Quantum dot spin effect on the conductance of a quantum wire

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A numerically exact calculation of the $T=0$ transport properties of a quantum wire interacting with a lateral two-level quantum dot is presented. The wire conductance is calculated for all different states of charge and spin of the quantum dot. For a dot with two electrons we obtain an enhancement of the Kondo temperature at the singlet-triplet transition and a nonuniversal scaling law for its dependence upon the dot energy spacing. We find that the Kondo correlation is stronger for a dot spin $S_D \sim 1$ than for $S_D \sim 1/2$. In both cases the wire current is totally quenched by the Kondo effect. When the dot is in the mixed-valence regime and $1/2 \lesssim S_D \lesssim 1$ the wire conductance is partially quenched except in a very small region of gate potential where it reaches the maximum value e^2/h.

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In recent years an important experimental and theoretical effort has been dedicated to the understanding of the physical properties of a system constituted by a dot connected to two leads under the effect of an external potential.[1–6] This system has shown to be a versatile device to study the Kondo effect for a variety of regimes that can be accessed by changing continuously the values of the parameters that define the system. For temperatures below T_K, in the Kondo regime, the electrons circulate along the system through a channel at the Fermi level that disappears as the temperature is increased.

Recently, in a very interesting experiment,[7] the measurement of the transport through a dot with energy levels tuned by the application of an external magnetic field has demonstrated that the current through an even-charged dot connected to two leads is controlled by the Kondo correlation between the $S_D=1$ spin of the dot triplet state and the conduction-electron spins. This correlation gets stronger as the magnetic-field energy splitting is increased, and reaches its maximum value when the system is in the singlet-triplet transition, beyond which the Kondo effect dies out very rapidly.

This problem was theoretically studied by using poor man's scaling arguments and the mapping of a generic model of a dot undergoing a singlet-triplet transition onto the two impurity Kondo model.[8,9] These theoretical works focus their attention on the middle of the Coulomb blockade valley, a situation where the dot has an integer well-defined number of electrons, so that all mixed-valence regimes are eliminated. Assuming that the system is in the immediate vicinity of the singlet-triplet transition with an even number of electrons in the dot, they show that the Kondo effect is enhanced by the competition between the triplet and the singlet states.

In this paper we report the results of a numerically exact solution for a two-level quantum dot (QD) interacting with a wire, at $T=0$, for the whole range of parameters that permits the investigation of all possible regimes and states of charge and spin of the system. By varying the gate potential applied to the dot and the dot level energy spacing we are able to study the wire conductance for the dot in the mixed-valence regime and in the triplet ($S=1$), doublet ($S=1/2$), and singlet ($S=0$) spin states.

The system we consider consists of a dot laterally connected to a conducting wire. This is a very interesting configuration as it mimics the situation of a metal doped by magnetic impurities, where the localized spins belong to an electronic state outside the conduction band.[10] In this configuration, as shown in a recent theoretical work[11] restricted to a one-level dot, the Kondo correlation among the dot spin $S_D=1/2$ and its neighboring conducting spins provides a scattering mechanism for the electrons that quenches the circulating current. This behavior was explained using the mean-field slave boson infinite Coulomb repulsion approximation, assuming that the system is a Fermi liquid that satisfies the Friedel-Langreth sum rule.

In our calculations we use parameter values that are compatible with the experimental situation. In particular, as we take the Coulomb interaction to be finite we have the appropriate energy scale for the Kondo temperature. Since we use a Lanczos diagonalization our analysis is restricted to $T=0$. For the dot with a fixed number of two electrons and total spin $S_D \sim 1$, we obtain an enhancement of the Kondo effect when the dot energy spacing is equal to the exchange interaction, at the singlet-triplet transition. In this case, the wire conductance is canceled due to strong interference effects. As the number of particles and spin of the dot are varied, the conductance goes from zero to e^2/h, according to the different regimes of the dot. We find stronger correlation for the $S=1$ Kondo regime than for the usual $S=1/2$. Our results are compatible with experimental observations of a system where the current goes through the dot.[7]

In order to be able to incorporate the physics associated with the singlet-triplet transition the dot is described by two levels. We allow it to have different states of charge, as it occurs in any experiment where the gate potential is varied. Part of the system, consisting of a cluster which includes the two-level dot, is exactly solved using a Lanczos algorithm[12] and then embedded into the rest of the wire. We show that, for reasonably reduced cluster sizes, due to the way in which the embedding is done, the results are independent of the cluster size.[13] As the diagonalization of an infinite cluster would give an exact result for the Hamiltonian taken, con-

vergence for the cluster sizes we use implies a numerically exact result for our model. We calculate the states of charge and spin at the dot, the density of states (DOS) projected onto the QD, and the current circulating through the wire, as a function of the gate potential applied to the QD and of its energy-level energy spacing.

The system is represented by an Anderson impurity first-neighbor tight-binding Hamiltonian. In a cluster of $2(M+1)$ sites (the number is taken to be even to maintain the cluster symmetry), the two states of the QD are denoted by α and β and the other $2M+1$ sites belonging to the wire numbered from $-M$ to M. The QD is connected to site 0. The total Hamiltonian can be written as

$$H=\sum_{\substack{r=\alpha,\beta\\ \sigma}}(V_g+\epsilon_r)n_{r\sigma}+\frac{U}{2}\sum_{\substack{r=\alpha,\beta\\ \sigma}}n_{r\sigma}n_{r\bar{\sigma}}+U\sum_{\sigma\sigma'}n_{\alpha\sigma}n_{\beta\sigma'}$$

$$+J(S_\alpha S_\beta)+t'\sum_{\sigma}[(c_{\alpha\sigma}+c_{\beta\sigma})c^{+}_{0\sigma}+\text{c.c.}]$$

$$+\sum_{i,\sigma}t_{ij}c^{+}_{i\sigma}c_{j\sigma}, \tag{1}$$

where U, J, and V_g are, respectively, the Coulomb repulsion in the dot, the exchange energy, and the gate potential applied to the two dot states with energies ϵ_α and ϵ_β. The hopping matrix elements between the dot states and the wire state at site 0, taken for simplicity to be equal, are given by t', and the $t_{ij}=t$ are the nearest-neighbor hopping elements within the wire. The Fermi energy is taken to be $\epsilon_F=0$. The dot levels, with energy spacing $\Delta=\epsilon_\alpha-\epsilon_\beta$, interact through the exchange coupling and can be changed continuously by varying the gate potential applied to the QD.

To obtain the properties of the system we calculate the one-particle Green functions G_{ij}. They are made 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. In order to guarantee consistency the charge of the dressed and undressed clusters is imposed to be the same. We calculate $\hat{g}$ as a combination of the Green function of n and $n+1$ electrons with weight $1-p$ and p,$\hat{g}=(1-p)\hat{g}_n+p\hat{g}_{n+1}$. The charge of the undressed cluster is $q_c=(1-p)n+p(n+1)$.[14] The charge of the cluster when linked to the leads can be expressed as $Q_c=2\int_{-\infty}^{\epsilon_F}\Sigma_i \text{Im}Gii(\omega)d\omega$, where i runs over all the cluster sites. This equation plus the condition $q_c=Q_c$ constitute a system of two equations which requires a self-consistent solution to obtain p and n. Using the Keldysh[15] formalism the conductance can be written as

$$G=\frac{e^2t^2}{h}|G_{00}|^2[\rho(\epsilon_F)]^2, \tag{2}$$

where G_{00} is the Green function of the wire site connected to the dot, while $\rho(\epsilon_F)$ is the density of states at the Fermi level at the first neighbors of site 0, when disconnected from it.

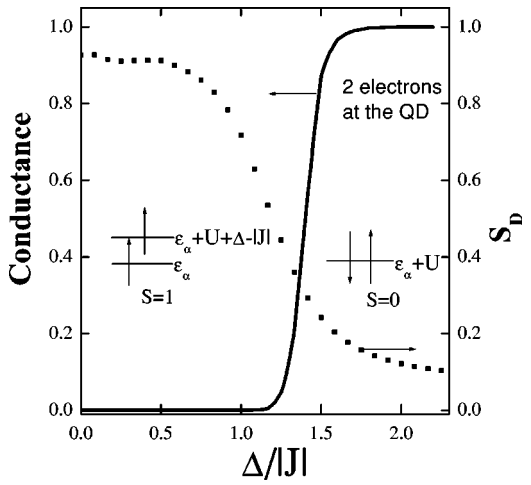

FIG. 1. Conductance in units of e^2/h (continuous line) and QD total spin (squares) as a function of $\Delta/|J|$, for two electrons at the dot. The singlet-triplet transition corresponds to $\Delta/|J|=1$.

We discuss first the transport properties in the wire as a function of the QD energy spacing Δ, maintaining fixed the number of electrons at the dot; then, for a fixed value of Δ, we vary the number of particles at the QD by changing V_g. All energies are in units of U. We take $\Gamma=t'^2/W=0.08$, where W is the wire bandwidth, a value compatible with experiments.[5]

In order to analyze the singlet-triplet transition we fix the gate potential such that the dot is charged with two particles. The results for the current in the wire and for the total spin at the dot are presented in Fig. 1 as a function of $\Delta/|J|$. As Δ increases, the QD spin goes from a triplet to a singlet state. The conductance is a function which interpolates between the value for a perfect insulator (for $S_D\sim 1$) and for a perfect conductor (for $S_D\sim 0$). The transition from one behavior to the other is reflected in a rapid increase of the current for $\Delta/|J|>1$ due to the weakening of the Kondo effect and the consequent decrease of the scattering of the conduction electrons. This result is the counterpart obtained by the poor man's scaling calculation in the case of a system in which the current goes through the dot itself.[8,9] To incorporate the temperature in the calculation would require a huge computational effort, outside our capabilities. However, it is possible to obtain the Kondo temperature as a function of Δ in an approximate way from the density of states of the system. We find that the imaginary part of the many-body contribution to the self-energy of the Green function at the dot, in the vicinity of the Fermi level, is proportional to $(w-E_f)^2$, a characteristic of a Fermi liquid. The density of states around E_f, depicted in the lower inset of Fig. 2, can be well represented by a Lorentzian, $Z(T_k)/E-\epsilon_F+iT_k$, where the Kondo weight $Z(T_k)$ is a function of the Kondo temperature and the width coincides with T_k.[16] Based on these considerations we obtain the curve of Fig. 2 showing that T_k increases with Δ, has its maximum at the singlet-triplet transition, and decreases rapidly for $\Delta/|J|>1$. This is compatible with experimental results for the conductance through a dot embedded into a wire as a function of the magnetic-field

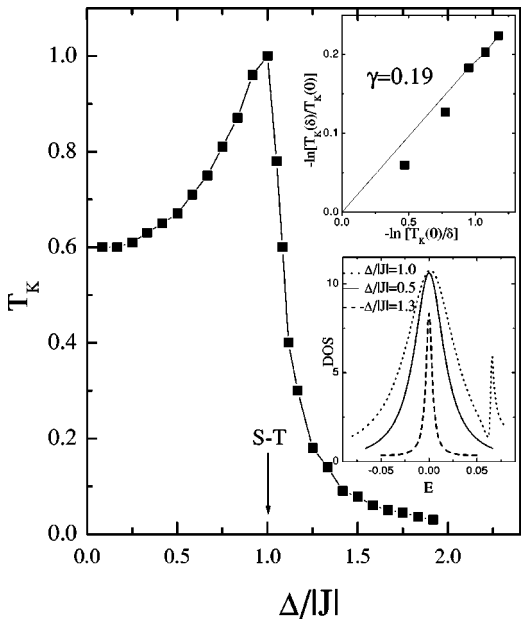

FIG. 2. Kondo temperature, normalized to one at the singlet-triplet transition, as a function of $\Delta/|J|$. In the upper inset the exponent γ is obtained from the logarithm of the equation $T_K(\delta) = T_K(0)[T_K(0)/\delta]^{\gamma}, \delta = |J| - \Delta$; the lower inset shows the Kondo peak in the DOS, for $\Delta/|J| = 0.5$, 1.0, and 1.3.

energy splitting,[7] where the Kondo effect is strong and only clearly observed near the singlet-triplet transition.

For the limit $T_k(0) \ll \delta$, where $\delta = |J| - \Delta$, we have obtained a power-law dependence of the Kondo temperature on δ,

$$T_K(\delta) = T_K(0)\left[\frac{T_K(0)}{\delta}\right]^{\gamma}. \tag{3}$$

In the upper inset of Fig. 2 we show this relation in a logarithmic scale from which we obtain an exponent $\gamma = 0.19$. We have found that this value is not universal and depends on Γ. A similar power law has been obtained for a different geometry where the current goes through the dot, although the Kondo temperature has been defined in a different way.[8,9]

With the purpose of studying other experimentally accessible regimes we fix the dot level energy spacing and calculate the current in the wire for all possible states of charge and spin of the dot by varying continuously the number of electrons in the QD. In this way we are able to study the mixed-valence regime and the evolution of the spin state of the QD from the doublet ($S = 1/2$), when the dot has an odd number of electrons, to the triplet ($S = 1$) or the singlet ($S = 0$), when the number of electrons in the dot is even.

The results as a function of V_g are displayed in Fig. 3, for $\Delta/|J| = 1$. The wire conductance and the total spin and charge at the QD are shown in Figs. 3(a) and 3(b); the Kondo correlation, between the dot total spin and the spin of the conduction electrons at the neighboring site, $\langle \vec{S}_D \vec{S}_c \rangle$, as well as the spin correlation of the two states of the QD, $\langle \vec{S}_\alpha \vec{S}_\beta \rangle$, are shown in Fig. 3(c). Since we choose the lowest dot energy $\epsilon_\alpha = 0$, for $V_g > 0$ both dot levels are above the Fermi level and the charge at the dot is approximately zero. As V_g reduces, charge enters into the dot and the system goes through a charge fluctuation regime up to $V_g \sim -0.4$ where the dot has nearly one electron and a total spin $S_D \sim 0.4$. At this point the Kondo correlation has a local maximum. This situation corresponds to the usual $S = 1/2$ Kondo regime, which is reflected in the cancellation of the conductance due to strong scattering of the conduction electrons. As V_g continues to decrease the system goes again into a mixed-valence regime—the lowest level rearranges its charge between spin up and down and extra charge enters into the second dot level. The Kondo correlation diminishes and has a minimum around $V_g = -0.75$, where the current circulating along the wire acquires its maximum value. As charge keeps entering into the dot the Kondo correlation begins to increase again, reaching an absolute maximum value at $V_g \sim -1.9$, when there are just two electrons at the dot and the singlet and triplet states are degenerate. At this point the total dot spin as well as the dot spin-spin correlation $\langle \vec{S}_\alpha \vec{S}_\beta \rangle$ have maximum values, and the current cancels again. The $S = 1$

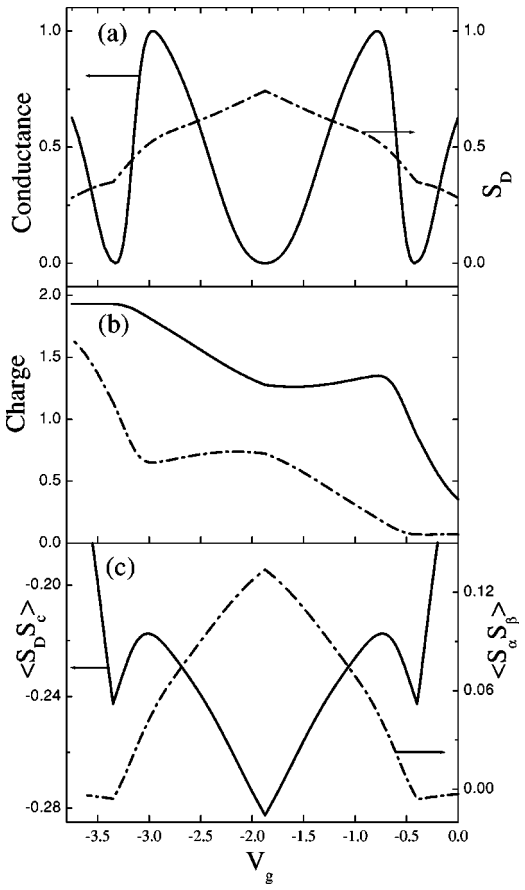

FIG. 3. Conductance, spin, charge, and spin correlation as a function of V_g, for $\Delta/|J| = 1$. (a) Conductance (continuous line) in units of e^2/h and QD total spin (dash-dotted line); (b) charge in state α (continuous line) and in state β (dash-dotted line) in units of the electronic charge; (c) Kondo spin correlation $\langle \vec{S}_D \vec{S}_c \rangle$ (continuous line) and spin correlation between the two states of the QD $\langle \vec{S}_\alpha \vec{S}_\beta \rangle$ (dash-dotted line).

Kondo regime is responsible for this strong scattering effect. As reflected on the curve for conductance as a function of V_g the system has electron-hole symmetry with respect to $V_g = -1.9$.

Notice the strong correlation between the behavior of the current and of the Kondo spin correlation as V_g is varied. The bigger the Kondo correlation, the stronger the interference effects which cause the degradation of the current. Moreover, the Kondo correlation is stronger for the dot with two electrons and a maximum total spin $S_D \sim 1$, in the singlet-triplet transition, than for the usual case of $S_D \sim 1/2$, as shown in Fig. 3(c). This result is compatible with the measurements[7] of the conductance as a function of gate voltage in a system with the dot embedded into the wire, where the $S=1/2$ Kondo effect is much weaker, and almost not observable, than the $S=1$ Kondo effect in the singlet-triplet transition. Notice, also, the way in which the charge enters into the dot, continuously rather than in steps as in the Coulomb blockade regime, reflecting the gradual way the Kondo peak moves through the Fermi level as V_g is varied.

In summary, we present numerically exact results for the transport properties of a system consisting of a two-level quantum dot laterally coupled to a wire, where the dot energy spacing is varied in order to mimic the effect of a magnetic field. In the special case where the dot has an integer number of electrons equal to two, the wire conductance shows a crossover behavior from a perfect insulator to a perfect conductor for values of the energy spacing such that the dot singlet and triplet spin states are nearly degenerate. Our results show a maximum Kondo temperature at this singlet-triplet transition and a nonuniversal power-law dependence of T_K with the dot energy splitting. We have also explored the intermediate-valence regime by varying the gate potential applied to the dot. We study the influence of the different states of charge and spin of the dot upon the wire conductance. As the dot occupation is changed the Kondo correlation is found to be stronger when the dot has $S_D \sim 1$ and is in the singlet-triplet transition than for the usual $S_D \sim 1/2$ Kondo regime. The dependence of the conductance on the gate potential as well as on the dot level splitting is in agreement with the experiments[7] done in a system where the current goes through the dot. We hope that our results stimulate measurements of the transport properties in a wire with the dot in a lateral configuration, as discussed in this work.

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