Kondo Regime of a Quantum Dot Molecule: A Finite-$U$ Slave-Boson Approach

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Abstract

We study the electronic transport in a double quantum dot structure connected to leads in the Kondo regime for both series and parallel arrangements. By applying a finite-$U$ slave boson technique in the mean field approximation we explore the effect of level degeneracy in the conductance through the system. Our results show that for the series connection, as the energy difference of the localized dot levels increases, the tunneling via the Kondo state is destroyed. For the parallel configuration, we find an interesting interplay of state symmetry and conductance. Our results are in good agreement with those obtained with other methods, and provide additional insights into the physics of the Kondo state in the double dot system.

Key words: Electronic Transport, Double Quantum Dot, Kondo Effect

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Transport properties of small structures such as atoms, molecules and quantum dots have received a great deal of attention in recent years. Electron coherence at these nanoscales bring out interference effects that are inherent to the system and are explorable in experiments [1]. Confinement of electrons in these structures results in strong Coulomb effects. The combination of Coulomb interaction and strong coupling to reservoirs, for example, gives rise to interesting spin-singlet correlations observed at energies of the order of the Kondo temperature $T_K$, typically in the sub-kelvin regime. This Kondo effect has been extensively studied theoretically and experimentally in different quantum dot systems [1,2,3]. Rich behavior is anticipated when coherence and correlations compete in different geometries, and we address some of these issues in this work.

Although theoretical studies have been presented utilizing different approaches [4,5,6,7], the physical richness of these systems deserves more attention. In this paper we focus our efforts on describing the transport properties of the double quantum dot system connected to leads either in series or in parallel while in the Kondo regime. We apply a finite-$U$ slave boson mean field technique [8], which has been shown to capture the interesting physics in this regime. We find that the strong interdot coupling either directly or through the leads, results in interesting sub- and super-tunneling transport regimes, associated with the characteristic bonding and anti-bonding states of a diatomic molecule. It is fascinating that these features are projected into the Kondo regime, and result in
H and d doubly occupied electron states respectively. Within
where the constraints establish the couplings. We model the leads in
H(QDs) before they are coupled to the leads; Hleads describes the two semi-infinite leads, and Hdot−leads establishes the couplings. We model the leads in the tight-binding approximation, which can be described by Hleads = \sum_{\sigma,i=\pm 1} \left( t_{\alpha \sigma} c_{i-1 \sigma} + H.c. \right) + \sum_{\sigma,i\geq 1} \left( t_{\alpha \sigma} c_{i+1 \sigma} + H.c. \right). In the finite-U slave boson approach, one enlarges the Hilbert space of the dots by
introducing a set of boson operators, ci (ei), pσ (pσ), and di (dσ), which project onto the empty, singly and
doubly occupied electron states respectively. Within
this approach we can write the Hamiltonian Hdot as:

\begin{align}
H_{dot} = & \sum_{i=\alpha \beta} (\epsilon_i + eV_i) c_i^\dagger c_i + U \sum_{i=\alpha \beta} d_i^\dagger d_i \\
+ & \sum_{\sigma,i=\pm 1} \left( t_{\alpha \sigma} z_{\alpha \sigma} c_i^\dagger c_{i+1 \sigma} + H.c. \right) \\
+ & \sum_{i=\alpha \beta} \left( \lambda^{(1)}_{i} P_i + \sum_{\sigma} \lambda^{(2)}_{i\sigma} Q_{i\sigma} \right),
\end{align}

where

\begin{align}
z_{i\sigma} = & \left( 1 - d_i^\dagger d_i - p_i^\dagger p_i \right)^{-1/2} \left( e_i^\dagger p_i + p_\beta^\dagger d_i \right) \\
\times & \left( 1 - e_i^\dagger e_i - p_\alpha^\dagger p_\sigma \right)^{-1/2}.
\end{align}

The constraints

\begin{align}
P_i = & \sum_{\sigma} p_i^\dagger p_i + e_i^\dagger e_i + d_i^\dagger d_i - 1 = 0
\end{align}

and

\begin{align}
Q_{i\sigma} = & c_i^\dagger c_\sigma - p_i^\dagger p_\sigma - d_i^\dagger d_\sigma = 0
\end{align}

are enforced in the problem through their respective Lagrange multipliers in Hdot, \lambda^{(1)}_{i\sigma} and \lambda^{(2)}_{i\sigma}, in order to eliminate unphysical states. Finally,

\begin{align}
H_{dot−leads} = & \sum_{\sigma,j=\alpha,\beta} \left( \tilde{t}_{ij} z_{i\sigma} c_i^\dagger c_{j\sigma} + H.c. \right)
\end{align}

allows electrons to travel through the QD region.

In the mean field approximation we replace all the
boson operators by their expectation values. This procedure results in a convenient non-interacting Hamiltonian for the quasi-electrons with effective energy \( \epsilon_i + \lambda \). The effective Hamiltonian is a function of 14 free
parameters which are determined by the minimization of the free energy \( \langle H \rangle \) with respect to all of them. The
information about the strong correlation is however captured by these parameters. Utilizing the Hellman-Feynman theorem, the condition for minimal free energy requires \( \partial \langle H \rangle / \partial x = 0 \), where \( x \) runs over all the
parameters. This results in a set of non-linear coupled equations that is solved numerically. The expectation values appearing in these equations are calculated by Green’s functions techniques. Expressions for the
Green’s functions can be obtained straightforwardly by the equation of motion method, using the effective
mean-field Hamiltonian. From the Keldysh formalism the equilibrium conductance can be written as \( G = 4n^2 e^2 \rho(\epsilon_F) \rho(\epsilon_F) G_{11}(\epsilon_F)^2 \), where \( \rho(\epsilon) = \rho_\alpha(\epsilon) = \rho_\beta(\epsilon) \) is the spectral density of states of the semi-
infinite chain and \( G_{11} \) is the propagator that promotes one electron from site 1 to site 1 and \( \epsilon_F \) is the Fermi energy.

One can transform Fig. 1 into a series configuration
if we take \( t_{\alpha \beta} = t_{\beta \beta} = 0 \). The lead bandwidth is \( D = 4t \) and
the Fermi level is set to zero \( (\epsilon_F = 0) \); hereafter we take the broadening \( \Gamma = \pi t^2 \rho_\gamma \) due to the coupling to the
leads as the energy unit and show results for temperature \( T = 0 \). Figure 2 shows the conductance for
the case of two dots coupled in series for several values of the energy difference \( \Delta \epsilon = \epsilon_\beta - \epsilon_\alpha \) and for \( t_{\alpha \beta} = 1 \).
For this relatively small value of \( t_{\alpha \beta} \), the role of the
direct interdot connection is only to provide a bridge
between the two dots so that electrons can go through.
Here, the level repulsion between the original dot levels
is essentially negligible (within the level broadening), and the conductance has a maximum at the particle-hole symmetry condition ($V_g = -U/2$). For the degenerate case, $\Delta \epsilon = 0$, the dots are in the Kondo regime for the same $V_g$, and the peaks in the density of states at the Fermi level provide a resonant tunneling condition with unitary value. This limiting case agrees well with results obtained in previous works [5]. As $\Delta \epsilon$ increases the dots reach the Kondo regime for slightly different $V_g$ values and the conductance is suppressed. Larger $t_{\alpha \beta}$ values result in sizable level repulsion and two conductance peaks.

Figure 3 shows the conductance as function of gate voltage for the parallel configuration for $\Delta \epsilon = 0$ and different values of the interdot coupling $t_{\alpha \beta}$. Notice that this configuration resembles the one used in Ref.[9] to study the persistent current of a quantum dot side-coupled to a ring. For the data displayed in Fig. 3, we have chosen $U = 12.5$ and $t_{\alpha 1} = t_{\beta 1} \equiv t' = 0.2t$. For $t_{\alpha \beta} = 0$ we see the typical unitary limit conductance region around $V_g = -U/2$. In this case we have both dots in the Kondo regime. The half-filled case results in a total spin $S = 1$, provided by the two electrons in the dots. One can distinguish two well-defined regimes on the conductance curves. The original flat region around $V_g = -U/2$ for $t_{\alpha \beta} = 0$ is split into two regions for larger interdot coupling. Let us analyze this behavior in more detail.

As $t_{\alpha \beta}$ increases, level mixing and repulsion takes place, creating bonding and antibonding states in the dot system. These coherently-mixed states created between the two QDs have typical symmetric/antisymmetric configurations, resulting also in very different effective coupling to the leads. The antibonding state, for example, contributes a delta-like peak to the density of states (see Fig. 4) and is completely uncoupled to the leads, due to destructive interference between the two paths. This interference is akin to the “subradiant” state discussed in the context of coupled radiant units, while here is more natural to call it the “sub-tunneling” state [10]. The contribution to the conductance, however, comes from the bonding state. The bonding/symmetric state has a much larger effective coupling to the leads, as in the “superradiant state”, and is therefore termed the “super-tunneling state” [10]. The super-tunneling state results in the broad density of states feature seen in Fig. 4 at higher energies.

It is the competition between the bonding and antibonding states that results in the conductance curves in Fig. 3. In the flat region present for $t_{\alpha \beta} \neq 0$, the antibonding state is found pinned around the Fermi level for a large range of gate voltage, as we can see in Fig. 4. In that regime, the contribution to the conductance comes from the tail of the bonding state that is slightly above the Fermi level. Since the bonding state is not in
resonance with the Fermi level, the conductance does not reach the unitary limit, until the antibonding state is filled and moves well below the Fermi level. Notice that the energy difference between bonding and antibonding states is determined by $t_{\alpha\beta}$. As the tail of the bonding state is increasingly occupied, the sharp antibonding state reaches the Fermi level. It remains there until it fills, while contributing nothing to the conductance. Notice further that a change in the sign of $t_{\alpha\beta}$ produces a mirror reversal (left to right) of Figs. 3 and 4. This is in agreement with the single-particle results in Ref. [11].

Breaking the degeneracy between dots, $\Delta \epsilon \neq 0$, significantly changes the conductance of the system. The conductance for the non-degenerate case is shown in Fig. 5. We have chosen here $t' = 0.1t$ and $\Delta \epsilon = 0.075\Gamma$, so as to have significant separation of the levels. We obtain a structure of three clear peaks, analogous to those obtained in previous works [6,7], where exact diagonalization plus embedding methods are used to study the Kondo regime. The three peaks can be understood as follows. The peak around $V_g = 0$ is due to electrons travelling through the dot $\alpha$ with energy $\epsilon_\alpha = V_g - \Delta \epsilon/2$, which is in the Kondo regime ($S = 1/2$). As the levels shift with gate, the dot $\beta$ with energy $\epsilon_\beta = V_g + \Delta \epsilon/2$ becomes then accessible and the conductance starts dropping due to the destructive interference of electrons travelling through the two different paths, totally vanishing the conductance at $V_g \approx -0.2U$. The peak at the particle-hole symmetry position ($V_g/U = -0.5$) reaches unity when both dots are in the Kondo regime ($S = 1$). The following valley in the conductance has a similar interpretation as the first one. Finally, in the last peak (at $V_g \approx -0.8U$) the $\epsilon_\alpha$ is well below the Fermi level and the contribution comes only from the dot $\beta$ in the Kondo regime.

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