Nonequilibrium spintronic transport through an artificial Kondo impurity: Conductance, magnetoresistance and shot noise

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We investigate the nonequilibrium transport properties of a quantum dot when spin flip processes compete with the formation of a Kondo resonance in the presence of ferromagnetic leads. Based upon the Anderson Hamiltonian in the strongly interacting limit, we predict a splitting of the differential conductance when the spin flip scattering amplitude is of the order of the Kondo temperature. We discuss how the relative orientation of the lead magnetizations strongly influences the electronic current and the shot noise in a nontrivial way. Furthermore, we find that the zero-bias tunneling magnetoresistance becomes negative with increasing spin flip scattering amplitude.

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Introduction.—The Kondo effect in quantum dots (QD’s) occurs because of a strong antiferromagnetic coupling between the conduction band electrons in the electrodes and the localized spin in the QD through higher-order tunneling processes. The resulting correlated motion gives rise to a Kondo singularity in the quasiparticle density of states at the Fermi level $E_F$.[1]. As a consequence, the conductance is enhanced below the Kondo temperature $T_K$.[2]. The fact that the parameters that define $T_K$ are fully controllable and the ability to apply external fields in QD’s have spurred a good deal of works addressing nonequilibrium situations[3]. At the same time, recent advances in the control and manipulation of the spin degree of freedom in magnetic environments[4] has paved the way for startling potentialities in spintronic devices[5] and quantum computation[6]. A single spin-1/2 confined in a discrete level reaches the ultimate degree of miniaturization in semiconductor physics. Thus, it is crucial to understand the properties of spintronic transport in QD’s. The main focus has so far been to investigate magnetic effects in QD’s in the Coulomb blockade regime[2,3]. In comparison, the issue of spin-dependent physical effects in the Kondo resonance, which seems to be much richer, has been relatively unexplored. In particular, one might ask to what extent the Kondo cloud is sensitive to the lead magnetization. Or, is the many-body Kondo state robust against spin flip processes? Answering these questions is not only interesting for QD’s but also for similar coherent phenomena in molecular transistors[7].

Consider first a noninteracting QD with a single energy level $E_0$ attached to two ferromagnetic contacts. Intradot spin flip processes lift the level degeneracy, yielding $E_0 \pm R$, where $R$ is a phenomenological spin flip scattering amplitude. When $R$ is greater than the tunneling induced broadening $\Gamma$, the linear conductance will show a splitting sensitive to the lead polarization alignment. Similarly, in the strongly interacting case we expect the Kondo induced spin fluctuations to become affected by the combined influence of ferromagnetic leads and spin flip processes. Our main findings reflect this physics, summarized in Figs. 1 and 2a: (i) Let $T_K$ denote the Kondo temperature of a QD for a given magnetic configuration ($R \neq 0$ and lead magnetization $\eta \neq 0$). For $R/T_K < 1$ the differential conductance $G \equiv dI/dV_{dc}$ ($V_{dc}$ is the bias voltage) shows the distinctive zero bias anomaly (ZBA) of Kondo physics[2] whereas for $R/T_K > 1$ the ZBA smoothly splits at finite $V_{dc}$ into two peaks separated by a distance $\delta$. With decreasing $T_K$ (e.g., by lowering $E_0$ with a gate voltage), the spin flip scattering is shown to suppress the Kondo state. (ii) We find that the exact form of $G$ depends on whether the relative orientation of the lead magnetizations is parallel (P) or antiparallel (AP). In addition, in the P case the ZBA splitting develops at different $R$ with regard to the AP case. We find that in the AP configuration the variation of the Kondo temperature with $R$ is independent of $\eta$. Strong effects of $R$ and $\eta$ in the measurement of the magnetoresistance and the current fluctuations at $T = 0$ (shot noise) are predicted as well.

Model.—There exist in the literature very scarce theoretical investigations that deal with Kondo transport in QD’s in the presence of ferromagnetic leads[10,11,12]. To the best of our knowledge, no complete picture of the Fermi-liquid behaviour (i.e., at temperatures $T \ll T_K$) of the Kondo effect in ultrasmall magnetic tunnel junctions has been yet put forward. We consider a QD (region 0) with large on-site Coulomb interaction $U$ coupled via $V_{ko}$ to two Fermi-liquid reservoirs labeled with $\alpha = \{L, R\}$ with chemical potentials $\mu_L$ and $\mu_R$. We describe the system with a $N = 2$ fold degenerated Anderson Hamiltonian allowing for intradot spin flips. In the limit $U \rightarrow \infty$, QD double occupancy is forbidden and the slave-boson representation[13] may be used to write the Hamiltonian as follows:

$$
\mathcal{H} = \sum_{k, \alpha} \varepsilon_{k, \alpha} c_{k, \alpha}^\dagger c_{k, \alpha} + \sum_\sigma \varepsilon_0 f_\sigma^\dagger f_\sigma + (R f_\uparrow^\dagger f_\downarrow + \text{H.c.}) + \frac{1}{\sqrt{N}} \sum_{k, \alpha} (V_{ko} c_{k, \alpha}^\dagger b^\dagger f_\sigma + \text{H.c.}) + \lambda (b^\dagger b + \sum_\sigma f_\sigma^\dagger f_\sigma - 1)
$$
where \(c_{k\sigma}^\dagger \) is the creation (annihilation) operator for an electron in the state \(k\) with spin \(\sigma = \{\uparrow, \downarrow\}\) in the lead \(\alpha\). Ferromagnetism in the leads arises through spin-dependent densities of states \(\nu_{\sigma}\). We have assumed implicitly that both ferromagnetic leads possess the same \((z)\) easy axis. The generalization to noncollinear magnetic moments is straightforward [11]. In Eq. 10, the spin flip term is assumed to be coherent in the sense that \(R\) does not involve spin relaxation since each flip-flop process can be reversible [14]. Only when \(\eta = 0\) (no magnetization) do we include in the QD a vanishingly small Zeeman splitting to intentionally break the SU(2) spin symmetry (\(\varepsilon_{0\uparrow} - \varepsilon_{0\downarrow} = \Delta Z \rightarrow 0^+\)). Finally, \(f_{\sigma}^\dagger \) (\(f_{\sigma}\)) is a pseudofermion operator that creates (annihilates) a singly occupied state and the auxiliary boson operator \(b^\dagger \) (\(b\)) creates (annihilates) an empty state in the QD. The last term is a constraint enforced by the replacement of the QD second-quantization operators by the \(f\)'s and \(b\)'s when \(U \rightarrow \infty\) with an associated Lagrange multiplier \(\lambda\) [13].

The solution of the Hamiltonian (11) can be found in the mean field approach, which is the leading order in a \(1/N\) expansion, extended to deal with nonequilibrium situations [14]. This way one sets \(b(t)/\sqrt{N}\) to a c-number corresponding to its expectation value \(\bar{b} \equiv \langle b(t) \rangle/\sqrt{N}\), thereby neglecting charge fluctuations. This is correct as long as we are interested only in spin fluctuations. Now, by calculating the equation of motion for \(b\) and taking into account the QD constraint we arrive at:

\[
\sum_{k,\sigma} \varepsilon_{k\sigma} G_{0,0\sigma}^{<}(t, t) = -iN\lambda \langle \bar{b} \rangle^2, \quad (2a)
\]

\[
\sum_{\sigma} G_{0,0\sigma}^{>}(t, t) = i(1 - N\langle \bar{b} \rangle^2), \quad (2b)
\]

which self-consistently determine the unknowns \(\langle \bar{b} \rangle^2\) and \(\lambda\). We have defined \(\varepsilon_{k\sigma} = \langle \bar{b} \rangle^2 V_{k\sigma}\). The nondiagonal (in the layer indices) Green function \(G_{0,0\sigma}^{<}(t, t) = i(c_{k\sigma}^\dagger(t) f_{\sigma}(t))\) can be cast in terms of \(G_{0,0\sigma}^{>}(t, t) = i(f_{\sigma}^\dagger(t) f_{\sigma}(t))\), with the help of the equation of motion of the operators and then applying the analytical continuation rules in a complex time contour [17]. After lengthy algebra, the Fourier transform of \(G_{0,0\sigma}^{<}\) becomes

\[
G_{0,0\sigma}^{<}(\varepsilon) = 2\sum_{\alpha} \varepsilon_{\alpha} f_{\alpha}(\varepsilon) (|M_{\sigma\alpha}\varepsilon + R^2\varepsilon_{\bar{\alpha}}|/|M_{\sigma\alpha}\varepsilon - R^2|^2), \quad \text{where} \quad f_{\alpha}(\varepsilon) = \text{the Fermi function of lead } \alpha \text{ and} \quad M_{\sigma\alpha} = \varepsilon - \varepsilon_{\sigma\alpha} \pm i \sum_{\alpha} \Gamma_{\alpha}. \quad \text{Notice that by virtue of Kondo correlations, the original energy level } \varepsilon_{\sigma\alpha} \text{ is transformed into } \bar{\varepsilon}_{\sigma\alpha} = \varepsilon_{\sigma\alpha} + \lambda. \quad \text{Likewise, the linewidths } \Gamma_{\sigma\alpha} = \langle \bar{b} \rangle^2 T_{\sigma\alpha} \text{ normalize the bare couplings } \Gamma_{\sigma}^{\alpha}(\varepsilon) = (\pi i/2) \sum_{k,\sigma} |V_{k\sigma}|^2 \delta(\varepsilon - \varepsilon_{k\sigma}). \quad \text{In what follows, } \Gamma_{\sigma}^{\alpha} \text{ is taken as } \Gamma_{\sigma}^{\alpha} = \Gamma_{\sigma}^{\alpha}(E_F) \text{ for } -D \leq \varepsilon \leq D \text{ (}D\text{ is the energy cutoff).} \quad \text{Within the slave-boson mean-field theory, Kondo physics arises when the auxiliary boson field } b \text{ is condensed. At that point, } \Gamma_{\sigma}^{\alpha} \text{ gives roughly } T_K \text{ and } \lambda \text{ shifts the resonant level up to } E_F. \quad \text{The magnetization at reservoir } \alpha \text{ is } \eta_{\alpha} = \langle \nu_{\alpha}^+ - \nu_{\alpha}^\dagger \rangle/\langle \nu_{\alpha}^+ + \nu_{\alpha}^\dagger \rangle. \quad \text{As } -1 \leq \eta \leq 1, \text{ the linewidths } \Gamma_{\sigma}^{\alpha} \text{ will be generally spin dependent: } \Gamma_{\sigma}^{\alpha} = (1 \pm \eta_{\alpha}) \Gamma_{\sigma}^{\alpha}/2. \quad \text{Hereafter we shall deal with symmetric leads so that } \Gamma_{\alpha} = \Gamma_{\alpha} = \Gamma/2. \quad \text{Notice that spin flip effects are fully included due to the presence of } R \text{ in the denominator of } G_{0,0\sigma}^{<}(\varepsilon). \quad \text{Hence, the closed form of } G_{0,0\sigma}^{<}(\varepsilon) \text{ given above represents the distribution function of a QD in the presence of spin flips, ferromagnetic leads and Zeeman splitting [13]. For } R = 0 \text{ and } \eta_{\alpha} = 0 \quad \text{we get at equilibrium the position of the Kondo resonance of the impurity at } \varepsilon_0 = \varepsilon_0 = \varepsilon_0 = \varepsilon_0 \text{ with width } \Gamma_\alpha = \Gamma_\alpha + \Gamma_\alpha \text{ and Kondo temperature } T_K = (\varepsilon_0^2 + \varepsilon_0^2)^{1/2} = D \exp(-\pi |\varepsilon_0|/\Gamma). \quad \text{From the solution of Eq. 2, we can obtain the current traversing the dot: } I = (-e/\hbar) \sum_{\nu} \Gamma_{\nu}^{\alpha} \int \frac{G_{0,0\sigma}^{<}(\varepsilon) f_{\nu}(\varepsilon) + G_{0,0\sigma}^{>}(\varepsilon) f_{\nu}(\varepsilon)}{f(\varepsilon)} \, d\varepsilon, \quad \text{(f being the Fermi function). In the following, we shall present mainly nonequilibrium results for } \mu_L = -\mu_R = eV_{dc}/2, \quad c_0 = -3.5\Gamma \text{ and } D = -60\Gamma \quad (T_K \approx 10^{-3}\Gamma). \quad \text{The reference energy is set at } E_F = 0. \quad \text{Results.— Let us first focus on the case of polarized reservoirs with parallel (P) alignment (\(\eta_L = \eta_R = \eta\)). Figure 1(a) shows } G \text{ for partial lead magnetization (}\eta = 0.5\text{) and different values of } R. \quad \text{As seen, } G \text{ is a direct measure of how the spin flip mechanisms weaken the Kondo effect. For relatively small values of } R \quad (R < T_K) \text{ the height of the ZBA decreases but } G \text{ does not split. The appearance of a splitting } \delta \neq 0 \text{ occurs at } R \sim T_K. \quad \text{Importantly, due to that coexistence of the Kondo state and the intradot spin flips, the positions of the peaks in } G \text{ are renormalized by Kondo correlations, i.e., these peak positions are not trivially related with their single-particle counterparts (which should be centered around } V_{dc} = \pm 2R. \quad \text{For } R > T_K^0, \text{ the mean field approach predicts a complete quenching of the ZBA (}T_K = 0\text{) because the solution of Eq. 2 is the trivial one (}b = 0\text{), which}

![FIG. 1: (a) Differential conductance \(G\) versus bias voltage \(V_{dc}\) in the parallel case with lead magnetizations \(\eta_L = \eta_R = \eta = 0.5\) for four different values of the spin flip amplitude \(R\). (b) Dependence of the \(G-V_{dc}\) curves on \(R\) for \(R = 0.75T_K^0\). Inset: Kondo temperature of the QD (\(T_K\)) as a function of \(R\) for the lead polarizations depicted in (b). The crossing points with the straight line \(T_K = R\) marks the transition to a nonzero splitting in \(G(V_{dc})\).]

is unphysical. A more detailed theory including charge fluctuations (noncrossing approximation) would correct this. They price that one has to pay, however, is the appearance of spurious peaks in the conductance. Only for illustrative purposes have we also plotted in Fig. 1(a) the case with $\delta = 0$ as a function of the bias voltage $V_{dc}$ for the first four values of $R$ plotted in Fig. 2(a).

In Fig. 3(b) we plot the dependence of $G$ on the lead polarization (for P alignment) at a fixed value of $R$. The overall effect of $\eta$ is to diminish $G$. In particular, the ZBA quenching can be ascribed to a weaker Kondo state because of a smaller $T_K$. The Kondo temperature can be easily obtained from Eq. [2], but for $R \neq 0$ and $\eta \neq 0$ we find an explicit equation that can be worked out numerically (in contrast to the AP case, see below). We depict the results in the inset of Fig. 3(b). The splitting $\delta \neq 0$ takes place at a lower $R$ upon increasing $\eta$, in agreement with Fig. 3(b). We have checked that our numerical results fulfill two requirements, namely: (i) they are independent of the sign of $\eta$, for $T_K$ must be invariant after flipping simultaneously all the electron spins in both reservoirs, and (ii) with increasing $\eta$, $T_K$ decreases [see inset in Fig. 3(b) along the vertical axis $R = 0$] and eventually vanishes for full lead polarization ($\eta \to 1$), i.e., no Kondo effect may arise in the case of half-metallic leads.

Unlike the P case, for the AP alignment ($\eta_L = -\eta_R = \eta$) the ZBA splitting is generated at larger values of $R$ [see Fig. 3(a) for $\eta = 0.5$]. Nevertheless, we observe that the ZBA height is reduced even for $R = 0$. The reason is that $G$ decreases roughly by a factor $1 - \eta^2$ when the magnetic moments point along the opposite directions. More interesting is the fact that the ZBA width is given by a $|\eta|$-independent Kondo temperature. We find $T_K = \sqrt{(T_K^P)^2 - R^2}$, i.e., $T_K$ does not depend on $|\eta|$ [see inset of Fig. 2(a)]. The underlying physics for this is that both spin channels are coupled to the QD in the same way (i.e., $\Gamma_L^P + \Gamma_R^P = \Gamma_L^\uparrow + \Gamma_R^\downarrow = \Gamma$) so that $T_K$ persists regardless of the value of $\eta$. As a result, the splitting in $G(V_{dc})$ takes place always at the same point independently on the degree of lead magnetization.

We have found as well interesting features in the tunneling magnetoresistance $M \equiv (G^P - G^{AP})/G^{AP}$ [see Fig. 2(b)]. For definiteness, let us focus on the $V_{dc} = 0$ case. In conventional magnetic tunnel junctions, it is usual that the P current is larger than the AP current, thereby resulting in an increase of the impedance of the system when the configuration is switched from the P to the AP alignment [21]. This is really the case for the Kondo ZBA in the absence of spin flips [see Fig. 2(b) for $R = 0$]. However, increasing $R$ does not lead only to a reduction of $M$ but also to a reversal of the sign of $M$. This arises from the fact that the Kondo effect is more robust against spin flips in the AP configuration than in the P alignment, as stated above.

**Shot noise.**—As known, current fluctuations due to charge granularity (shot noise) can provide information additional to the averaged current [21]. The shot noise is given by the current-current correlation function $S(t - t') = \langle \delta I(t) \delta I(t') \rangle$, where $\delta I = I - \langle I \rangle$ measures the current fluctuations. (Because we consider a two-terminal system, we have dropped the lead indices.) An important figure of merit is the Fano factor: $\gamma = P(0)/2e\langle I \rangle$, where $P(0)$ is the noise power spectrum at zero-frequency [i.e., the Fourier transform of $S(t - t')$]. The Fano factor determines the deviations of the shot noise away from the Poissonian value of a classical con-
ductor due to, e.g., strong electron-electron interactions as those giving rise to the Kondo effect. Figure 3 shows the influence of spin flips (a) and lead magnetization (b) in $\gamma$. At low bias, $\gamma$ behaves as $1 - T(E_F) \mathcal{T}$, where $\mathcal{T}$ is the transmission probability. As shown in Fig. 3(a) for $R = 0$, the Kondo unitary limit is reached for a partial lead magnetization in the parallel case. Because of the correlated motion of the electrons which lead to the singlet formation there is a suppression of $\gamma$ at zero bias. As $R$ is turned on, the transmission departs from its unitary limit [see inset of Fig. 3(b)] because the Kondo effect is quenched and $\gamma$ takes on a nonzero value. Finally, for the largest $R$ the Fano factor tends to its Poissonian limit as spin flip processes reduce the Kondo resonance and a two-peak structure arise in the transmission probability. Thus, while the splitting of $G$ requires large applied voltages to be observable, the shot noise shows the same effect already in the zero voltage limit. On the other hand, the behavior of $\gamma$ at larger $V_{dc}$ depends on the specific transport mechanism. At $R = 0$, correlations between the band electrons and the localized electron dominate so that $\gamma$ increases with $V_{dc}$. For $R/T_K \rightarrow 1$, the Kondo resonance is split [see inset in Fig. 3(b)] and transport is maximized as $V_{dc}$ sweeps across the new resonances. For comparison between normal metals and ferromagnetic electrodes, we observe from Fig. 3(b) ($R \rightarrow 0$) that (i) $\gamma$ increases more rapidly for the P than for the unpolarized case due to the $\eta$ dependence of $T_K$, and (ii) for AP alignment the ZBA diminishes by a factor $1 - \eta^2$ and therefore we find $\gamma \sim \eta^2$ at low bias.

**Conclusion.** Using a slave-boson mean-field theory, we have shown that the combined influence of ferromagnetic electrodes and spin flip transitions in the Kondo physics of a QD manifests itself in the nonequilibrium transport properties of the system. The Kondo temperature (which can be regarded as the coupling strength of the singlet formation) is shown to be suppressed with increasing lead magnetization in the parallel alignment but the Kondo state is remarkably stable in the antiparallel case. This may lead to negative tunneling magnetoresistance at zero-bias when the spin flip scattering amplitude is enhanced. The overall behavior is confirmed with shot noise calculations. Experimentally, we believe that the effects addressed in this paper should be visible within the scope of present techniques as our energies are within the Kondo scale.

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