Transport through Quantum Dots in Mesoscopic Circuits

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We study the transport through a quantum dot, in the Kondo Coulomb blockade valley, embedded in a mesoscopic device with finite wires. The quantization of states in the circuit that hosts the quantum dot gives rise to finite size effects. These effects make the conductance sensitive to the ratio of the Kondo screening length to the wires length and provide a way of measuring the Kondo cloud. We present results obtained with the numerical renormalization group for a wide range of physically accessible parameters.

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Since the pioneer work of Goldhaber-Gordon and coworkers reporting the observation of Kondo effect in a single quantum dot (QD) [1], many different circuit and dot configurations have been designed and studied [2]. In a single electron transistor or QD built on a semiconductor heterolayer, the most relevant parameters can be controlled by applying voltages. The possibility of their continuous variation allows one to investigate different regimes with different numbers of electrons localized in the dot [3]. States with a well-defined number of electrons tend to be stabilized by the Coulomb interaction, a phenomenon known as Coulomb blockade. When an odd number of electrons is stable in the dot and the total spin is $S = 1/2$, the coupling with the leads gives rise to the usual Kondo effect. The Kondo effect is the magnetic screening of the dot spin by the electrons of the host [4]. The screening occurs by the formation of a spin singlet involving the dot spin and the host electron's spins. This screening is nearly fully developed below a characteristic temperature T_K known as the Kondo temperature. The size of the screening cloud, the spatial extension of the singlet wave function, is the Kondo screening length $\xi_K \approx \hbar v_F/T_K$ where v_F is the Fermi velocity. For a typical QD the Kondo temperature T_K is of the order of magnitude of 1° and the Kondo screening length can be up to 1 μm. A logical step in the development of molecular electronics is the connection of quantum wires to single electron transistors to be used as building blocks. The reduction of the quantum wires dimensions down to the micron length scale may change the system properties. For such devices to be useful, a detailed knowledge of the behavior of the transmission phase shift and the conductance through this system is needed.

In GaAs circuits with a QD, the smallness of T_K makes it possible to alter the Kondo ground state by finite size effects. It was shown that whenever the characteristic size of the system is reduced and the mean level spacing Δ becomes of the order of or larger than T_K, finite size effects become important [5–9]. Then, in any nanoscopic system with a QD coupled to one dimensional leads or wires of the order of 1 μm of length, the Kondo effect may be subject to size effects. Based precisely on these effects, Simon and Affleck made two proposals to measure the Kondo screening length [8,9]. The first one concerns a closed loop with a QD. The persistent current induced by a magnetic flux threading the ring is sensitive to the screening length and is reduced when the circumference of the ring is smaller than ξ_K. The second proposal, which is also the subject of the present work, considers a QD coupled to mesoscopic leads.

In what follows we study a QD attached to quantum wires as schematically shown in Fig. 1(a). By a quantum wire we mean a narrow wire with a small number of channels participating in the conductance. The wires are weakly coupled at one end to the QD and at the other to three dimensional macroscopic contacts that act as a reservoir. The Hamiltonian of the system is then given by

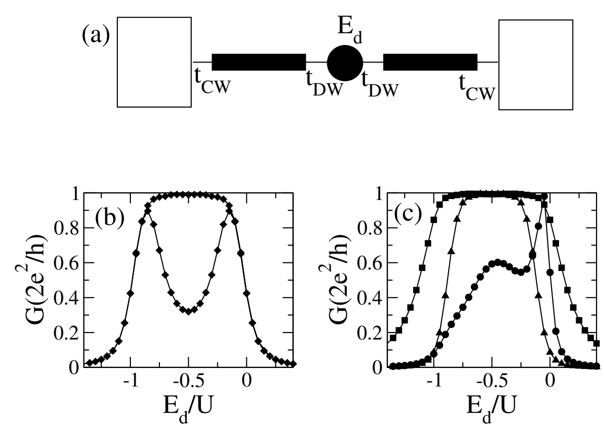

FIG. 1. (a) Mesoscopic circuit with an embedded quantum dot. (b) Conductance as a function of the QD level position for a system with infinite wires ($t_{DW} = 0.14\, t_0$) and $U = t_0$. $T = 0$ (open diamonds) $T \simeq 10\, T_K^0$ (filled diamonds). (c) Zero temperature conductance as a function of the QD level position for a system with finite wires ($\Delta \simeq 10\, T_K^0$ and $t_{CW} = 0.6\, t_0$) and different values of ϵ_W: at-resonance (squares), off-resonance (triangles), and intermediate case $\epsilon_W = 0.4\, \Delta$ (circles).

$$H = H_D + H_W + H_C + H_{DW} + H_{CW}, \quad (1)$$

where the first two terms corresponding to the dot and wire Hamiltonians are

$$H_D = \sum_\sigma E_d d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow, \quad (2)$$

where $d_\sigma^\dagger$ creates an electron with spin σ and energy E_d in the quantized state of the QD and U is the Coulomb repulsion for electrons in this state,

$$H_W = \sum_{\eta,\sigma,n=1}^{N} \varepsilon_W c_{\eta n\sigma}^\dagger c_{\eta n\sigma} - t_0 \sum_{\eta,\sigma,n=1}^{N-1} [c_{\eta n\sigma}^\dagger c_{\eta(n+1)\sigma} + \text{H.c.}], \quad (3)$$

with $\eta = R, L$ denoting the right and left wires described by the conventional one dimensional tight binding model. For simplicity, as in Ref. [9], the contact Hamiltonian H_C describes two linear chains with a hopping matrix element t_0. The last two terms of the Hamiltonian describe the coupling of these three components: $H_{DW} = -t_{DW}\sum_{\eta,\sigma}(d_\sigma^\dagger c_{\eta 1\sigma} + \text{H.c.})$ and $H_{CW} = -t_{CW}\sum_{\eta,\sigma}(c_{\eta N\sigma}^\dagger a_{\eta 1\sigma} + \text{H.c.})$, where $a_{\eta 1\sigma}^\dagger$ creates an electron in the first site of the contact η. The parameters E_d and U can be estimated and related to a gate voltage using a capacitance model for the QD [10].

If $t_{DW} = t_{CW} = 0$ the wires are isolated and each energy spectrum corresponds to a set of N states. Around the Fermi energy these states are separated by a characteristic energy $\Delta \simeq \hbar v_F \pi/L \simeq 4t_0/N$ where $L = a(N-1)$ is the wire length and a the lattice constant. When the wires are connected to the contacts with a nonzero t_{CW}, the wire states become resonances of width γ. The local density of states at the wire end $\rho_W(\omega)$, consists of a collection of resonant states characterized by the two energy scales Δ and γ [7]. This structure of the system that hosts the QD may drastically change the Kondo screening and consequently the linear conductance of the circuit. Using the Keldysh formalism [11] the conductance can be put as follows:

$$G(T) = \frac{2e^2}{h} 2\pi \int d\omega \left[-\frac{\partial f(\omega)}{\partial \omega}\right] \Gamma(\omega)\rho_D(\omega), \quad (4)$$

where $f(\omega)$ is the Fermi function, $\Gamma(\omega) = \pi(t_{DW})^2\rho_W(\omega)$, and $\rho_D(\omega)$ is the QD spectral density [4]. This simple formula gives the conductance of the central part of the circuit: QD plus wires. It can be obtained calculating the current through the CW links [11] and expressing it in terms of the QD spectral density. The spectral densities are calculated using the numerical renormalization group (NRG) technique [12–14]. The linear conductance as function of E_d is shown in Fig. 1(b) for $t_{CW} = t_0$ corresponding to infinite wires ($L \to \infty$) without constrictions. At high temperatures two Coulomb peaks and the central Coulomb blockade valley are clearly observed. The Coulomb peaks are due to E_d or $E_d + U$ being aligned with the Fermi energy. The central valley, away from the Coulomb blockade peaks, has one electron localized at the dot and corresponds to the Kondo regime. As the temperature is lowered, the conductance at the central Kondo valley increases indicating the occurrence of the Kondo screening. In this case $\rho_W(\omega)$ is constant around the Fermi level and $\rho_D(\omega)$ develops a narrow Kondo resonance at the Fermi level. At zero temperature, at the center of the Kondo valley $2\pi\Gamma(E_F)\rho_D(E_F) = 1$, a situation known as the unitary limit, and the conductance is simply $2e^2/h$. For finite wires with a constriction ($t_{CW} < t_0$), the low temperature conductance shows finite size effects in the whole range of E_d as shown in Fig. 1(c). At these low temperatures, the conductance becomes sensitive to the relative position of the Fermi energy E_F and the structure of $\rho_W(\omega)$. We distinguish three cases: (i) the Fermi level lying at a wire resonant state, a maximum in $\rho_W(\omega)$ (the at-resonance case), (ii) exactly between two resonances, a minimum in $\rho_W(\omega)$ (the off-resonance case), and (iii) intermediate situations. As shown in 1(c) for the at-resonance and off-resonance cases, a conductance of $2e^2/h$ is obtained at the Coulomb blockade valley, while for intermediate situations strong anomalies are obtained. These results correspond to the low temperature limit, for $T > \Delta$ the structure of $\rho_W(\omega)$ becomes unimportant and all three curves of Fig. 1(c) collapse into a single one that reproduces the high temperature behavior of Fig. 1(b).

The behavior of the transmission close to the Coulomb peaks can be understood in terms of a simple single particle resonant state lying above (for $E_d \gtrsim 0$) or below (for $E_d \lesssim -U$) the Fermi energy. If $E_d \simeq -U/2$, the center of the Coulomb blockade valley, the behavior is dominated by the Kondo physics. Let us now concentrate on the Kondo regime ($E_d < 0$ and $E_d + U > 0$) and define a reference Kondo temperature T_K^0 [12] at the center of the valley ($E_d = -U/2$) of the system with infinitely long quantum wires ($L \to \infty$). If a system with finite wires is such that $T_K^0 \gg \Delta$, on the scale of the characteristic Kondo energy the host local density of states can be averaged to its mean value and the finite size effects are washed out for any temperatures $T \gtrsim T_K^0$. This means that as the temperature is lowered and the Kondo screening starts to develop, the finite size effects are unimportant. The Kondo peak in $\rho_D(\omega)$ keeps its width ($\sim T_K^0$) unchanged but it is modulated in the scale of Δ [7]. Conversely, if the system were such that $T_K^0 \ll \Delta$, we expect strong finite size effects both in the spectral properties and in the conductance at any temperature $T \lesssim \Delta$, i.e., even before the Kondo effect of the reference system starts to develop. For high temperatures $T > \Delta$, the finite size effects are washed out and the behavior of the system is independent of Δ.

In a circuit built on a semiconductor heterolayer, the position of E_F relative to the wire structure as well as the coupling to the reservoirs (t_{CW}) can be varied applying gate voltages [2]. In Fig. 2 the conductance as a function of temperature for different values of the parameters is shown. For an ideal coupling ($t_{CW} = t_0$) the conductance presents a universal behavior [solid line in Figs. 2(a) and 2(b)] and reaches the value $2e^2/h$. In what follows we analyze these results according to the position of the Fermi level relative to the structure of the wire density of states $\rho_W(\omega)$.

(i) At-resonance case.—The conductance obtained from Eq. (4) for a relatively long quantum wire with $T_K^0 \simeq 3\Delta$ is shown in Fig. 2(a) for different values of the wire-contact coupling strength t_{CW}/t_0. For $t_{CW} < t_0$, as T is lowered and approaches the energy scale Δ, the structure in $\rho_D(\omega)$ becomes relevant and the conductance departs from the $t_{CW} = t_0$ case. As $T \rightarrow 0$, the ideal value is recovered generating a minimum in the conductance. In the low temperature regime, the QD acts as a perfect link between the right and left wires creating a single wire of length $2L$. The at-resonance condition implies that the Fermi level is aligned with a wire state giving an ideal conductance. For short wires with $T_K^0 < \Delta$, the screening develops for temperatures $T \sim \Delta$ [6] and, for the parameters studied ($\gamma \lesssim \Delta$), the conductance is not very sensitive to the confinement effects [Fig. 2(b)]. In the regime $\gamma \ll \delta$ confinement effects are expected to be much stronger as shown in Ref. [9].

(ii) Off-resonance case.—For $T_K^0 > \Delta$ and low temperatures, the QD acts again as a perfect link, the resulting effective wire of length $2L$ has resonant states separated by $\Delta/2$, rather than by Δ, and one of them is aligned with E_F. Although the at-resonance and off-resonance spectral densities are different [7] the temperature dependence of the conductance is similar [Fig. 2(a)], in fact the product $\Gamma(\omega)\rho_D(\omega)$ has qualitatively the same structure in both cases giving a conductance that does not clearly distinguish the two situations. For $T_K^0 \ll \Delta$, as the temperature increases, the conductance departs from its low temperature value $G \sim 2e^2/h$ [Fig. 2(b)] at a very small temperature ($\ll T_K^0$) which can be identified as the off-resonance Kondo temperature of the system.

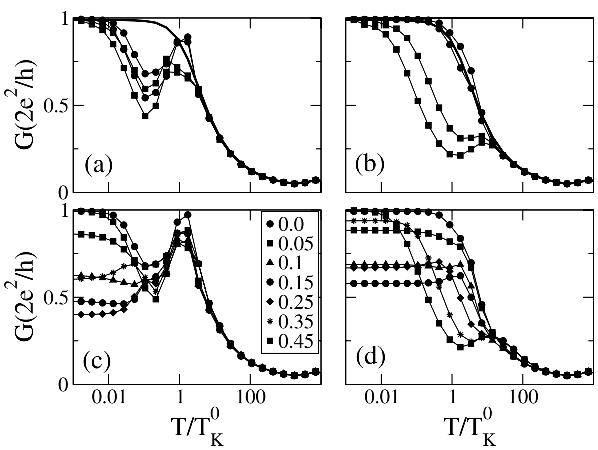

FIG. 2. Conductance as a function of temperature for a $\Delta \simeq T_K^0/3$ system (a) and (c), and a $\Delta \simeq 10\,T_K^0$ system (b) and (d). (a) and (b) At-resonance (circles) and off-resonance (squares) situations with $t_{CW} = 0.5\,t_0$ (filled symbols), and $t_{CW} = 0.6\,t_0$ (open symbols). (c) and (d) Conductance for different values of ϵ_W/Δ and $t_{CW} = 0.5\,t_0$. The other parameters are $E_d = -0.5\,U$, $U = t_0$, $T_K^0 \simeq 5 \times 10^{-5} t_0$, and $t_{DW} = 0.14\,t_0$ [$\gamma \sim T_K^0$ for (b) and (d)]. The solid line in (a) and (b) is the conductance for an infinite wire.

(iii) Intermediate case.—This situation where the Fermi level lies at an arbitrary position with respect to wire states generates a quite different behavior at low temperatures. The conductance never reaches the value $2e^2/h$ even for $T \rightarrow 0$ [see full symbols in Figs. 2(c) and 2(d)] essentially for reasons not involving interactions. Even with the QD behaving as a perfect link, the resulting wire states would not be aligned with E_F. For very long wires the conductance will be close to $2e^2/h$ in the temperature range $[\Delta, T_K^0]$.

The conductance as a function of ε_W for short ($T_K^0 < \Delta$) wires is shown in Fig. 3 for different temperatures. As discussed above, for low temperatures both the at-resonance and off-resonance cases give a conductance close to its ideal value $2e^2/h$, as shown in Fig. 3(a). In agreement with the results of Ref. [9], for intermediate temperatures ($T \sim T_K^0$), the off-resonance case gives a small conductance [see Fig. 3(b)]. This change of behavior looks like a change in the periodicity of G vs ε_W. Finally at high enough temperatures the amplitude of the oscillations goes to zero [see Fig. 3(c)]. For long wires, as can be deduced from Fig. 2(c), the intermediate regime is never observed, i.e., the system does not show a doubling of periodicity in G vs ε_W. In quantum wires with one channel, the condition $T_K^0 \gtrsim \Delta$ is equivalent to $L \gtrsim \xi_K^0$ and these results of $G(T)$ vs ε_W could be used to measure the Kondo screening length. The amplitude of the oscillations is given by the width of the wire levels γ and the periodicity by their spacing Δ. For short finite systems with weaker links to the leads, the oscillations with

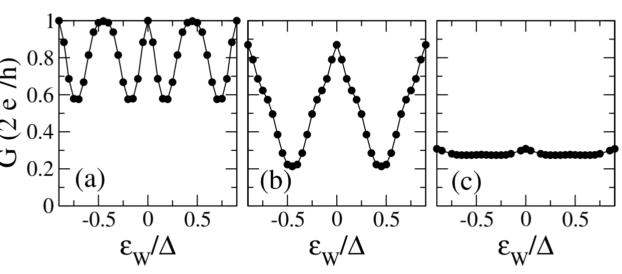

FIG. 3. Conductance as a function of ϵ_W for a $\Delta \simeq 10\,T_K^0$ system at $T = 0$ (a), $T \simeq T_K^0$ (b), and $T \simeq \Delta$ (c). $\varepsilon_W/\Delta = 0$, ± 0.5 correspond to the at-resonance and off-resonance cases, respectively.

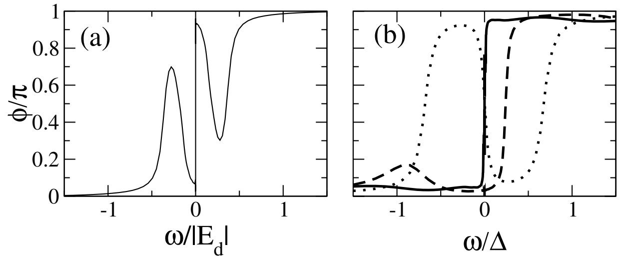

FIG. 4. (a) Zero temperature transmission phase shift for a $\Delta \simeq 10\, T_K^0$ system. (b) Low energy detail for the at-resonance case (dotted style), off-resonance case (solid style), and an intermediate case (dashed style).

maxima in the conductance separated by $\Delta/2$ will occur only at extremely low temperatures, and for intermediate temperatures only sharp peaks separated by Δ, in the at-resonance situation, are to be expected.

Finally we analyze the finite size effects on the phase shift introduced by the QD [15]. We define an energy dependent transmission as $t_\sigma(\omega) = \Gamma(\omega) G_{D\sigma}(\omega)$ where $G_{D\sigma}(\omega)$ is the retarded Green's function for a spin-σ electron in the QD level. The conductance as given by Eq. (4) is the thermal average of $-1/\pi \sum_\sigma \mathrm{Im}[t_\sigma(\omega)]$. The phase of the transmission for a spin-σ electron, $\phi_\sigma(\omega) = \arg[t_\sigma(\omega)]$, is shown in Fig. 4 for a system with finite wires. On a large energy scale, the low temperature behavior of $\phi_\sigma(\omega)$ qualitatively reproduces the results of Gerland *et al.* [16], it has a maximum (minimum) for $\omega \approx E_d/2$ $[\omega \approx (E_d + U)/2]$ and a large phase lapse for $\omega \approx 0$. This large phase lapse at zero frequency shows novel features due to the confinement effects. A zoom of the low frequency details in Fig. 4(b), shows the behavior of $\phi_\sigma(\omega)$ for $\omega \lesssim \Delta$ with a superstructure consistent with that of the Kondo peak. These effects in the transmission phase shift may affect the current in Aharonov-Bohm interferometers with two arms and an embedded QD.

In this Letter we have shown how the transport properties change when the QD is connected to finite quantum wires. In particular, the behavior of the system is very sensitive to the length of the quantum wires and to the position of the Fermi level relative to the structure of the local density of states. The confinement introduces anomalous features in the temperature dependence of the conductance and the energy dependence of the phase shift. For long wires ($T_K^0 > \Delta$), the Kondo effect is nearly fully developed at the temperatures the level spacing of the wires becomes a relevant energy scale. The finite size effects, as the nonmonotonous behavior of the conductance observed at low temperature are related to the quantization effects of the wire and not to the Kondo physics. The conductance oscillations observed at very low temperatures as a function of ϵ_F have the maxima with a period $\Delta/2$ that are related to the energy levels of the $2L$ length wire (the QD acts as a perfect link) being aligned with the Fermi level. For short wires, the Kondo effect is strongly dependent on the position of the Fermi level relative to the structure of the density of states. In the off-resonance situation, the Kondo effect is suppressed and the Kondo temperature is much smaller than that of the reference system. At intermediate temperatures the conductance at the off-resonance situation is small due to the Coulomb blockade and the oscillations have now the maxima only at the at-resonance situation, i.e., with a period Δ.

For single channel wires in the Kondo regime the response of the system depends on whether the Kondo screening length is shorter or larger than the quantum wire length. The finite size effects are also present in the Coulomb blockade peaks of the conductance, and in the general case they will manifest as an asymmetry between peaks.

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