Phase effects on the conductance through parallel double dots

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Phase effects on the conductance of a double-dot system in a ring structure threaded by a magnetic flux are studied. The Aharonov-Bohm effect combined with the dot many-body charging effects determine the phases of the currents going through each arm of the ring. The cases for zero magnetic flux or half a quantum of flux are discussed in detail. It is shown that, depending upon the magnetic flux and the state of charge of the dots, controlled by gate potentials, the dephasing of the upper and lower arm current gives rise to a $S=1/2$ or $S=1$ Kondo regime.

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I. INTRODUCTION

In the last years attention has been focused on the properties of double quantum dot systems[1] since they are expected to be basic building blocks for quantum computing.[2] In this context mesoscopic coherent transport is a key phenomenon that can probe entanglement[3] and phases accumulated by electrons traversing the system. The phase-coherent transport effects can be analyzed by embedding the dots into an Aharonov-Bohm ring threaded by a magnetic flux and connected to leads. Theoretical[4] and experimental[5] works have discussed the transmission phase shifts of single and double quantum dot systems in the Coulomb blockade regime. More recently the effect of Kondo correlation on the transmission phase of a quantum dot has been measured[6] and theoretically discussed.[7–12]

The two quantum dot system is particularly interesting since, when each dot is inserted into one arm of a ring connected to leads, as represented in Fig. 1, it presents two paths for the electrons to go through, producing interferences that depend upon the phase in each arm. The effect of the interferences on the spectral densities of such a system has been studied,[13] taking the intra- and interdot Coulomb repulsion to be infinite. This limit restricts the study of the Kondo phenomenon and the phase-shift interference effects to a situation in which the number of electrons in the system cannot be greater than 1. However, depending on the magnetic flux enclosed by the ring, very interesting physics appear when both dots are charged and in the Kondo regime. Moreover, the general problem of the transmission phases in this system as the magnetic flux and the state of charge of the dots are varied has not been yet clarified. The dephasing between the two contributions to the current do not depend exclusively upon the state of charge of each dot, as a naive interpretation of the Friedel sum rule could predict. This is a consequence of the fact that the phases associated to the arms are not independent objects because one is renormalized by the other.[7,8]

The purpose of this paper is to contribute to the understanding of this problem. We discuss phase effects on the conductance of this system using an exact numerical diagonalization algorithm that provides only the ground state of the system. Our study is therefore restricted to zero temperature. This procedure permits us to take into account in an adequate way the interference effects due to the interaction between the two ring arms. Different Kondo regimes are accessed by varying the magnetic flux and the charge in the dots controlled by the gate potentials. The Aharonov-Bohm effect combined with the dot many-body charging effects determine the phases of the currents going through each arm of the ring. In order to have reliability in the numerical results, we adopt a dot-lead interaction such that the Kondo cloud is of the order of the cluster we exactly diagonalize.[14] In this case the plateau shape of the conductance, when the system is in the Kondo regime, is more like a Lorentzian. The conductance shows quite different behaviors for the magnetic flux $\Phi=0$ and $\Phi=\Phi_0/2$. In the first case the dots act coherently and the system is in a Kondo state of total spin $S\sim 1$ while in the second, the dots are uncorrelated and in a $S=\frac{1}{2}$ Kondo regime. For other fluxes the conductance shows intermediate behavior between these two extremes.

II. THEORY

An Anderson two-impurity first-neighbor tight-binding Hamiltonian represents the system shown in Fig. 1,

$$H=\sum_{\substack{r=\alpha,\beta\\ \sigma}}\left(V_r+\frac{U}{2}n_{r\bar{\sigma}}\right)n_{r\sigma}+t\sum_{i,j}c_{i\sigma}^{+}c_{j\sigma}+t'[e^{i(\pi/2)(\Phi/\Phi_0)}\times(c_{\alpha\sigma}^{+}c_{1\sigma}+c_{1\sigma}^{+}c_{\beta\sigma}+c_{\beta\sigma}^{+}c_{\bar{1}\sigma}+c_{\bar{1}\sigma}^{+}c_{\alpha\sigma})+\text{c . c . }], \quad (1)$$

where V_α and V_β are the gate potentials applied to the dots,

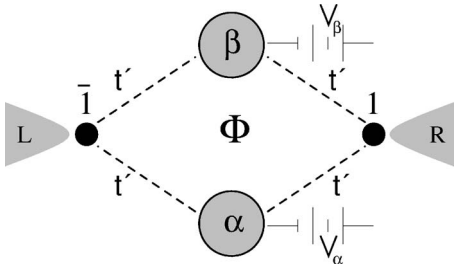

FIG. 1. Aharonov-Bohm interferometer with two embedded quantum dots, threaded by a magnetic flux Φ, connected to leads.

U is the Coulomb repulsion, considered to be equal for the two dots, and Φ is the magnetic flux threading the ring. The parameters t' and t are, respectively, the hopping matrix element between the dots and their neighbors and between sites in the leads. The one-particle Green functions G are imposed to satisfy a Dyson equation $\hat{G}=\hat{g}+\hat{g}\hat{T}\hat{G}$ where $\hat{g}$ is the Green-function matrix of a cluster containing the ring with the dots and a number of atoms of each lead and $\hat{T}$ is the matrix Hamiltonian that couples the cluster to the rest of the system. The undressed Green function $\hat{g}$ is calculated using the cluster ground state obtained by the Lanczos method. This approximation[14] has been shown to be very accurate when the cluster is of the size of the Kondo cloud hv_F/T_K, where v_F is the Fermi velocity and T_K is the Kondo temperature, although it gives qualitatively reliable results even for smaller clusters, compatible with the Friedel sum rule and the Fermi-liquid properties of the system.

The conductance of the system is defined as $G=dI/dV$ where I is the current that flows from the left lead, at a chemical potential μ_L, to the right lead, at a chemical potential μ_R ($\mu_L>\mu_R$). Denoting by $L(R)$ the site at the left (right) lead nearest neighbor to site $\bar{1}$ (1), as shown in Fig. 1, the total current along the system can be written as[15,16]

$$I=\frac{2e}{h}t_{1R}\int_{-\infty}^{\infty}d\omega[G_{1R}^{-+}(\omega)-G_{R1}^{-+}(\omega)] \tag{2}$$

where $t_{1R}=t$ is the hopping between two nearest-neighboring sites in the leads, in our case sites 1 and R, and the G^{-+} are nonequilibrium Green functions defined as $G_{l,j}^{-+}(\omega)=i\langle c_j^+c_l\rangle_\omega$, whereas c_j^+ and c_j are, respectively, the creation and annihilation operators for electrons. To obtain these functions in the context of the Keldysh formalism the system is partitioned in such a way that one subsystem is in thermodynamic equilibrium with the left reservoir and the other with the right one so that the advanced and retarded equilibrium Green functions can be calculated. The Green functions of the complete nonequilibrium system are expanded in terms of the ones in equilibrium taking the connection between the two subsystems as a perturbation. In our case it is more convenient to partition the system at two points, between sites L and $\bar{1}$ and sites 1 and R, so that site $L(R)$ is at the chemical potential $\mu_L(\mu_R)$ while the ring sites $\bar{1}$, 1 and the two dots α and β can be assumed to have no electrons. Since inelastic processes are not taken into account[16] and the Hamiltonian describing the leads is noninteracting the G^{-+} can be expressed in terms of the dressed retarded and advanced Green functions, G^r and G^a, as[17]

$$G^{-+}=(1+G^r\Sigma^r)g^{-+}(1+\Sigma^aG^a), \tag{3}$$

where g^{-+} is the density of states of the disconnected subsystems multiplied by the Fermi distribution function and $\Sigma^r=\Sigma^a=t$ is the interaction that restitutes the nonequilibrium situation. Since $g_{i,j}^{-+}=0$ for $i,j=\bar{1}$, 1, α, and β, G_{1R}^{-+} and G_{R1}^{-+} are given by

$$G_{1R}^{-+}(\omega)=G_{11}^rtg_R^{-+}+t^2[G_{11}^rg_R^{-+}G_{1R}^a+G_{1\bar{1}}^rg_L^{-+}G_{\bar{1}R}^a] \tag{4a}$$

and

$$G_{R1}^{-+}(\omega)=g_R^{-+}tG_{11}^a+t^2[G_{R1}^rg_R^{-+}G_{11}^a+G_{R\bar{1}}^rg_L^{-+}G_{\bar{1}1}^a] \tag{4b}$$

where

$$g_i^{-+}(\omega)=\rho_i(\omega)f_{\mu_i}(\omega),\quad i=L,R. \tag{5}$$

$\rho_{L(R)}$ is the density of states at the disconnected lead site $L(R)$ and $f_{\mu_{L(R)}}$ is the corresponding Fermi distribution function.

Substituting Eqs. (4) into Eq. (2), after some manipulations we arrive at a simple expression for the total current in the system,

$$I=\frac{2et^4}{h}\int_{-\infty}^{\infty}d\omega|G_{\bar{1}1}^r|^2\rho_R(\omega)\rho_L(\omega)[f_{\mu_L}-f_{\mu_R}] \tag{6}$$

that at $T=0$ reduces to

$$I=\frac{2et^4}{h}\int_{\mu_R}^{\mu_L}d\omega|G_{\bar{1}1}^r|^2\rho_R(\omega)\rho_L(\omega). \tag{7}$$

For infinitesimal bias voltage the differential conductance of the system reads,

$$\mathbf{G}=\frac{2e^2}{h}t^4|G_{\bar{1}1}^r|^2\rho^2(\epsilon_F), \tag{8}$$

where we have supposed that the density of states of the left and right contacts are equal, $\rho_R(\omega)=\rho_L(\omega)=\rho(\epsilon_F)$, and all the quantities are calculated at the Fermi energy.

III. RESULTS AND DISCUSSIONS

The transport properties are studied as a function of the gate potentials applied to the dots, for two values of the magnetic flux $\Phi=0$ and $\Phi=\Phi_0/2$. Taking the energies in units of the Coulomb interaction U, we set the leads bandwidth $W=8$ and $\Gamma=t'^2/W=0.05$. The Fermi level is chosen to be $\epsilon_F=0$. The conductance obtained from Eq. (8) for two values of the magnetic flux, $\Phi=0$ and $\Phi_0/2$, is represented in Fig. 2 as a function of the energy of the dot levels. It results to be weakly dependent upon the magnetic flux in the regions of the parameter space where only one dot is active so that current flows essentially along one arm of the ring. It possesses the characteristics of the one-dot conductance with a width, as a function of the gate potential, of the order of U due to the Kondo effect of the charging dot. On the other hand, when $V_\alpha\sim V_\beta$, the conductance is strongly dependent upon the magnetic flux, showing special different features for the cases $\Phi=0$ and $\Phi_0/2$. Let us focus on the region $-1<V_\alpha, V_\beta<0$ of Fig. 2. The differences in the conductance between these two cases are more striking when the dot level energies are similar, $\Delta E\sim 0$ (diagonal continuous line). In this case the two arms are at resonance since both dots are in the Kondo regime. For $\Phi=0$ the two arm currents are in phase and interfere constructively and the conductance has one broad peak. As the magnetic flux is turned on, the currents along the two arms are no longer in phase and the

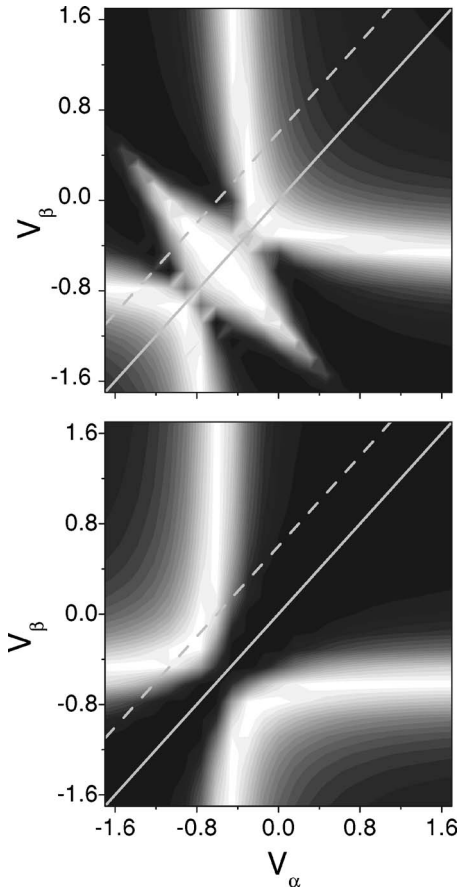

FIG. 2. Conductance (white, maximum; black, minimum) as a function of the gate potentials at the dots, V_α and V_β. $\Phi=0$ (upper panel), $\Phi=\Phi_0/2$ (lower panel); $\Delta E=0$ (continuous line), $\Delta E=0.6$ (dashed line).

transport properties change qualitatively. For $\Phi=\Phi_0/2$, the current arm amplitudes are out of phase and the conductance for $\Delta E=0$ cancels out for all values of the gate potentials, as shown in Fig. 2 (lower panel).

For small values of ΔE, the conductance presents two peaks for $\Phi=\Phi_0/2$, and three for $\Phi=0$, the most interesting case. The spin-spin correlation, the charge at the dots, and the conductance are displayed in Fig. 3 as a function of V_α for $\Delta E=0.6(V_\alpha=V_\beta-0.6)$, corresponding to the dashed line in Fig. 2. We first analyze the case $\Phi=0$. As V_α decreases from the value 0.5 and charge begins to enter into dot α its spin gets negatively correlated to the conduction electrons. The dot is in the Kondo regime and the conductance increases up to a quantum of conductance maximum around $V_\alpha=-0.2$. At $V_\alpha=-0.5$ the conductance cancels out and the various spin-spin correlations change abruptly. In the region $-0.5<V_\alpha<-1.1$ the Kondo correlation of both dots, $\langle\vec{S}_\alpha\vec{S}_c\rangle$ and $\langle\vec{S}_\beta\vec{S}_c\rangle$, gets stronger [Fig. 3(b)] and the conductance grows again reaching a second maximum at the electron-hole symmetry condition, $V_\alpha=-0.8$, where the system has just two electrons.

The most interesting aspect of the conductance is that the lateral and the central peaks are due to different Kondo regimes. This conclusion can be reached by analyzing the spin-

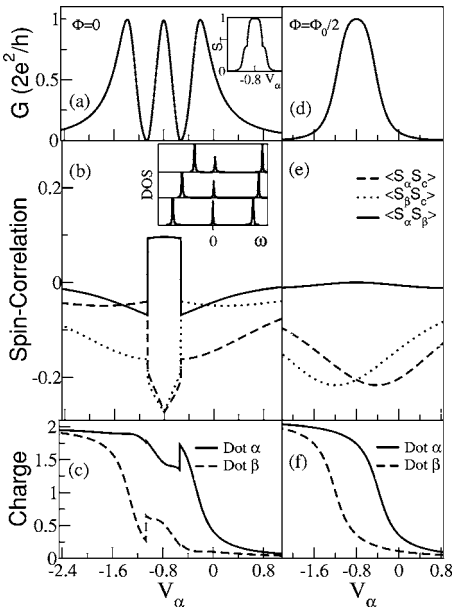

FIG. 3. Conductance, spin correlation, and charge occupancy for $\Delta E=0.6(V_\beta=V_\alpha+0.6)$, as a function of V_α. $\Phi=0$ (left) and $\Phi=\Phi_0/2$ (right). Conductance (a) and (d); spin correlation (b) and (e): $\langle\vec{S}_\alpha\vec{S}_\beta\rangle$ (continuous line), $\langle\vec{S}_\alpha\vec{S}_c\rangle$ (dashed line), and $\langle\vec{S}_\beta\vec{S}_c\rangle$ (dotted line); charge occupancy (c) and (f): dot α (continuous line), dot β (dashed line). The insets in (a) shows the total dot spin and in (b) the Kondo peak ($\omega=0$) in the DOS for $V_\alpha=-0.6,-0.7,-0.8$.

spin correlations of the two dots, the total dot spin, and the density of states (DOS) projected on the two dots.

When the gate potential is reduced from $V_\alpha=0.5$, dot α enters into resonance and in the Kondo regime, while the other is well above the Fermi level and without charge. The current circulates only along dot α giving rise to the first peak of the conductance. It is a typical one-dot $S=1/2$ Kondo effect. As the gate potential is further reduced the electronic charge begins to drop also into dot β, giving rise to a new Kondo peak that, due to level repulsion, pushes the Kondo peak related to dot α towards values below the Fermi level. This reduces the DOS at the Fermi level, diminishing the conductance of the system, and raises the dot α charge to a value above unity [Fig. 3(c)], increasing the energy of the ground state due to Coulomb repulsion. As a consequence, a level crossing takes place and an excited state with less charge at dot α becomes the new ground state of the system. This process gives rise to an abrupt reduction of the dot charge and to a restoration of the Kondo resonance at the Fermi level. While in the gate potential region corresponding to the original ground state the two dots are weakly antiferromagnetic correlated, in this new ground state they adopt a coherent behavior and have a strong ferromagnetic spin-spin correlation, $\langle\vec{S}_\alpha\vec{S}_\beta\rangle$, independent of the gate potential, and a total spin $\langle S_T\rangle\sim 1$, as shown in Figs. 3(b) and 3(a). The system is in a $S=1$ Kondo regime. This is confirmed in the inset of Fig. 3(b) where the DOS close to the Fermi level shows the Kondo peak pinned to the Fermi level as the gate potential varies and the two Coulomb blockade satellites.

The two crossing states have opposite parity. The crossing and the abrupt change of the physical properties are derived

from the fact that the system is spatially invariant under reflection so that parity is a good quantum number. When this symmetry is broken by introducing a small magnetic field (note that we are analyzing the case $\phi=0$) or an asymmetric perturbation to the Hamiltonian, the ground state results to be a linear combination of these two previous states. In this case the level crossing transforms into a crossover behavior and the abrupt changes of the physical quantities are eliminated. This phenomenon is enhanced when the interaction among the dots and the conduction electrons is increased. When this interaction is large enough, the Kondo cloud is reduced to the size of the cluster we exactly diagonalize. In this region of the parameter space, our approximation is almost numerically exact and independent of the cluster size we adopt for sizes greater than the Kondo cloud.

The physics of the $\Phi=\Phi_0/2$ case is diverse from that previously discussed. In this situation the dot spins are weakly correlated while each dot is independently Kondo correlated to the electrons of the leads, as appears in Fig. 3(e). This different behavior can be clarified by a perturbation-theory argument. The effective correlation between the dots can be obtained by taking the nondiagonal matrix elements that connect the dots to the rest of the circuit, t', as a perturbation. Due to the system topology it is clear that to get the dominant contribution to the effective interdot interaction it is necessary to go to fourth order in perturbation theory. In this case, while for $\Phi=0$ the contributions that go from one dot to the other and return along the same path sum-up with the circulating contributions, for $\Phi=\Phi_0/2$ these two contributions, having opposite signs, tend to cancel each other, giving rise to a weak interdot correlation. For small ΔE the conductance [Fig. 3(d)] possesses only one peak that develops into two as ΔE increases. The charge at the dots has a smooth dependence upon the gate potential, as shown in Fig. 3(f).

The quantum interference between the electrons going along the two ring arms depends on the relative phases of the transmissions through these two paths and cannot be obtained through the current that is proportional to the square modulus of $G^r_{\bar{1},1}$, as shown in Eq. (7). These phases can, however, be made explicit by analyzing the relation between the Green function $G^r_{\bar{1},1}$ and the Green functions $G^r_{\alpha,1}$ and $G^r_{\beta,1}$ that represent the contributions from the ring arms containing dots α and β, respectively. Using the equation of motion for the Green functions, $G^r_{\bar{1}1}$ satisfies the exact relationship,

$$G^r_{\bar{1},1} = g_{\bar{1}}(t^*_\Phi G^r_{\alpha,1} + t_\Phi G^r_{\beta,1}), \tag{9}$$

where $g_{\bar{1}}$ is the diagonal element of the retarded Green function of the disconnected lead at the site $\bar{1}$. Since we are interested in phase differences we can take the contribution from arm α as a reference and write the total transmission as

$$|G^-_{\bar{1},1}|^2 = |A_\alpha + A_\beta e^{i(\phi_{\alpha,\beta})}|^2, \tag{10}$$

where A_α and A_β are, respectively, proportional to the modulus of $G^r_{\alpha,1}$ and $G^r_{\beta,1}$, and $\phi_{\alpha,\beta}$ is their phase difference. It is important to notice that $G^r_{\alpha,1}$ and $G^r_{\beta,1}$ incorporate all the renormalization of one arm due to the existence of the other. As a consequence, the phase of each trajectory is a function not only of its own dot charge but also of the charge of the other dot, and depends as well upon the topology of the whole system.[7]

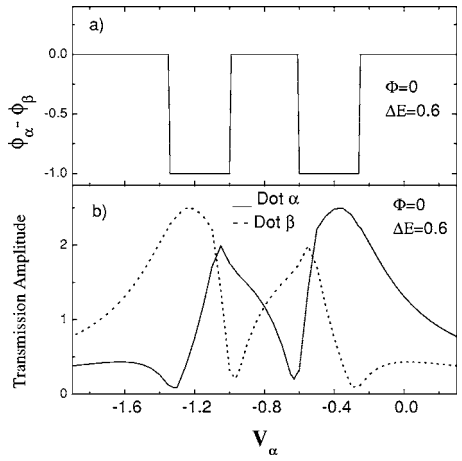

FIG. 4. Transmission through the two ring arms as a function of V_α, for $\Phi=0$ and $\Delta E=0.6$. (a) phase difference (units of π); (b) modulus (arbitrary units).

The results for the case $\Phi=0$ and $\Delta E=0.6$ are shown in Fig. 4. The calculated phase difference oscillates between two values, $\phi_{\alpha,\beta}=0$ or π, as the state of the dot charges changes by the application of gate potentials. This is in agreement with the Onsager relation that predicts, for a system that possesses a closed geometry like ours, that the conductance is an even function of the applied magnetic flux threading it. The calculated transmission amplitudes are also shown in Fig. 4 as a function of the gate potential for the case $\Phi=0$, $\Delta E=0.6$. These results help in the understanding of the dependence of the total current with gate potential, shown in Fig. 3(a). When the transmission amplitudes are equal, $A_\alpha=A_\beta$, the conductance cancels or has a maximum depending upon the phase difference being $\phi_{\alpha,\beta}=\pi$ ($V_\alpha=-0.5$ and -1.1) or $\phi_{\alpha,\beta}=0$ ($V_\alpha=-0.8$), respectively.

IV. CONCLUSIONS

We have studied a double dot system in a ring threaded by a magnetic flux and connected to leads. The cases $\Phi=0$ and $\Phi_0/2$ are discussed. It is shown that the dephasing of the upper and lower arm current determines whether the system is in a $S=1$ Kondo regime, when the two dots behave coherently, or in a $S=1/2$ Kondo regime, when they are uncorrelated. A recent experiment on Pt nanocontacts has shown that their electronic transports are strongly modified by the presence of hydrogen.[18] It has been theoretically shown[19] that this system has a topology similar to the one studied in this work, where the hydrogens play the role of the quantum dots. Due to the large electronic correlation at the hydrogens and the strength of the hydrogen Pt interactions, a Kondo system with a small screening length could be expected. We believe it could be a good candidate to study the properties we analyzed in this work.

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