Kondo effect in side coupled double quantum-dot molecule

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Abstract

Electron tunneling through a double quantum dot molecule side attached to a quantum wire, in the Kondo regime, is studied. The mean-field finite-U slave-boson formalism is used to obtain the solution of the problem. We found conductance cancelations when the molecular energies of the side attached double quantum-dot cross the Fermi energy. We investigate the many body molecular Kondo states as a function of the parameters of the system.

Key words: Quantum dots, Fano resonance, Kondo effect
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1 Introduction

Quantum dots (QDs) are man-made nanostructures in which electrons are confined in all three space dimensions [1]. Energy and charge quantization results from this confinement. As both features are present in real atomic systems, an useful analogy has been used between “real” and “artificial” atomic systems.

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Like-wise, a system of coupled QDs is called an “artificial molecule”. Enforcing this analogy, in QDs configurations Kondo effect and Fano resonance are also present.

The Kondo effect is the name given to describe the resistivity minimum for decreasing temperature in certain alloys with a minute concentration of a magnetic impurity [2,3]. It is important to emphasize that in this case, the so-called traditional Kondo effect, magnetic impurities act as scattering centers, increasing the sample resistivity (for a review see Ref. [4]). The opposite behavior is found in the Kondo effect in QDs, the so-called anti Kondo effect. Experimentally [5,6,7] and theoretically [8,9], the situation considered usually consists of a QD connected to two leads. In these configuration electrons transmitted from one electrode to the other necessarily pass through the QD.

The Kondo effect in QDs has been extensively studied in the last years [5,6,7] (for a review see Ref. [10]). The experimental evidence has confirmed that many of the phenomena that characterize strongly correlated metals and insulators, as it is the case of the Kondo effect, are present in QDs. The QDs allow to study systematically the quantum-coherence many-body Kondo state, due to the possibility of continuous tuning the relevant parameters governing the properties of this state, in equilibrium and nonequilibrium situations. Recently Kondo effect has been studied in double quantum dot molecule in series [11,12,13,14,15]. This system allows the study of the many body molecular Kondo states in equilibrium and nonequilibrium situation. The type of coupling between the QDs determines the character of the electronic states and the transport properties of the artificial molecule. In the tunneling regime, the electronics states are extended across the entire system and form a coherent state based on the bonding or anti-bonding levels of the QDs.

An alternative configuration consists of a side-coupled QDs attached to a perfect quantum wire (QW). This structure is reminiscent of T-shaped quantum wave guides known as electron stub tuners [16] (see also Refs. [17,18]). In this case, the QDs acts as scattering centers in close analogy with the traditional Kondo effect [19,20,21,22,23].

Recent electron transport experiments showed that Kondo resonance occurs simultaneously with the Fano resonance [24,25]. Multiple scattering of traveling electronic waves on a localized magnetic state are crucial for a formation of both resonances. The condition for the Fano resonance [26] to appear is a presence of at least two scattering channels: the discrete level and the broad continuum band [27,28].

In this work we study the transport properties of a double quantum dot molecule side attached to a quantum wire in the Kondo regimen. We use the finite-$U$ slave boson mean-field approach which was initially developed by
Koliar and Ruckenstein [29] and used later by Bing Dong and X. L. Lei to study the transport through coupled double quantum dots connected in series to leads [30,31,32,33]. We found that the antiresonances of the linear conductance reflect the spectral properties of the artificial molecule. We investigate the many body molecular Kondo states as a function of the parameters of the system.

Fig. 1. Scheme of double quantum dot (DQD) attached to a lead (perfect quantum wire (QW)). The QW is coupled to the left (L) and right (R) “reflectionless” contacts.

2 Model

Let us consider a double quantum dot (DQD) side coupled to a perfect quantum wire (QW) (see Fig. 1). We adopt the two-fold Anderson Hamiltonian, that is diagonalized using the finite-$U$ mean field slave boson formalism. Each dot has a single level $E_i$ (with $i = 1, 2$) and intradot Coulomb repulsion $U$, and is coupled to each other with interdot tunneling coupling $t_c$. The QW has an energy $\varepsilon_{i,\sigma}$ for site and has a hopping parameter $t$.

In analogy with the infinite-$U$ slave boson approach [34,35,36] the Hilbert space is enlarged at each site, to contain in addition to the original fermions a set of four bosons [29] represented by the creation (annihilation) operators $e_i^\dagger (e_i)$, $p_{i,\sigma}^\dagger (p_{i,\sigma})$, and $d_i^\dagger (d_i)$ for the $i$-th dot, which act, respectively, as projectors onto empty, single occupied (with spin up and down) and doubly occupied electron states. Then the Hamiltonian is written as,

$$
H = \sum_{i,\sigma} \varepsilon_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) - t_0 (c_{0,\sigma}^\dagger \tilde{Z}_{1,\sigma} f_{1,\sigma} + \text{H.c.}) \\
+ \sum_{i=1}^2 \sum_{\sigma} (\varepsilon_{d_i} + \lambda_{i,\sigma}^{(2)}) f_{i,\sigma}^\dagger f_{i,\sigma} - t_c \sum_{\sigma} (f_{1,\sigma}^\dagger \tilde{Z}_{1,\sigma}^\dagger \tilde{Z}_{2,\sigma} f_{2,\sigma} + \text{H.c.}) \\
+ \sum_{i=1} \left\{ U d_i^\dagger d_i + \lambda_{i}^{(1)} \left( p_{i,\uparrow}^\dagger p_{i,\uparrow} + p_{i,\downarrow}^\dagger p_{i,\downarrow} + e_i^\dagger e_i + d_i^\dagger d_i - 1 \right) \\
- \sum_{\sigma} \lambda_{i,\sigma}^{(2)} \left( p_{i,\sigma}^\dagger p_{i,\sigma} + d_i^\dagger d_i \right) \right\} \tag{1}
$$
where $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) is the creation (annihilation) operator of a electron with spin $\sigma$ in the $i$-th site on quantum wire; $f_{i,\sigma}^\dagger$ ($f_{i,\sigma}$) is the creation (annihilation) operator of a electron with spin $\sigma$ in the $i$-th QD. The operator $\tilde{Z}_{i,\sigma}$ is chosen to reproduce the correct $U \to 0$ limit in the mean field approximation,

$$\tilde{Z}_{i,\sigma} = \left(1 - d_i^\dagger d_i - p_i^\dagger p_i,\sigma\right)^{-1/2} \left(\epsilon_i^\dagger p_i,\sigma + p_i^\dagger d_i\right) \left(1 - \epsilon_i^\dagger \epsilon_i - p_i^\dagger p_i,\sigma\right)^{-1/2}.$$

The constraint, i.e., the completeness relation $\sum_\sigma p_{i,\sigma} p_{i,\sigma} + b_i^\dagger b_i + d_i^\dagger d_i = 1$ and the condition for the correspondence between fermions and bosons $f_{i,\sigma}^\dagger f_{i,\sigma} = p_{i,\sigma} p_{i,\sigma} + d_i^\dagger d_i$, have been incorporated with Lagrange multipliers $\lambda_{i,\sigma}^{(1)}$ and $\lambda_{i,\sigma}^{(2)}$ into the Hamiltonian. Then we use the mean-field approximation in which all the boson operators are replaced by their expectation value. These expectation values and the Lagrange multipliers are then determined by minimization of the free energy with respect to these variables. So, the effective Hamiltonian is $H_{\text{eff}} = H_{TB} + H_B$, where:

$$H_{TB} = -t \sum_{i,\sigma} \left(c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}\right) - \sum_{\sigma} \tilde{t}_{0,\sigma} \left(c_{0,\sigma}^\dagger f_{1,\sigma} + \text{H.c.}\right)$$

$$+ \sum_{i=1}^2 \sum_{\sigma} \tilde{\varepsilon}_{d_i,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} - \sum_{\sigma} \tilde{t}_{c,\sigma} \left(f_{1,\sigma}^\dagger f_{2,\sigma} + \text{H.c.}\right)$$

$$H_B = \sum_{i=1}^2 \left\{ U d_i^2 + \lambda_{i,\sigma}^{(1)} \left(p_{i,\uparrow}^2 + p_{i,\downarrow}^2 + \epsilon_i^2 + d_i^2 - 1\right) - \sum_{\sigma} \lambda_{i,\sigma}^{(2)} \left(p_{i,\sigma}^2 + d_i^2\right) \right\},$$

with $\tilde{\varepsilon}_{d_i,\sigma} = \varepsilon_{d_i} + \lambda_{i,\sigma}^2$, $\tilde{t}_{0,\sigma} = t_0 \langle \tilde{Z}_{1,\sigma} \rangle$, and $\tilde{t}_{c,\sigma} = t_c \langle \tilde{Z}_{1,\sigma} \tilde{Z}_{2,\sigma} \rangle$, and we set $\varepsilon_{i,\sigma} = 0$ in the QW. The Hamiltonian tight binding, $H_{TB}$, corresponds to an effective free-particle Hamiltonian on a lattice with spacing set as unity, and whose eigenfunctions are expressed as Bloch solutions

$$|k\rangle = \sum_{j=-\infty}^{\infty} e^{ikj} |j\rangle,$$

where $|k\rangle$ is the momentum eigenstate and $|j\rangle$ is a Wannier state localized at site $j$. The dispersion relation associated with these Bloch states reads $\omega = -2t \cos k$. Consequently, the Hamiltonian supports an energy band from $-2t$ to $+2t$ and the first Brillouin zone expands the interval $[-\pi, \pi]$. The stationary states of the entire Hamiltonian $H$ can be written as

$$|\psi_k\rangle = \sum_{j=-\infty}^{\infty} a_j^k |j\rangle + \sum_{l=1}^2 b_l^k |l\rangle,$$

where the probability amplitude to find the electron in the state $k$ in the $j$-th site of the QW is the coefficient $a_j^k$, and to find it in $l$-th QD is the coefficient $b_l^k$. 

4
From $H_{TB} |\psi_k\rangle = \omega |\psi_k\rangle$, the amplitudes $a_j^k$ and $b_j^k$ obey the following linear difference equations

\begin{align}
\omega a_j^k &= -t(a_{j+1}^k + a_{j-1}^k), \quad j \neq 0, \quad (7a) \\
\omega a_0^k &= -t(a_1^k + a_{-1}^k) - \tilde{t}_0 b_1^k, \quad (7b) \\
(\omega - \tilde{\varepsilon}_{d1}) b_j^k &= -\tilde{\tau}_l b_{j+1}^k - \tilde{t}_0 a_j^k, \quad (7c) \\
(\omega - \tilde{\varepsilon}_{d2}) b_j^k &= -\tilde{\tau}_r b_{j+1}^k. \quad (7d)
\end{align}

We can express the amplitudes $b_j^k$ in terms of $a_0^k$, therefore the equation for $a_j^k$ can be cast into the form

\begin{align}
(\omega - \delta_{j,0} \tilde{\varepsilon}) a_j^k &= -t(a_{j+1}^k + a_{j-1}^k), \quad (8)
\end{align}

where let us define the effective energy $\tilde{\varepsilon}$ as

\begin{align}
\tilde{\varepsilon} &\equiv \frac{\tilde{t}_0^2 (\omega - \tilde{\varepsilon}_{d2})}{(\omega - \tilde{\varepsilon}_{d1})(\omega - \tilde{\varepsilon}_{d2}) - \tilde{t}_c^2}. \quad (9)
\end{align}

This contains all the information about the side-attached quantum-dot molecule. Thus, the problem reduces to one of an impurity of effective energies $\tilde{\varepsilon}$.

In order to study the solutions of (8), we assume that the electrons are described by a plane wave incident from the far one side with unity amplitude and a reflection amplitude $r$, and at the far other side by a transmission amplitude $\tau$. That is,

\begin{align}
a_j^k &= e^{ikj} + re^{-ikj}, \quad (j < 0, k > 0), (j > 0, k < 0), \quad (10a) \\
da_j^k &= \tau e^{ikj}, \quad (j > 0, k > 0), (j < 0, k < 0) \quad (10b)
\end{align}

Inserting (10b) into (8), we get a inhomogeneous system of linear equations for $\tau$, $r$ and $a_j^k$, leading to the following expression

\begin{align}
\tau = \frac{(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)}{(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+) + i(\omega - \tilde{\varepsilon}_{d2})\tilde{\Gamma}}, \quad (11)
\end{align}

where the bonding energy $(\tilde{\varepsilon}_-)$ and antibonding energy $(\tilde{\varepsilon}_+)$ are defined by $\tilde{\varepsilon}_\pm = (\tilde{\varepsilon}_{d1} + \tilde{\varepsilon}_{d2})/2 \pm \sqrt{(\tilde{\varepsilon}_{d1} + \tilde{\varepsilon}_{d2})^2/4 + \tilde{t}_c^4}$ and $\tilde{\Gamma} = \pi \tilde{t}_0^2 \rho(\omega)$ is the renormalized coupling between the double quantum-dot and the quantum wire. The transmission probability is given by $T = |\tau|^2$,

\begin{align}
T(\omega) &= \frac{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)]^2}{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+) + [(\omega - \tilde{\varepsilon}_{d2})\tilde{\Gamma}]^2]. \quad (12)
\end{align}

In the limit of zero bias and at zero temperature we obtain the expression for
the linear conductance,
\[
G = \frac{2e^2}{h} T(0) = \frac{2e^2}{h} \frac{(\bar{\varepsilon}_-\bar{\varepsilon}_+)^2}{(\bar{\varepsilon}_-\bar{\varepsilon}_+)^2 + (\bar{\varepsilon}_{d2}\Gamma)^2}.
\] (13)

Additionally, from the amplitudes $b^k_1$ and $b^k_2$ we can obtain the local density of states (LDOS) in the quantum dots,

\[
\rho_1 = \frac{1}{\pi} \frac{\tilde{\Gamma}(\omega - \bar{\varepsilon}_{d2})^2}{[\omega - (\bar{\varepsilon}_-\bar{\varepsilon}_+)]^2 + [\omega - \bar{\varepsilon}_{d2}\Gamma]^2},
\] (14)

\[
\rho_2 = \frac{1}{\pi} \frac{\tilde{\Gamma}^2 t_c^2}{[\omega - (\bar{\varepsilon}_-\bar{\varepsilon}_+)]^2 + [\omega - \bar{\varepsilon}_{d2}\Gamma]^2}.
\] (15)

And then we can calculate the density of states of the DQD molecule.

\[
\rho = \frac{1}{\pi} \frac{\tilde{\Gamma}(\omega - \bar{\varepsilon}_{d2})^2 + \tilde{t}_c^2}{[\omega - (\bar{\varepsilon}_-\bar{\varepsilon}_+)]^2 + [\omega - \bar{\varepsilon}_{d2}\Gamma]^2}.
\] (16)

3 Results

We study a model with $t = 25\Gamma$, $t_0 = 7.07\Gamma$. From here on we use $\Gamma = \pi t_0^2 \rho_{QW}(0)$ as the energy unit.

First we consider the situation when the energies are varied simultaneously by a gate voltage $V_g$, i.e. $\varepsilon_{d1} = \varepsilon_{d2} = V_g$.

Fig. 2. Transmission spectrum for $V_{1g} = V_{2g} = V_g = -3\Gamma$, $t_c = 0.5\Gamma$ (solid line) and $t_c = \Gamma$ (dashed line), for various values of the on site energy $U$, a) $U = 2\Gamma$, b) $U = 4\Gamma$, c) $U = 8\Gamma$ and d) $U = 16\Gamma$.

Figure 2 displays the transmission probability $T$ for various values of $U$. For all values of $U$ the transmission probability reaches the minimum values 0 at $\omega = \bar{\varepsilon}_-$ and $\bar{\varepsilon}_+$ and its maximum value the unity at $\omega = \bar{\varepsilon}_{d2}$. With increasing
A sharp feature develops close to the Fermi energy \((\omega = 0)\), which is a signature of a Kondo resonance. In fact, for \(U\) sufficiently large the transmission can be written approximately as the superposition of two Fano-Kondo line shapes, one with a zero \(q\) factor and another one with a \(q\) factor no null,

\[
T(\omega) \approx \frac{(\epsilon' + q')^2}{(\epsilon')^2 + 1} + \frac{(\epsilon'' + q'')^2}{(\epsilon'')^2 + 1},
\]

where \(\epsilon' = (\omega - \tilde{\varepsilon}_{d2})/\tilde{\Delta}\), \(q' = (\tilde{\varepsilon}_{d2} - \tilde{\varepsilon}_{-})/\tilde{\Delta}\), \(\epsilon'' = (\omega - \tilde{\varepsilon}_{+})/\Gamma\) and \(q'' = 0\), with \(\tilde{\Delta} = \tilde{\Gamma}/\Gamma\).

The density of states of the quantum-dot molecule can give us a better understanding of the transport properties of the system. Figure 4 displays DOS for various values of \(U\). We can observe that the density of states is the superposition of a narrow Kondo peak and a broad Kondo peak with a width that tends to \(2\tilde{\Gamma}\). In fact, from Eq. (16) the density of states can be written as the superposition of two Lorentzians,

\[
\rho \approx \frac{1}{\pi} \frac{\tilde{\Gamma}}{(\omega - \tilde{\varepsilon}_{+})^2 + \tilde{\Gamma}^2} + \frac{1}{\pi} \frac{\tilde{\Delta}}{(\omega - \tilde{\varepsilon}_{d2})^2 + \tilde{\Delta}^2}.
\]

Fig. 3. DOS for \(t_c = 0.5\Gamma\), \(V_{1g} = V_{2g} = -3\Gamma\), for various values of the on site energy, \(U = 16\Gamma\) (solid line), \(U = 8\Gamma\) (dashed line), \(U = 4\Gamma\) (dotted line) and \(U = 2\Gamma\) (dash-dot line).

Additionally, the LDOS give us more details about the formation of the Kondo resonance. The LDOS are displayed in Figure 4. The local density of states \(\rho_2\) develops a Kondo resonance peak near the Fermi energy \((\omega = 0)\). As the outside dot (dot 2) develops a Kondo resonance, the density of states \(\rho_1\) is depleted near to the Fermi energy. From the LDOS we can see that the Kondo resonance is developed in the outside dot. This behavior is explained by the fact that the outside dot is weakly connected to the continuum and therefore it is favorable the formation of a localized state there. The coherent coupling of this localized state and the conduction states give origin to this Kondo resonance.
Figure 5 display the linear conductance versus the gate voltage, when the two gates voltages are varied simultaneously \((\varepsilon_{d1} = \varepsilon_{d2} = V_g)\), for various values of the on-site energy \(U\). The linear conductance shows two Fano antiresonances corresponding to the bonding and antibonding energies of the quantum-dot molecule and one resonance between them. The separation between the two antiresonance grows linearly with \(U\). From the equation (13) the conductance vanishes when \(\bar{\varepsilon}_-\) or \(\bar{\varepsilon}_+\) coincide with the Fermi energy \((\omega = 0)\). On the other hand the conductance reaches the unitary limit when \(\bar{\varepsilon}_{d2}\) crosses the Fermi energy.

Fig. 4. Local density of states a) quantum-dot 1, b) quantum-dot 2, \(V_{1g} = V_{2g} = -3\Gamma\), for various values of the on site energy, \(U = 16\Gamma\) (solid line), \(U = 8\Gamma\) (dashed line), \(U = 4\Gamma\) (doted line) and \(U = 2\Gamma\) (dash-dot line).

Fig. 5. Linear conductance \(G\) vs \(V_g\) for \(t_c = 0.5\Gamma\) (solid line) and \(t_c = \Gamma\), for various values of the on site energy, a) \(U = 2\Gamma\), b) \(U = 4\Gamma\), c) \(U = 8\Gamma\) and d) \(U = 16\Gamma\).

Let us consider now the situation where only one of the gate potential is varied while the other one is maintained constant \((\varepsilon_{d1} = V_{1g} = -U/2, \varepsilon_{d2} = V_{2g})\). The Figure 6 shows the \(G\) versus \(V_{2g}\) for \(U = 8\Gamma\). In this situation the occupation number of the quantum dot 1 (QD1) is \(n_1 \approx 1\) and its energy level is near the Fermi energy. A Kondo singlet state is formed between the QD1 and the adjacent wire. For large positive values of \(V_{2g}\), the occupation number of the quantum-dot 2 (QD2) is almost zero and the position of the antibonding
energy, $\tilde{\varepsilon}_+ \approx V_{2g}$ and the position of the bonding energy is close to zero and negative, $\tilde{\varepsilon}_- \approx -t_c^2/V_{2g} \approx 0$. Consequently, according to Eq. (13) the conductance is close to zero. Decreasing $V_{2g}$ the occupation number of the QD2 grows up to $n_2 = 1$, and its energy level tends to the Fermi energy. Then the QD2 enters into the Kondo regime and the conductance reaches the quantum limit ($G = 2e^2/h$). The energy level of the QD2 is pinned at the Fermi energy and the conductance shows a plateau in its maximum. For $V_{2g} < U$ the QD2 is doubly occupied and a localized spin-singlet is formed, consequently the Kondo effect of the coupling of this quantum dot with the quantum wire is destroyed. On the other hand, QD1 charge is kept almost constant with one electron and the Kondo singlet state between this quantum dot and the wire remains. In this situation $\tilde{\varepsilon}_+ + t_c$ tends asymptotically to the Fermi energy and the conductance decreases to zero.

Figure 7 displays the density of states of the DQD for $V_{2g} = -U/4$, $t_c = 0.5 \Gamma$ (solid line) and $t_c = \Gamma$ (dashed line). For $t_c = 0.5 \Gamma$ the density of states is the superposition of a broad and a narrow peaks centered at the Fermi energy with widths $\tilde{\Gamma}$ and $\Delta$ respectively. Then, in this case the side-coupled DQD
has two Kondo temperatures, $T_{1K} = \tilde{\Gamma}$ and $T_{2K} = \Delta = \tilde{t}_c^2/\tilde{\Gamma}$. On the other hand, for $t_c = \Gamma$ the density of states shows two peaks at the bonding and antibonding energies. Both QDs tend to form a coherent spin-singlet state. This state coexists with the Kondo states formed between the QD and the QW.

4 Summary

In conclusion, we have studied the transport through a side-coupled double quantum-dot molecule using the finite-$U$ slave boson mean field approach. We have found that the transmission spectrum shows a structure with two antiresonances localized at the bonding and antibonding energies of the quantum-dot molecule, and one resonance at the site energy of the outside quantum-dot. Moreover the density of states shows that the outside quantum-dot develops a strong Kondo effect with the quantum-wire and its Kondo temperature depends strongly on the interdot coupling tunneling. The linear conductance reflects the transmission spectrum properties as the gate potential is varied.

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