomb repulsion $U$ is reduced to an effective noncorrelating one described by the effective Hamiltonian (1) with the slave-boson operators treated as $c$-numbers. The retarded (advanced) Green’s function can be expressed in the form renormalized due to dot-lead couplings: $G_{d\sigma}^\sigma(\omega) = \frac{1}{1 - \Omega_{\sigma}^{l(\sigma)}}$, in which $\Omega_{\sigma}^{l(\sigma)} = \xi_{\sigma} (\xi_{\sigma} + \lambda^{(2)}_{\sigma})$ and $\Omega_{\sigma}^{l(\sigma)} = \frac{1}{2} |z_{\sigma}|^2 (\Gamma_{L\sigma} + \Gamma_{R\sigma})$ reflects the dot-level broadening, and $\Gamma$ is a unit matrix. The correlation Green’s function $G_{d\sigma}^{-\sigma}$ can be obtained by the Keldysh equation: $G_{d\sigma}^{-\sigma} = G_{d\sigma}^\sigma \Sigma_{d\sigma}^{-\sigma} G_{d\sigma}^\sigma$, with

$$
\Sigma_{d\sigma}^{-\sigma} = i|z_{\sigma}|^2 (f_L\Gamma_{L\sigma} + f_R\Gamma_{R\sigma}) \delta_{\sigma'\sigma},
$$

The electric current flowing from the left lead into the QD is obtained from the rate of change of the electron number operator of the left lead:\(^{11,18}\)

$$
I_L = \frac{ie}{\hbar} \int \frac{d\omega}{2\pi} \sum_{\sigma} \Gamma_{L\sigma} |z_{\sigma}|^2 [\{ (G_{d\sigma}^\sigma - G_{d\sigma}^{-\sigma}) f_L + G_{d\sigma}^{-\sigma} \}]. \quad (8)
$$

In the steady transport state, the current flowing from the QD to the right lead must be equal to the current from the left lead to the QD, and the formula (8) can be directly used for calculating the current flowing through the lead-dot-lead system under a bias voltage $V$ between the two leads: $I = I_L$.

We assume that the left and right leads are made from identical materials and that, in the wide band limit, the effective coupling strength functions are constants for each direction of magnetization, such that in the P configuration $\Gamma_{RT}(\omega) = \Gamma_{L}(\omega) = \Gamma_{R}(\omega)$ and in the AP configuration $\Gamma_{RT}(\omega) = \Gamma_{L}(\omega) = \Gamma_{R}(\omega)$. We will take $\Gamma = (\Gamma_{L} + \Gamma_{R})/2$ as the energy units and define the spin polarization as $P = (\Gamma_{L} - \Gamma_{R})/(2\Gamma)$. The Kondo temperature for finite-$U$ system in the case of $P = 0$, given by $T_K^0 = U/\sqrt{\beta} \exp(-\pi/\beta)/2\pi$ with $\beta = -2U/e(\mu_L + \mu_R)$, will be used as a reference dynamical energy scale. In the following we will study FM/QD/FM systems having a fixed finite Coulomb repulsion $U = 6$ and concentrate on the effects of the spin-flip scattering on linear and nonlinear transport. In calculating the dc current under a bias voltage $V$ between two leads, we choose the chemical potential $\mu_L = -\mu_R = eV/2$ for the left and right leads. The finite-$U$ SBMF method was known to yield qualitatively correct conduction behavior at low temperatures within the bare dot-level range $-1.2U \leq \epsilon_d \leq 0.2U$. Fig. 1 shows the calculated zero-temperature linear conductance $G = (dI/dV)_{V=0}$ as a function of $\epsilon_d$ of the QD having spin-flip scattering of different amplitude $R$ at fixed polarization $P = 0.7$ in AP and in P configurations.

In the case of $R = 0$, the $G$-vs-$\epsilon_d$ curve contains three regimes, covering the resonance peak due to the dot level around $\epsilon_d = 0$, the charging peak around $\epsilon_d = -U$, and the Kondo peak centered at $\epsilon_d = -U/2$. In the AP configuration, all the renormalized parameters are identical for up and down spin indices at arbitrary $P$ and electrons with up-spin and down-spin are equally available in the whole lead-dot-lead system, favoring the formation of the Kondo-correlated state within a relatively wide dot-level range centered at $\epsilon_d = -3$. The $G$-vs-$\epsilon_d$ curves appear to be gentle-top hump structure. On the other hand, in the AP configuration the available minority-spin (e.g. up-spin) states in the right lead decline due to $P > 0$ and the transfer of the majority-spin (up-spin) electrons from the left lead to the right lead is suppressed by the finite polarization, such that the conductance of the system goes down with increasing polarization from $P = 0$ and vanishes at $P = 1$. The effect of a finite polarization is to reduce the height of the $G$-vs-$\epsilon_d$ hump, while the shape of the curve remains essentially unchanged.
in the P configuration, the spin-flip scattering reduces the central Kondo peak sharply while slightly shifts the resonance peak and charging peak apart, finally turning the three-peak $G$-$\epsilon_d$ curve into a Coulomb blockade type double-peak one. In the AP configuration, a deep valley develops progressively at the center $\epsilon_d = -3$ from the previous $G$-$\epsilon_d$ hump, leading also to a Coulomb blockade type double peak one with enhanced heights of and enlarged distance between two peaks.

Effects of changing polarization strength on linear conductance in the presence of spin-flip process are shown in the right part of Fig.1 for the system of $\epsilon_d = -2$ in the Kondo regime. In the P configuration, $G$ always goes down with growing $P$ for fixed $R$ and with growing $R$ for fixed $P$, indicating that both the polarization and the spin-flip scattering suppress the Kondo resonance. In the AP configuration, although the linear conductance $G$ still declines with increasing $P$ in the case of $R = 0$ or with increasing $R$ in the case of $P = 0$, anomaly shows up at finite $P$ and finite $R$ due to the competing effects of polarization and spin-flip scattering on Kondo correlation and resonance tunneling. At $R = 0.1$ the conductance descends much slower than at $R = 0$, and $G$ even rises with increasing polarization for $R \geq 0.2$.

A coherent spin-flip scattering ($R > 0$) in the dot plays three important roles. (1) It lifts the degenerate dot level $\epsilon_d$ to $\epsilon_d \pm R$ even in the presence of a strong on-site Coulomb repulsion, with states being the linear combinations of the up- or down-spin ones. This level splitting may lead to somewhat broadening of the resonance peak and charging peak. (2) It strongly suppresses the Kondo correlation, such that the conductance maximum at $\epsilon_d = -3$, which is fully Kondo-induced, drops sharply when $R > 0$. (3) In the AP configuration, $R > 0$ makes it possible for the majority-spin electrons of the left lead to change their spin orientations after tunneling into the dot, in favor of their continuing to tunnel into the right lead, and thus enhances the tunneling related conductance. As can be seen in Fig.1, the tunneling peaks and the charging peaks in the cases of $R = 0.1, 0.2, 0.3$ and 0.4 are all higher than those of $R = 0$. In the P configuration, however, the tunneling-related conductance is essentially not affected by the presence of spin-flip process. The $G$-$\epsilon_d$ curves in Fig.1 are the result of competition and compensation of the above three effects. We see that,
configuration has not yet been able to split the broadened Kondo peak. We have essentially the conventional zero-bias anomaly of Kondo correlation in both AP and P configurations for $R = 0$. Turning on the intradot spin-flip scattering suppresses the Kondo effect and lifts the dot-level degeneracy of order of $R$, giving rise to a significant drop of the height of the zero-bias anomaly and, up from $R = 0.1$ ($\sim 0.7T_K$), $dI/dV$ begins to split into two peaks centered around $eV = \pm 2R$ in both configurations. This result is in agreement with the recent prediction of López and Sánchez.\textsuperscript{10} Note that, however, our $dI/dV$ for this system does not show any sign of complete quenching of the zero-bias conductance. The spin-flip process suppresses the Kondo contribution while keeps the latter essentially unchanged. Therefore the drop of the zero-bias $dI/dV$ is modest in comparison with that in the left part of Fig. 2. On the other hand, the peak splitting develops progressively due to the increase of $R$-induced level splitting. The appearance of three-peak structure in the curves of $R = 0.2, 0.3$ and 0.4 is just the result of these two effects. In the AP configuration, there is no dot-level splitting and the differential conductance remains a zero-bias single-peak curve for any strength of the lead polarization in the case of $R = 0$. The spin-flip scattering, while suppressing the Kondo contribution, helps to enhance the resonance-tunneling related conductance. For $\epsilon_d = -1$ system the latter overcompensates the Kondo reduction, such that we see the whole $dI/dV$ curve of $R = 0.1$ rising over that of $R = 0$. Note that at $R = 0.1$, the spin-flip induced level splitting has not yet been able to destroy the single-peak structure and we have only a broadened peak. The $R = 0.2$ induced level splitting leads to the appearance of shoulders on both sides. Two side peaks clearly show up at larger spin-flip scattering amplitudes. We see three-peak $dI/dV$ curves for $R = 0.3$ and 0.4 in the AP configuration.

In summary, we have demonstrated that a spin-flip scattering in QD always suppresses the Kondo correlation at arbitrary polarization strength in both P and AP alignment of the lead magnetizations, and the effect is stronger for P configuration at larger $P$. It effectively reinforces the tunneling related conductance in the AP configuration. For systems deep in the Kondo regime, the zero-bias single Kondo peak in the differential conductance is split into two peaks by the intradot spin-flip scattering; while for system somewhat further from the symmetric point, the spin-flip process in the dot may turn the single-peak conductance curve into a three-peak form. The predicted positions and widths of the split peaks are in rough agreement with the spin-flip induced energy splitting and the tunneling induced level broadening, renormalized by the many-body effect. The main physics concerned in this Letter is in the energy scale of the Kondo temperature $T_K$ or the effective coupling strength $\Gamma$, which are easily accessible experimentally.

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