Transport in coupled quantum dots: Kondo effect versus antiferromagnetic correlation

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The interplay between the Kondo effect and the interdot magnetic interaction in a coupled-dot system is studied. An exact result for the transport properties at zero temperature is obtained by diagonalizing a cluster, composed by the double dot and its vicinity, which is connected to leads. It is shown that the system goes continuously from the Kondo regime to an antiferromagnetic state as the interdot interaction is increased. The conductance, the charge at the dots, and the spin-spin correlation are obtained as a function of the gate potential.

In the last years electron transport through a quantum dot (QD) has been the subject of many experimental and theoretical[1–6] investigations. The possibility of measuring the Kondo effect in a system with a QD has been proposed by several theoretical studies.[1,4] Its detection is a difficult task since small size dots are required. Such a small QD was recently obtained and the Kondo effect was measured.[5] This confirms the possibility of studying many of the properties of strongly correlated metals and insulators in artificial constructed mesoscopic structures. The advantage of these systems is that their parameters can be continuously changed by modifying the applied external potentials so that different regimes can be studied.

The physics associated with heavy-fermion compounds in the vicinity of what is called the quantum phase transition is identified by the competition between the spin correlation among the magnetic atoms and between the atoms and the conduction electrons.[7] The latter gives rise to the Kondo effect and the former tends to create a ferromagnetic or antiferromagnetic ground state destroying the Kondo regime. The study of the two-impurity Kondo Hamiltonian was proposed to clarify this important problem, as it includes in the model the two interactions responsible for this competing behavior.[8,9]

There have been extensive experimental transport studies in the double-dot system.[10] They were mainly designed to analyze the double-dot molecule. From the theoretical viewpoint transport through a double dot has received considerable attention mainly restricted to the study of high-temperature Coulomb blockade phenomenon.[11]

At very low temperature, the study of a completely different physics, created by the interplay of the Kondo effect and the interdot antiferromagnetic correlation, is now feasible due to the recent possibility of constructing very small dots. An interesting analysis of these phenomena in a two-QD system, based on qualitative arguments and slave-boson mean-field theory (SBMFT), has recently appeared.[6] The behavior of the conductance was studied for a system where the double occupancy at the dots was eliminated from the Hilbert space. Although this method becomes exact when the number of spin degrees of freedom is infinite, some caution is necessary when applying it to spin-1/2 systems.

The purpose of this paper is to present a numerically exact calculation of the transport properties of a double-dot system to investigate the competition between the Kondo effect and the antiferromagnetic correlation. The parameters are chosen to reflect real experimental conditions and, in particular, the intradot Coulomb repulsion is taken to be finite. The conductance is obtained for several interdot coupling constants. The density of states, the charge inside the dots and the various spin-spin correlation functions are calculated in order to characterize the state of the system.

The properties of the system for temperatures well below the Kondo temperature T_K is obtained by using the Lanczos method[12] to calculate the ground state of a small cluster containing the two dots, which is embedded into the leads. The conductance calculated according to this procedure tends very rapidly to its exact result as the size of the cluster is increased. From this viewpoint our calculation is numerically exact since we were able to reach convergence, within 1% error, for a small cluster. For $T > T_K$ we use a self-consistent solution for the equation of motion for the one-particle Green function.[13] This approximation eliminates all the low-lying excitations in the vicinity of the Fermi level and, as a consequence, the Kondo effect. However, it provides an adequate description of the Coulomb blockade high-temperature regime.[2]

The system is represented by an Anderson two-impurity first-neighbor tight-binding Hamiltonian,

$$H = V \sum_{\substack{\sigma \\ r=\alpha,\beta}} n_{r\sigma} + \frac{U}{2} \sum_{r\sigma} n_{r\sigma} n_{r\sigma}^{-} + t'' \sum_{\sigma} (c_{\alpha\sigma}^{\dagger} c_{\beta\sigma} + \text{c.c.}) + t' \sum_{\sigma} (c_{\alpha\sigma}^{\dagger} c_{\bar{1}\sigma} + c_{\beta\sigma}^{\dagger} c_{1\sigma} + \text{c.c.}) + t \sum_{\substack{\sigma \\ i,j}} c_{i\sigma}^{\dagger} c_{j\sigma} \qquad (1)$$

The expression above includes the Hamiltonian for the cluster containing the two dots and their first neighbors denoted by α, β, 1, and $\bar{1}$, respectively. The parameters U and V represent the electronic repulsion and the gate potential at the dots, t'' is the interdot interaction, t' the coupling between the dots and the leads, t the nearest-neighbor hopping, and the subindices i and j, in the last term, run over all sites

other than the dot sites. We restrict our analysis to the case of two identical dots. An interdot magnetic exchange term J is not explicitly included in the Hamiltonian since it is not an independent parameter but a function of the interdot tunneling ($J \sim t''^2/U$).[7] We neglect also the interdot Coulomb repulsion, which only contributes to strengthen the antiferromagnetic interaction in the very-strong-coupling limit, without introducing qualitative changes in the physics of the system.

To describe the very-low-temperature properties, we calculate the one-particle Green functions $G_{\alpha\beta}$ at the dots. They are imposed to satisfy a Dyson equation $\hat{G}=\hat{g}+\hat{g}\hat{T}\hat{G}$, where $\hat{g}$ is the cluster Green function matrix and $\hat{T}$ is the matrix of the coupling Hamiltonian between the cluster and the rest of the system. The undressed Green function $\hat{g}$ is calculated using the cluster ground state obtained by the Lanczos method. The Dyson equation proposed is equivalent to the chain approximation in a kinetic energy diagrammatic expansion for the Hubbard Hamiltonian.[14] To be consistent, the charge of the dressed and undressed cluster is imposed to be the same. We calculate $\hat{g}$ as a combination of the Green functions of n and $n+1$ electrons with weights $1-p$ and p, $\hat{g}=(1-p)\hat{g}_n+p\hat{g}_{n+1}$.[15] In this case the charge of the undressed cluster is $q_c=(1-p)n+p(n+1)$. The charge of the cluster linked to the leads can be expressed as $Q_c=2\int_{-\infty}^{\epsilon_F}\Sigma_i \mathrm{Im}\, G_{ii}(\omega)d\omega$, where i runs through all the cluster sites and the factor 2 includes the electronic spin. This equation together with the imposed condition $q_c=Q_c$ constitute a system of two equations, which requires a self-consistent solution to obtain p and n as a function of the parameters of the system. Due to the symmetry of the problem, it is useful to represent the Hamiltonian using the two-dot bonding and antibonding states. In this case, according to the Keldysh formalism,[16] the conductance can be written as $\sigma=e^2/h[t'^2\rho(\epsilon_F)]^2|G_d^+-G_d^-|^2$ where $\rho(\epsilon_F)$ is the density of states at the Fermi energy and $G_d^{\pm}=1/[\omega-\epsilon^{\pm}-\Sigma_c(w)-\Sigma_d^{\pm}(w)]$ are the one-particle Green functions at the dots represented in the bonding and antibonding wave functions, with energies $\epsilon^{\pm}=V\pm t''$. $\Sigma_c(w)$ and $\Sigma_d^{\pm}(w)$ are the self-energies corresponding to the leads and to the many-body interaction, respectively.

The expression for the current is obtained by considering explicitly that the system is a Fermi liquid $\lim_{\omega\to 0}\mathrm{Im}\,\Sigma_d^{\pm}(\omega)\propto\omega^2$, which implies that there are no dissipative processes taking place at the Fermi level. It is important to point out that our diagonalization self-consistent procedure satisfies, without any imposition, the Luttinger-Ward identity $\mathrm{Im}\int_{-\infty}^{\epsilon_F}[\partial\Sigma_d^{\pm}(\omega)/\partial\omega]G_d^{\pm}(\omega)d\omega=0$.[17] This ensures the fullfilment of the Fridel sum rule and of the Fermi liquid properties.

We have as well studied this problem through the equation of motion for the G^+ and G^- using a self-consistent decoupling procedure, proposed by Hubbard.[13] Since it eliminates all the low-lying excitations involved in the Kondo effect and properly describes the high-energy states, we suppose it to be an adequate solution for high temperatures, $T>T_K$. It has been used with success to study the Coulomb blockade behavior of the current going through a highly confined region, as in a QD.[2] Within this approximation the many-body self-energy can be expressed as $\Sigma_d^{\pm}(w)=n^{\pm}U(\omega-\epsilon_{\pm})/[\omega-i\eta-\epsilon^{\pm}-(1-n^{\pm})U]$. It requires the self-consistent calculation of the charge at the bonding and antibonding state $n^{\pm}$. As shown below the two treatments are equivalent in the limit of strong antiferromagnetic interdot coupling regime, where there is no Kondo ground state. In order to provide a complete characterization of the ground state we have compared the interdot spin-correlation $\langle\vec{S}_{d\alpha}\cdot\vec{S}_{d\beta}\rangle$ with the spin correlation of one dot and its nearest-neighbor conduction electrons $\langle\vec{S}_{c1}\cdot\vec{S}_{d\beta}\rangle$.

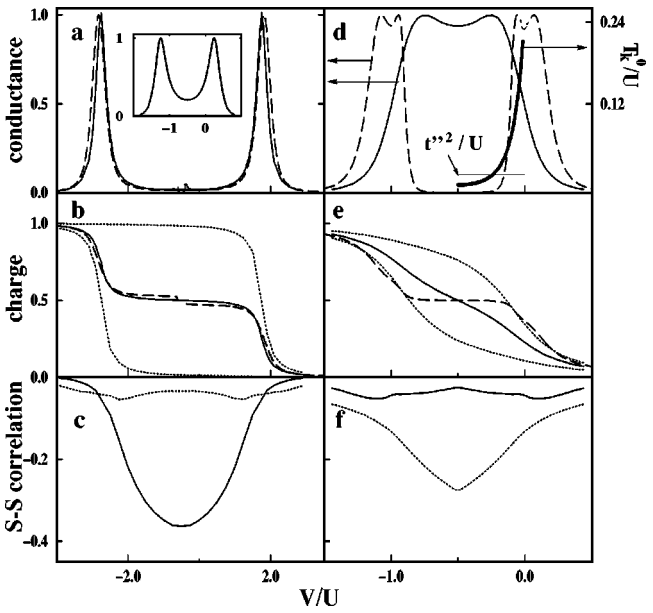

FIG. 1. Conductance, charge and spin correlation with $\Gamma/U=0.12$, for weak ($t''/U=0.16$) and strong ($t''/U=2.0$) coupling. Conductance in units of e^2/h: strong (a) and weak (d) coupling; exact-cluster (continuous) and Hubbard approximation (dotted). The thick line in (d) represents the single-dot Kondo temperature. The value t''^2/U is also indicated. The inset in (a) corresponds to the intermediate coupling ($t''/U=0.4$) in the exact-cluster approximation. Charge: strong (b) and weak (e) coupling; exact-cluster results for charge per spin in each dot (continuous) and in the $+$ $-$ states (dotted); Hubbard approximation results for charge per spin in each dot (dashed). Spin correlation: strong (c) and weak (f) coupling; dot–conduction-electron, $\langle\vec{S}_{c1}\cdot\vec{S}_{d\beta}\rangle$, (dotted) and dot-dot, $\langle\vec{S}_{d\alpha}\cdot\vec{S}_{d\beta}\rangle$, (continuous).

The transport properties are studied for weak and strong interdot coupling. We solve an eight-atom cluster with the parameter $\Gamma/U=t'^2/WU=0.12$, where W is the lead bandwidth. This value corresponds approximately to the device where the Kondo effect has recently been measured[5] and is compatible with first-principle calculated parameters.[18] The current, the dot charge, and the spin-spin correlation for weak interdot coupling ($t''/U=0.16$), as a function of V, are presented in the right part of Fig. 1. For $V>0.3$ the dot levels are above the Fermi level and there is no current. As V is reduced, the two dots become partially charged because the antibonding state enters into resonance. When the total charge at the dots is $N\sim 1$ there is a peak in the conductance which reaches the value of e^2/h. As soon as the system enters into the fluctuating valence regime, corresponding to ϵ^- below the Fermi energy, the Kondo peak appears, creat-

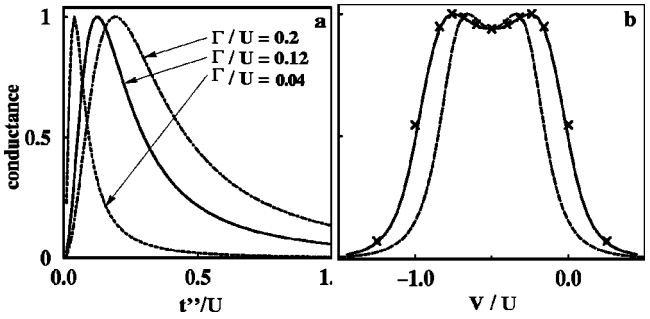

FIG. 2. Conductance (a) as a function of the interdot coupling for $V/U=-0.5$ and various values of Γ/U, (b) as a function of gate potential for $\Gamma/U=0.12$ and a cluster of four sites (dashed), eight sites (continuous), twelve sites (crosses).

ing a new channel for the electrons to flow. These features are shown in Figs. 1(d) and 1(e). The spin correlation $\langle \vec{S}_{c1}\cdot\vec{S}_{d\beta}\rangle$, continuous line in Fig. 1(c), increases. As V is further decreased extra charge enters into the dots and the conductance diminishes. As ϵ^- goes far beyond the Fermi energy the single-dot Kondo temperature, $T_K^0=\sqrt{U\Gamma/2}\exp[-\pi|V|(U+V)/(2U\Gamma)]$, represented in Fig. 1(d), decreases so that for $V/U\sim-0.5$, $t''^2/U>T_K^0$, reducing the Kondo effect. This reduction appears as a minimum of the conductance at $V/U=-0.5$ when the system has electron-hole symmetry and $N\sim 2$. However, as discussed below, the system is well in the Kondo regime, suggesting that T_K is enhanced relative to T_K^0 due to interdot coupling.[6] For $U\sim 2$ meV,[5] T_K^0 varies within the experimentally accessible range $0.2\ \mathrm{K}<T_K^0<4$ K. The large conductance in the interpeak region is therefore due to the channel created by the Abrikosov-Suhl resonance within Kondo regime, which is reflected as well in the relationship $\langle \vec{S}_{d\alpha}\cdot\vec{S}_{d\beta}\rangle \ll \langle \vec{S}_{c1}\cdot\vec{S}_{d\beta}\rangle$, shown in Fig. 1(f). This channel is absent when $T>T_K$. The Hubbard solution, also shown in Fig. 1(d), can be taken to be a high-temperature description of the same problem. It preserves the structure of the Coulomb blockade, with no conductance between the peaks, which are split into two due to the interdot interaction.

It is important to notice the different way the charge enters into the dots in the Coulomb blockade and in the Kondo regimes. In the former, the charge presents a plateau due to electronic repulsion while in the latter, the Kondo peak permits a continuous entrance of the charge. This behavior is shown in Fig. 1(e).

Finally, in the case of the strong interdot interaction ($t''/U=2$), shown at the left part of Fig. 1, the Kondo regime is almost quenched by the antiferromagnetic coupling. The Kondo spin-spin correlation, although small, has its maximum in the near vicinity of the conductance peaks where the Kondo temperature is high, while in the whole intermediate region antiferromagnetism controls the conduction. In this case, the conductances obtained by the two approaches, shown in Fig. 1(a), are almost identical, reflecting the fact that the system is outside the Kondo regime.[19]

When the dot-dot interaction has an intermediate value ($t''/U=0.4$) the conductance in the region between the peaks is slowly dependent upon the gate potential, as shown in the inset of Fig. 1(a). The conductance within the SBMFT has a two-plateau structure and drops abruptly to zero as the gate

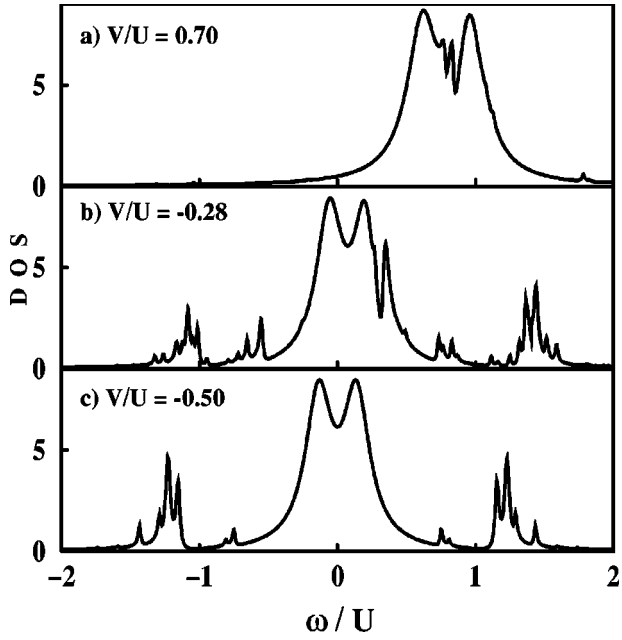

FIG. 3. DOS for the weak-coupling regime and three values of gate potential V. $\epsilon_F=0$, $\Gamma/U=0.12$, and $t''/U=0.16$.

potential is reduced.[6] However, we get neither a strict plateau structure nor a complete quenching of the Kondo effect. For a real situation where U is finite the current in the interpeak region is not zero although $t''^2/U\gg T_K^0$, reflecting an enhancement of T_K for coupled dots. Although the SBMFT has predicted this enhancement, its value for a real system, where $t\gg U$, requires further investigation.

The dependence of the conductance for the electron-hole symmetric situation as a function of the interdot coupling, for different values of Γ, is shown in Fig. 2(a). The conductance has a peak at $t''=\Gamma$, as obtained by SBMFT. The change in the conductance as t'' increases is more abrupt the smaller the value of Γ. As discussed below, our results for the two largest values of Γ are exact. However, for the smallest value it is only a good approximation because convergence with the size of the cluster is not completely reached in this case.

In order to study this convergence we calculate the conductance for three cluster sizes. We conclude that they are numerically exact, within 1%, for the experimental situation $\Gamma/U>0.08$. Results for $\Gamma/U=0.12$ for four-, eight-, and twelve-site clusters are shown in Fig. 2(b). In this region of Γ the Kondo effect is sufficiently local to be adequately described by our formalism using a small cluster.[20]

Our exact calculation confirms that the SBMF gets some important aspects of this problem correctly. However, as recognized in Ref. 6, the abrupt quenching of the Kondo effect obtained is an artifact of this approximation, which disconnects the dots from the leads, giving a zero conductance when the temperature is increased[21] or the interdot coupling augmented.[9] Fluctuation effects, not included in SBMFT, smooth out the transition, transforming it into a crossover behavior as shown in Fig. 2(b).

The analysis of the density of states (DOS) for various values of the gate potential helps to clarify the different circumstances involved. In Fig. 3(a) the DOS shows a relatively large and broad resonant peak above the Fermi energy,

which is split by the interdot interaction. It is approximately the DOS of a one-body problem since the dots are nearly empty, $N\sim 0$. The case of maximum conductance e^2/h and $N\sim 1$ is presented in Fig. 3(b). The Fermi level is located at one of the Abrikosov-Suhl subpeaks. Finally in Fig. 3(c) the electron-hole symmetric condition, $N\sim 2$ is represented. The Fermi energy coincides with the position of the pseudogap of the Kondo peak, which explains the reduction of the conductance in this case relative to the previous one. The figure shows also the lower and upper Hubbard resonances pushed far apart by the Kondo peak.

In summary, we have obtained a numerically exact $T=0$ solution for the transport properties of a coupled two-dot system. We show that the interplay between the interactions that give rise to the Kondo effect and the antiferromagnetic coupling are explicitly reflected on the conductance of the system. The different regimes have been characterized through a detailed study of the charge at the dots and the spin-spin correlations.

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