

# 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 cancellations when the molecular energies of the side attached double quantum-dot cross the Fermi energy. We investigate the many body molecular Kondo states and its interplay with the inter-dot antiferromagnetic correlation as a function of the parameters of the system.

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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. 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 in QDs has been extensively studied in the last years [2]. 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 [3,4]. 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 [5]. In this case, the QDs act as scattering centers in close analogy with the traditional Kondo effect [6].

Recent electron transport experiments showed that Kondo and Fano resonances occurs simultaneously [7]. Multiple scattering of travelling electronic waves on a localized magnetic state are crucial for a formation of both

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resonances. The condition for the Fano resonance is the existence of two scattering channels: A discrete level and a broad continuum band [8].

In this work, we study the transport properties of a double quantum-dot molecule side coupled to a quantum wire in the Kondo regimen. We use the finite- $U$  slave-boson mean-field approach, which was initially developed by Kotliar and Ruckenstein [9] and used later by Bing Dong and X. L. Lei to study the transport through coupled double quantum-dots connected to leads [10], which enforces the correspondence between the impurity fermions and the auxiliary fermions to a mean-field level to release the  $U = \infty$  restriction. In double quantum-dot molecules this approach allow to treat both the dot-lead coupling and the inter-dot tunneling nonperturbatively at an arbitrary strengths of the Coulomb correlation  $U$ , and thus an antiferromagnetic exchange coupling parameter appears naturally [10]. We found that the anti-resonances of the linear conductance reflect the spectral properties of the artificial molecule. We investigate the many body molecular Kondo ground state and the competing singlet ground state that results from the anti-ferromagnetic correlation between the dots, as a function of the parameters of the system. In the Kondo regime, each dot results to have its own Kondo temperature as a consequence of their different connections to the conduction electrons.

## 2. Model

Let us consider a double quantum-dot (DQD) side coupled to a perfect quantum wire (QW) (Fig. 1). We adopt the two-fold Anderson Hamiltonian. Each dot has a single level  $\varepsilon_{di}$  (with  $i=1,2$ ), intra-dot Coulomb repulsion  $U$ , is coupled to each other with inter-dot tunneling coupling  $t_c$ . The side attached double quantum-dot is coupled to the QW with coupling  $t_0$ . The QW has a site energy  $\varepsilon_{i,\sigma}$  and a hopping parameter  $t$ .

In analogy with the infinite- $U$  slave-boson approach [11] the Hilbert space is enlarged at each site, to contain in addition to the original fermions a set of four bosons [9] 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

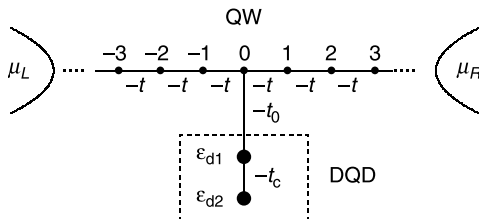


Fig. 1. Scheme of double quantum-dot (DQD) attached to a lead (perfect quantum wire (QW)). The QW is coupled to the left (L) and right (R) ‘reflectionless’ contacts.

(with spin up and down) and doubly occupied electron states. The Hamiltonian is written as,

$$\begin{aligned}
 H = & \sum_{i,\sigma} \varepsilon_{i,\sigma} c_{i,\sigma}^\dagger c_{i,\sigma} - t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) \\
 & - t_0 (c_{0,\sigma}^\dagger \tilde{Z}_{1,\sigma} f_{1,\sigma} + \text{H.c.}) \\
 & + \sum_{i=1}^2 \sum_{\sigma} (\varepsilon_{di} + \lambda_{i,\sigma}^{(2)}) f_{i,\sigma}^\dagger f_{i,\sigma} \\
 & - t_c \sum_{\sigma} (f_{1,\sigma}^\dagger \tilde{Z}_{1,\sigma} \tilde{Z}_{2,\sigma} f_{2,\sigma} + \text{H.c.}) + \sum_{i=1}^2 \left\{ U d_i^\dagger d_i \right. \\
 & + \lambda_i^{(1)} (p_{i,\uparrow}^\dagger p_{i,\uparrow} + p_{i,\downarrow}^\dagger p_{i,\downarrow} + e_i^\dagger e_i + d_i^\dagger d_i - 1) \\
 & \left. - \sum_{\sigma} \lambda_{i,\sigma}^{(2)} (p_{i,\sigma}^\dagger p_{i,\sigma} + d_i^\dagger d_i) \right\} \quad (1)
 \end{aligned}$$

where  $c_{i,\sigma}^\dagger(c_{i,\sigma})$  is the creation (annihilation) operator of an 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 an electron with spin  $\sigma$  in the  $i$ th QD. The operator  $\tilde{Z}_{i,\sigma}$  is chosen to reproduce the correct  $U \rightarrow 0$  limit in the mean field approximation,

$$\begin{aligned}
 \tilde{Z}_{i,\sigma} = & (1 - d_i^\dagger d_i - p_{i,\sigma}^\dagger p_{i,\sigma})^{-1/2} (e_i^\dagger p_{i,\sigma} + p_{i,-\sigma}^\dagger d_i) \\
 & \times (1 - e_i^\dagger e_i - p_{i,-\sigma}^\dagger p_{i,-\sigma})^{-1/2} \quad (2)
 \end{aligned}$$

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

$$\begin{aligned}
 H_{\text{TB}} = & -t \sum_{i,\sigma} (c_{i,\sigma}^\dagger c_{i+1,\sigma} + \text{H.c.}) \\
 & - \sum_{\sigma} \tilde{t}_{0,\sigma} (c_{0,\sigma}^\dagger f_{1,\sigma} + \text{H.c.}) + \sum_{i=1}^2 \sum_{\sigma} \tilde{\varepsilon}_{di,\sigma} f_{i,\sigma}^\dagger f_{i,\sigma} \\
 & - \sum_{\sigma} \tilde{t}_{c,\sigma} (f_{1,\sigma}^\dagger f_{2,\sigma} + \text{H.c.}) \quad (3)
 \end{aligned}$$

$$\begin{aligned}
 H_B = & \sum_{i=1}^2 \left\{ U d_i^2 + \lambda_i^{(1)} (p_{i,\uparrow}^2 + p_{i,\downarrow}^2 + e_i^2 + d_i^2 - 1) \right. \\
 & \left. - \sum_{\sigma} \lambda_{i,\sigma}^{(2)} (p_{i,\sigma}^2 + d_i^2) \right\} \quad (4)
 \end{aligned}$$

with  $\tilde{\varepsilon}_{di,\sigma} = \varepsilon_{di} + \lambda_{i,\sigma}^2$ ,  $\tilde{t}_{0,\sigma} = t_0 \langle \tilde{Z}_{1,\sigma} \rangle$ , 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 stationary states of the entire Hamiltonian  $H$  can be written as

$$|\psi_k\rangle = \sum_{j=-\infty}^{\infty} a_j^k |j\rangle + \sum_{l=1}^2 b_l^k |l\rangle \quad (5)$$

where  $a_j^k$  and  $b_l^k$  are the probabilities amplitudes to find the electron at the site  $j$  or at the  $l$ th QD, respectively, with energy at infinite  $\omega = -2t \cos k$ . The amplitudes  $a_j^k$  and  $b_l^k$  obey the following linear difference equations

$$\omega a_j^k = -t(a_{j+1}^k + a_{j-1}^k), \quad j \neq 0 \quad (6a)$$

$$\omega a_0^k = -t(a_1^k + a_{-1}^k) - \tilde{t}_0 b_1^k \quad (6b)$$

$$(\omega - \tilde{\varepsilon}_{d1}) b_1^k = -\tilde{t}_c b_2^k - \tilde{t}_0 a_0^k \quad (6c)$$

$$(\omega - \tilde{\varepsilon}_{d2}) b_2^k = -\tilde{t}_c b_1^k \quad (6d)$$

In order to study the solutions, given by the Eqs. (6)(a)–(d), we assume that the electrons are described by a plane wave with unitary incident amplitude, being  $r$  and  $\tau$  the reflection and transmission amplitudes. That is,

$$a_j^k = e^{ikj} + r e^{-ikj}, \quad (j < 0, k > 0), \quad (j > 0, k < 0) \quad (7a)$$

$$a_j^k = \tau e^{ikj}, \quad (j > 0, k > 0), \quad (j < 0, k < 0) \quad (7b)$$

Inserting Eqs. (7)(a) and (b) into Eqs. (6)(a)–(d), we get a inhomogeneous system of linear equations for  $\tau$ ,  $r$ ,  $a_j^k$  and  $b_l^k$ , leading to the following expression

$$\tau = \frac{(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)}{(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+) + i(\omega - \tilde{\varepsilon}_{d2})\tilde{I}} \quad (8)$$

where the bonding and antibonding energies ( $\tilde{\varepsilon}_{\pm}$ ) are defined by  $\tilde{\varepsilon}_{\pm} = (\tilde{\varepsilon}_{d1} + \tilde{\varepsilon}_{d2})/2 \mp \sqrt{((\tilde{\varepsilon}_{d1} - \tilde{\varepsilon}_{d2})/2)^2 + \tilde{t}_c^2}$  and  $\tilde{I} = \pi t_0^2 \rho_0$  ( $\omega$ ) is the renormalized coupling between the double

quantum-dot and the leads of density of states  $\rho_0(\omega)$ . The transmission probability is given by  $T = |\tau|^2$ ,

$$T(\omega) = \frac{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)]^2}{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)]^2 + [(\omega - \tilde{\varepsilon}_{d2})\tilde{I}]^2} \quad (9)$$

In the limit of zero bias and temperature we obtain the expression for the linear conductance,

$$G = \frac{2e^2}{h} T(0) = \frac{2e^2}{h} \frac{(\tilde{\varepsilon}_- \tilde{\varepsilon}_+)^2}{(\tilde{\varepsilon}_- \tilde{\varepsilon}_+)^2 + (\tilde{\varepsilon}_{d2} \tilde{I})^2} \quad (10)$$

From the amplitudes  $b_1^k$  and  $b_2^k$  we obtain the local density of states (LDOS) in the quantum dots,

$$\rho_1(\omega) = \frac{1}{\pi} \frac{\tilde{I}(\omega - \tilde{\varepsilon}_{d2})^2}{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)]^2 + [(\omega - \tilde{\varepsilon}_{d2})\tilde{I}]^2} \quad (11)$$

$$\rho_2(\omega) = \frac{1}{\pi} \frac{\tilde{I}^2}{[(\omega - \tilde{\varepsilon}_-)(\omega - \tilde{\varepsilon}_+)]^2 + [(\omega - \tilde{\varepsilon}_{d2})\tilde{I}]^2} \quad (12)$$

### 3. Results

We take typical values for the parameters that define the system,  $t = 25\Gamma$ ,  $t_0 = 7.07\Gamma$  where  $\Gamma = \pi t_0^2 \rho_0(0)$  is taken to be the unit of energy.

We consider first the situation where the two dots local state energies are varied simultaneously by a gate voltage  $V_g$ , i.e.  $\varepsilon_{d1} = \varepsilon_{d2} = V_g$ .

The transmission probability,  $T$ , is displayed in Fig. 2 for various values of  $U$ , and two values of  $t_c$ . The transmission probability always reaches zero at  $\omega = \tilde{\varepsilon}_-$  and  $\tilde{\varepsilon}_+$  and unitary value at  $\omega = \tilde{\varepsilon}_{d2}$ . The Fig. 2 permits to study the interplay between the Kondo effect and the inter-dot anti-ferromagnetic correlation. Increasing  $U$ , a sharp feature develops close to the Fermi energy ( $\omega = 0$ ), indicating the appearance of a Kondo resonance. We can see that this process is more rapidly defined for the case where  $t_c = 0.5\Gamma$  than for  $t_c = \Gamma$ . This behavior is due to the anti-ferromagnetic interaction between the spins of the dots, proportional to  $t_c^2/U$ , that destroys the Kondo effect when it is greater than the Kondo temperature creating a singlet ground state for the dot molecule.

For  $U$  sufficiently large the transmission can be written approximately as the superposition of two Fano–Kondo line shapes, one of which has zero  $q$  factor,

$$T(\omega) \approx \frac{(\varepsilon' + q')^2}{(\varepsilon')^2 + 1} + \frac{(\varepsilon'' + q'')^2}{(\varepsilon'')^2 + 1} \quad (13)$$

where  $\varepsilon' = (\omega - \tilde{\varepsilon}_{d2})/\tilde{\Delta}$ ,  $q' = (\tilde{\varepsilon}_{d2} - \tilde{\varepsilon}_-)/\tilde{\Delta}$ ,  $\varepsilon'' = (\omega - \tilde{\varepsilon}_+)/\Gamma$  and  $q'' = 0$ , with  $\tilde{\Delta} = \tilde{t}_c^2/\tilde{I}$  and  $\tilde{I}$ .

The DOS of the quantum-dot molecule gives us a better understanding of the transport properties of the system. The DOS is shown in Fig. 3 for various values of  $U$ , for the case  $t_c = 0.5\Gamma$ , where the Kondo spin correlation is dominant over the anti-ferromagnetic one. We can observe the

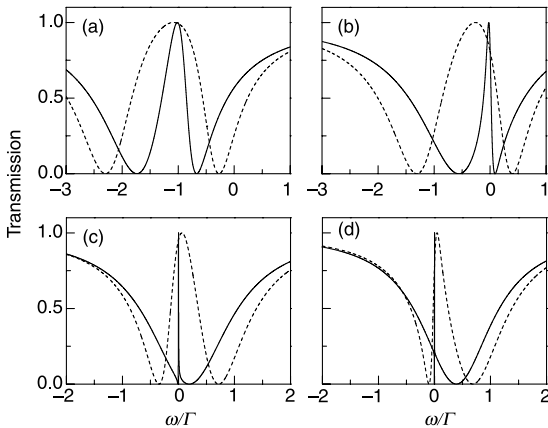


Fig. 2. Transmission spectrum for  $\varepsilon_{d1} = \varepsilon_{d2} = V_g = -3\Gamma$ ,  $t_c = 0.5\Gamma$  (solid line) and  $t_c = \Gamma$  (dashed line), for on site energy, (a)  $U = 2\Gamma$ , (b)  $U = 4\Gamma$ , (c)  $U = 8\Gamma$  and (d)  $U = 16\Gamma$ .

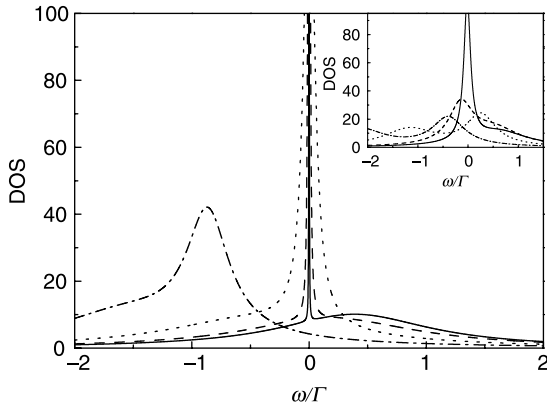


Fig. 3. DOS for  $t_c = 0.5T$ ,  $\varepsilon_{d1} = \varepsilon_{d2} = V_g = -3T$ , for on site energy,  $U = 16\Gamma$  (solid line),  $U = 8\Gamma$  (dashed line),  $U = 4\Gamma$  (dotted line) and  $U = 2\Gamma$  (dash-dot line). With  $t_c = \Gamma$  is displayed at the insert.

superposition of a narrow and a broad Kondo peaks with a widths  $\tilde{\Delta}$  and  $\tilde{\Gamma}$ . In fact, the DOS can be written as the superposition of two Lorentzian,

$$\rho(\omega) \approx \frac{1}{\pi} \frac{\tilde{\Gamma}}{(\omega - \tilde{\varepsilon}_+)^2 + \tilde{\Gamma}^2} + \frac{1}{\pi} \frac{\tilde{\Delta}}{(\omega - \tilde{\varepsilon}_-)^2 + \tilde{\Delta}^2} \quad (14)$$

As it can be seen from the Fig. 3, there is no Kondo peak for  $U = 2\Gamma$ , as it should because in this case the QDs are with two electrons each.

In order to confirm the destructive effect of anti-ferromagnetism on the Kondo regime, we display in the insert if the Fig. 3 the DOS of the DQD for the same parameters as before but with  $t_c = \Gamma$ . The DOS shows two peaks at the bonding and anti-bonding energies with no Kondo peak, showing that for this value of  $t_c$  anti-ferromagnetism is dominant.

The LDOS gives us more details about the formation of the Kondo resonance. The LDOS is displayed in Fig. 4. The LDOS  $\rho_2$  develops a sharp Kondo resonance peak near the Fermi energy ( $\omega = 0$ ). As the external dot (dot 2) develops a Kondo resonance, the LDOS  $\rho_1$  reduces near the Fermi

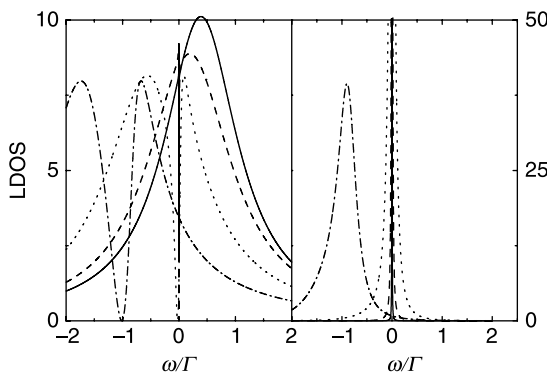


Fig. 4. Local density of states (a) quantum-dot 1, (b) quantum-dot 2,  $\varepsilon_{d1} = \varepsilon_{d2} = V_g = -3T$ , for on site energy,  $U = 16\Gamma$  (solid line),  $U = 8\Gamma$  (dashed line),  $U = 4\Gamma$  (dotted line) and  $U = 2\Gamma$  (dash-dot line).

energy. This behavior is understood considering that the Kondo regime of quantum-dot 2 (QD2) is a result of its weak coupling to the conduction electrons mediated by the intermediate quantum-dot 1 (QD1) that is as well at the Kondo regime. This coupling creates a very sharp Kondo peak at QD2, of width  $\tilde{\Delta}$  created by depleting, at the vicinity of the Fermi level, the larger Kondo peak of QD1 of width  $\tilde{\Gamma}$ . This is shown in Fig. 4(a) and (b). These results imply the existence of two Kondo temperature  $T_{1K} = \tilde{\Gamma}$  and  $T_{2K} = \Delta = \tilde{t}_c^2/\tilde{\Gamma}$ , associated to each dot. It is this depleting of the LDOS at the Fermi level of QD1 that permits the transmission to be unity at the Fermi level as shown in Fig. 2. In this case the side attached QD1, although being at the Kondo regime, cannot create a destructive interference for the conducting electrons going along the lead.

Fig. 5 displays 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 anti-resonances corresponding to the bonding and anti-bonding energies of the quantum-dot molecule and one resonance between them. The separation between the two anti-resonance grows linearly with  $U$ . From the Eq. (10) the conductance vanishes when  $\tilde{\varepsilon}_-$  or  $\tilde{\varepsilon}_+$  coincide with the Fermi energy ( $\omega = 0$ ). On the other hand, the conductance reaches the unitary limit when  $\tilde{\varepsilon}_{d2}$  crosses the Fermi energy.

Let us consider now the situation where only one of the gate potentials is varied while the other one is maintained constant ( $\varepsilon_{d1} = V_{1g} = -U/2$ ,  $\varepsilon_{d2} = V_{2g}$ ). Fig. 6 shows  $G$  versus  $V_{2g}$  for  $U = 8\Gamma$ . In this situation, the occupation number of the 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 QD2 is almost zero and the antibonding and bonding energies satisfy  $\tilde{\varepsilon}_+ \approx V_{2g}$  and  $\tilde{\varepsilon}_- \approx -\tilde{t}_c^2/V_{2g} \approx 0$ , respectively. This is the case of a single dot side connected to a wire at the Kondo regime that

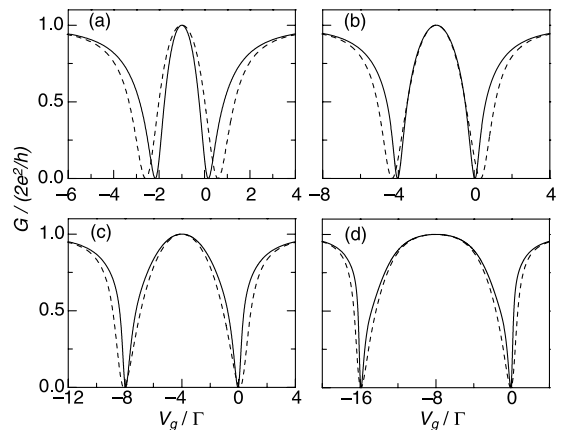


Fig. 5. Linear conductance  $G$  versus  $V_g$  for  $t_c = 0.5\Gamma$  (solid line) and  $t_c = \Gamma$ , for on site energy, (a)  $U = 2\Gamma$ , (b)  $U = 4\Gamma$ , (c)  $U = 8\Gamma$  and (d)  $U = 16\Gamma$ .

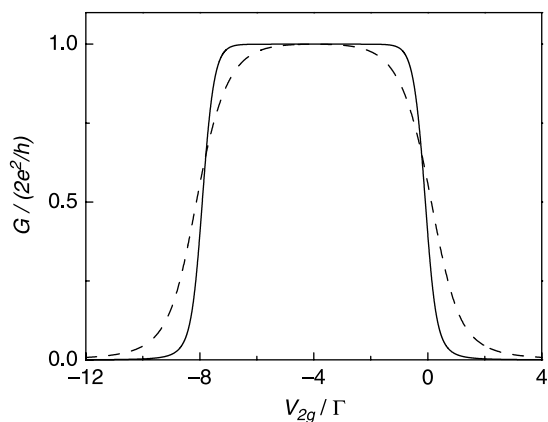


Fig. 6. Linear conductance  $G$  versus  $V_{2g}$  for  $U=8\Gamma$ ,  $t_c=0.5\Gamma$  (solid line) and  $t_c=\Gamma$  (dashed line).

produces a destructive interference at the leads that according to Eq. (10) reduces the conductance to zero. Decreasing  $V_{2g}$  the occupation number  $n_2=1$ , and QD2 enters into the Kondo regime. Then the QD2 depletes to zero the DOS of QD1 at the Fermi energy, as explained above eliminating the interference, which permits the conductance to reach 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 outside of the Kondo regime and QD1 recovers its destructive interference with respect to the flowing current reducing the conductance to zero.

#### 4. Summary

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 anti-resonances localized at the bonding and antibonding renormalized energies of the quantum-dot molecule, and one resonance at the renormalized site energy of the outside quantum-dot. The LDOS at each dot shows that when the Kondo correlations are dominant both dots are at the Kondo regime each one with its own Kondo temperature. Increasing the inter-dot interaction, the anti-ferromagnetic correlation becomes dominant destroying the Kondo effect and the physics associated with it. These phenomena have been analyzed as a function of the relevant parameters of the system. This study has been restricted to zero temperature. Using this same approach, finite temperature properties and systems with other topologies are currently being studied.

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