Kondo effect in a two-level quantum dot coupled to an external fermionic reservoir

A. L. Chudnovskiy and S. E. Ulloa
Department of Physics and Astronomy and Condensed Matter and Surface Sciences, Ohio University, Athens, OH 45701-2979 USA

Abstract

We investigate theoretically the linear conductance of a two-level quantum dot as a function of the gate voltage and different strength of coupling to the external electronic system (the reservoir). Apart from the weak coupling regime, characterized by the Kondo-enhancement of the conductance in the spinful ground state, a strong coupling regime, which can be called mixed-valence (MV), is found. This regime is characterized by a qualitative change of the energy level structure in the dot, resulting in sub- and super-tunneling coupling of the levels, which in turn yield a novel temperature dependence of the Kondo effect in the quantum dot.

The Kondo effect arises from the coherent screening between a localized spin and that of surrounding mobile electrons, producing for example anomalous transport properties in metals with magnetic impurities [1]. Recently, however, there has been a great deal of experimental activity in systems where an individual localized spin is probed directly in quantum dots defined in semiconductor systems [2, 3].

Previous investigations on both single- and multi-level models have uncovered interesting features of the Kondo effect, including Kondo peaks in the conductance and the associated density of states, their temperature dependence, and other features [2, 4]. However, the typical approximation made in models of multilevel quantum dots with discrete energy levels is to neglect the strong mixing between the energy levels of the dot due to the interaction with the external fermionic system. This approach incorporates the external fermionic system only as a broadening of the levels in the quantum dot [4].

In this paper we analyze the Kondo effect in a quantum dot coupled to an external fermionic system in addition to the coupling to the measuring leads. We explicitly take into account the mixing of the states in the dot due to the coupling to an external reservoir. A typical experimentally accessible example of such a system is a dot coupled to three leads with one lead playing the role of the reservoir and drawing no current. It is assumed that the coupling to the fermionic reservoir can be varied independently of the coupling to the measuring leads. In the case of weak coupling, the reservoir just leads to broadening of the energy levels in the dot, whereas strong coupling results in a qualitative rearrangement of the energy levels which influences the Kondo effect in a nontrivial manner.

In what follows we consider a two-level quantum dot in the linear (zero bias) regime at
zero temperature. The Hamiltonian of the model can be written as

\[ H = \sum_{l,\sigma} \{ E_l \hat{c}_{l,\sigma}^+ \hat{c}_{l,\sigma} + U_1 \sum_{l \neq l'} \hat{n}_l \hat{n}_{l'} + U \hat{n}_l \hat{n}_{l'} \} + \sum_{\nu=1}^{3} \gamma_\nu \sum_{l,\sigma} (\hat{c}_{l,\sigma}^+ \hat{a}_{\nu,0,\sigma} + \hat{a}_{\nu,0,\sigma}^+ \hat{c}_{l,\sigma}) + \sum_{\nu=1}^{3} H_{\nu}^r(\hat{a}_{\nu,\sigma}, \hat{a}_{\nu,r,\sigma}). \]  

(1)

Here, the fermionic operators \( \hat{c}_{l,\sigma}^+, \hat{c}_{l,\sigma} \) describe the states in the dot with orbital index \( l = 1, 2 \), and spin index \( \sigma \). \( \hat{n}_l = \hat{c}_{l,\sigma}^+ \hat{c}_{l,\sigma} \) is the particle number operator of the state \((l, \sigma)\), and \( \hat{n}_l = \hat{n}_l^+ + \hat{n}_l \). The dot is coupled by tunnel couplings \( \gamma_\nu \) to the two measuring leads, the right (\( R, \nu = 1 \)) and the left (\( L, \nu = 2 \)). The third lead couples the dot to a fermionic reservoir via the coupling \( \gamma_3 \). In what follows we consider the symmetric case, \( \gamma_1 = \gamma_2 = \gamma_3 = \gamma \). \( H_{\nu}^r \)'s denote the Hamiltonians of the leads. The fermions at the space position \( r = 0 \) are considered to be coupled directly to the dot.

The basic interactions in the quantum dot are the density-density repulsion between charges on different energy levels via the interaction constant \( U_1 \), and the Hubbard-like repulsion \( U \) between electrons on a given level of the dot. The interaction constants depend mostly on overlap integrals between the wave functions of the different energy levels. Therefore, they can be changed by changing the shape of the quantum dot, which is experimentally accessible [2].

To describe the effect of the quantum dot on the transport through the measuring leads, we integrate out the degrees of freedom related to the dot and reservoir. We then obtain the effective Lagrangian for the measuring leads only, which is given by

\[ L_{\text{eff}} = \sum_{\nu = R, L} L_{\nu}^0(\hat{a}_{\nu, \sigma}^+, a_{\nu, \sigma}) - \gamma_1^2 \sum_{\omega, \omega'} \left( \sum_{\nu = R, L} \hat{a}_{\nu, \sigma}^+ \right) \gamma_{\omega\omega'}^{\nu\nu'} \left( \sum_{\nu' = R, L} a_{\nu', \sigma} \right), \]  

(2)

where \( \gamma_{\omega\omega'}^{\nu\nu'}(i\omega_n) \equiv \langle \hat{c}_{\nu}(i\omega_n) \hat{c}_{\nu'}(i\omega_{n'}) \rangle \) is the fermionic one-particle Green’s function of the dot coupled to the reservoir but isolated from the measuring leads. \( L_{\nu}^0(\hat{a}_{\nu, \sigma}^+, a_{\nu, \sigma}) \) denotes the Lagrangian of the isolated lead \( (\nu = R, L) \), and \( \omega, \omega' \) are Matsubara frequencies. To find \( \gamma_{\omega\omega'}^{\nu\nu'}(i\omega_n) \), we integrate out the reservoir in the Hamiltonian (1). In the result, the effective Lagrangian acquires a new term \( i\kappa \sum_{l,\nu} \sum_{\sigma=1,2} c_{l,\sigma}^\nu c_{l,\sigma}^{\nu'} \) that describes broadening and mixing of the energy levels in the quantum dot. For Matsubara frequencies much less than the bandwidth of the reservoir \( D \), we obtain \( \kappa \approx \text{sign}(\omega_n) \pi \gamma^2 \rho_0 \), where \( \rho_0 \) is the density of states in the reservoir [1, 6].

We treat the many-body interaction in the dot in a Hartree approximation (the spin is assumed frozen in the \( z \)-direction) with subsequent expansion in spin fluctuations to take into account the Kondo effect. In the mean field (Hartree) approximation, the two level quantum dot with interactions is replaced by a non-interacting quantum dot with quasi-energy levels that depend on the ground state of the quantum dot. This approach allows one to describe correctly the properties of the quantum dot in the ground state and its gapless excitations, including the Kondo effect, which is the main aim of this treatment. Due to the mixing and broadening of the energy levels in the dot coupled to the reservoir, the effective energy levels for each spin projection become \( z_\pm^\sigma = (\epsilon_{1\sigma} + \epsilon_{2\sigma} \pm \sqrt{(\epsilon_{1\sigma} - \epsilon_{2\sigma})^2 - 2\kappa^2}) / 2 - i\kappa \text{sign}(\omega_n) \), where \( \epsilon_{\alpha\sigma} \) denote the effective energy level for the isolated dot. Detailed discussion of the mean-field equations and their solutions is given in Ref. [6].

In the limit of zero level mixing (zero tunnelling \( \gamma \)), the values of \( z_\pm \) coincide with \( \epsilon_{1,2} \). Small level mixing \( \kappa \) leads to small deviations from these solutions. On the other
hand, in the large level mixing regime, when the condition $2\kappa > |\epsilon_1 - \epsilon_2|$ is satisfied, the quasi-level structure changes qualitatively. The quasienergies are given by $z_{1,2} = (\epsilon_1 + \epsilon_2)/2 - i\kappa \left(1 \mp \sqrt{1 - (\epsilon_1 - \epsilon_2)^2/(4\kappa^2)}\right) \text{sign}(\omega_n)$, corresponding to two degenerate levels: one strongly broadened ($z_2$) “supertunneling” level, and the other one a “subtunneling” level with strongly suppressed broadening ($z_1$) \[5\]. The qualitative change of the effective energy level structure by going from small to large coupling to the external reservoir has a profound influence on the transport properties of the quantum dot, particularly in the Kondo ground state.

The physics of the Kondo effect is taken into account by considering spin fluctuations around the spinful saddle point. The charge fluctuations are massive and can be omitted \[6\]. The only modes of the spin fluctuation field $Q_{ll'}$ that can become massless and give rise to the Kondo effect are described by the correlators $\langle (\sigma^+ \otimes Q_{ll})(\sigma^- \otimes Q_{ll'}) \rangle_\omega = \langle (\sigma^- \otimes Q_{ll})(\sigma^+ \otimes Q_{ll'}) \rangle_{-\omega} = (16U^2)/(\omega + 4U(1 - \phi_{ll}/\pi))$ with $\phi_{ll} = \arccos(-z_{ll}'/|z_{ll}|) - \arccos(-z_{ll}'/|z_{ll}|)$. In the case of small broadening $\kappa$, $|z_{ll}| \approx |z_{ll}'|$. If the state of the level $l$ is spinful, then $z_{ll}' < 0$ and $z_{ll} > 0$, hence $\phi_{ll} = \pi$ and the correlator becomes massless. In the strong-coupling regime, which we will call “mixed valence” (MV), the subtunneling level has a very small broadening, and hence the fluctuations of the spin field for this level are massless, whereas the supertunneling level is strongly broadened and its spin fluctuations are massive. Physically, the electron on the supertunneling level is effectively delocalized, thus giving no Kondo effect in the usual sense, but having a different contribution in that regime (see below).

Expanding the function $Y$ in the Lagrangian \[2\] to lowest order of the fluctuation matrix $\hat{Q}$, we obtain the Kondo part of the interaction, from which we identify the Kondo constants. In the Kondo regime, $\kappa \ll |\epsilon_{1\sigma} - \epsilon_{2\sigma}|$, the Kondo coupling for the level $l$ assumes the form $J_{K}^l = -4U\gamma_1^2/\epsilon_{ll}\epsilon_{ll'}$. Since $\epsilon_{ll}\epsilon_{ll'} < 0$, the Kondo coupling is antiferromagnetic, $J_{K}^l > 0$. In the MV regime, only the subtunneling level contributes to the Kondo effect. For this level (let it be $l = 1$), we have $J_{K}^{sub} \approx -4U\gamma_1^2(E_1 - E_2)^2/(2\kappa^2(\epsilon_{1}\epsilon_{1} + \epsilon_{2}\epsilon_{2})).$ The Kondo coupling in the MV regime becomes ferromagnetic, and it is weaker that in the Kondo regime by the factor $(E_1 - E_2)^2/(8\kappa^2)$. The Kondo temperature can be evaluated as $T_{K} \sim D \exp[-1/(\nu_F J_{K})]$, where $\nu_F$ is the density of states at the Fermi level in the leads. It follows from the expressions for the Kondo couplings that whereas in the Kondo regime $T_{K}$ is determined by the position of a given level, in the MV regime $T_{K}$ is determined by the level mixing $\kappa$, as the positions of both levels enter symmetrically.

The behavior of the conductance versus gate voltage in the Kondo regime at different temperatures is illustrated in Fig.\[1\]a). The conductance is normalized by the value of the conductance through the leads. In the spinful state, the nonresonant conductance is enhanced due to the Kondo effect. The conductance drops with temperature, which is also characteristic for the Kondo effect temperature dependence. The levels in the dot are widely separated, so that one observes two subsequent Kondo states as the gate voltage is varied. The conductance versus the gate voltage in the MV regime is shown in Fig.\[1\]b). In this case, the enhanced scattering due to the Kondo effect involves scattering processes into the external reservoir, which leads to a reduction of the conductance through the dot. Therefore, in the spinful state we have a Kondo “dip” of the conductance instead of a Kondo peak. The Kondo dip in the conductance has an unusual temperature dependence. Notice that, in contrast to the Kondo regime, the position of the Kondo dip shifts with temperature in the
Figure 1: Conductance of the quantum dot versus the gate voltage ($E_1$). $U = 3, U_1 = 1$ at three different temperatures. (a) The Kondo (weak coupling) regime: $t = 15, \gamma_1 = \gamma = 0.5$. (b) The mixed valence (strong coupling) regime: $t = 50, \gamma_1 = \gamma = 4$.

MV regime. As it has been discussed above, in the MV regime, the Kondo contribution to the conductance is generated only by the subtunneling level. However, because of the large background conductance by the supertunneling level (through which the dot is practically open), the experimental identification of the Kondo dips shown in Fig. 1(b) might be difficult, especially in comparison with impurity effects in these systems (which would yield universal conductance fluctuations, for example). However, the large shifts in the dip position with temperature may help a great deal to isolate this effect.

We emphasize that the predicted effects would not be present for a single-level dot, where the broadening of the level suppresses the Kondo effect for strong coupling. Therefore, the mixing of the different energy levels in the dot by the coupling to the external fermionic system is essential for the observation of the Kondo effect in the MV regime.

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