Bohm-Aharonov and Kondo effects on tunneling currents in a mesoscopic ring

Maria A. Davidovich
Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, Caixa Postal 38071, 22452-970 Rio de Janeiro, Rio de Janeiro, Brasil

E. V. Anda
Instituto de Física, Universidade Federal Fluminense, Niterói, RJ Brasil, Avenida Litoranea s/n, Gragoatá, 24210-340 Niterói, Rio de Janeiro, Brasil

J. R. Iglesias
Instituto de Física, Univerisdade Federal do Rio Grande do Sul, Caixa Postal 15051, 91501-970, Porto Alegre, Rio Grande do Sul, Brasil

G. Chiappe
Departamento de Física, Universidad de Buenos Aires, Caixa Postal 1428-Nunez, Buenos Aires, Argentina
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We present an analysis of the Kondo effect on the Bohm-Aharonov oscillations of the tunneling currents in a mesoscopic ring with a quantum dot inserted in one of its arms. The system is described by an Anderson-impurity tight-binding Hamiltonian where the electron-electron interaction is restricted to the dot. The currents are obtained using nonequilibrium Green functions calculated through a cumulant diagrammatic expansion in the chain approximation. It is shown that at low temperature, even with the system out of resonance, the Kondo peak provides a channel for the electron to tunnel through the dot, giving rise to the Bohm-Aharonov oscillations of the current. At high temperature these oscillations are important only if the dot level is aligned to the Fermi level, when the resonance condition is satisfied. [S0163-1829(97)53012-8]

I. INTRODUCTION

The Bohm-Aharonov effect[1] has been the subject of many experimental and theoretical studies in the realm of mesoscopic transport. Under the effect of an external magnetic field the waves describing the currents propagating from left to right, along two branches of a mesoscopic ring, suffer a phase shift. According to this shift there is a constructive or destructive interference at the right contact of the device, which is reflected in the conductance as cycles of period $\phi_0 = hc/e$, depending on the magnetic flux ϕ encircled by the ring. This sensitivity of the interference pattern produced by the dephasing of the two waves can be exploited to study the nature of transport in a particular system. For example, recently the resonant tunneling of an electron going through a dot that belongs to one of the arms of a ring linked to two contacts has been measured[2] and theoretically studied.[3] From the experimental data it was possible to distinguish between coherent and sequential tunneling by studying the oscillations in the conductivity as a function of the magnetic flux threading the ring. Undoubtedly, a system of this kind is also extremely appropriate to study the effect of Coulomb repulsion on transport.

In the experiment mentioned[2] the system exhibits pronounced oscillations of the conductance when the gate potential on the dot is modified. The Coulomb blockade of an electron when it tries to go into a dot already occupied by another electron provides the theoretical explanation for the conductance oscillations. However, at low external applied potentials, when the system can be considered to be in equilibrium, another Coulomb repulsion effect, the Kondo[4] effect, shows up. Although its experimental detection is difficult[5] we believe that it can be clearly seen in a device of the kind described above, due to its sensitivity to interference effects. For temperatures below the Kondo temperature T_K the I-V characteristics should reflect this effect when the system operates in the so-called Kondo regime. This happens when the Fermi energy has an intermediate value between the energy of the localized level at the dot and the energy necessary to incorporate an extra electron to it.

The aim of this paper is to study the current going along a quantum dot in two different situations: at low temperature when the system is in the Kondo regime and at high temperature when the flowing charges are dominated by the resonant tunneling condition. We take advantage of the Bohm-Aharonov effect, which emphasizes the differences between the two regimes, by locating the dot in one of the arms of a ring connected to two contacts. A scheme of the ring with the dot is shown in Fig. 1. The ring is threaded by an external magnetic field and the dot is subjected to a gate potential. The electron-electron interaction gives rise to an Abrikosov-Suhl resonance or to Coulomb blockade behavior for temperatures below or above T_K, respectively. As we show below, these two situations are clearly distinguished in this Bohm-Aharonov device. The Kondo regime is characterized by a current that depends strongly upon the magnetic flux ϕ, due to interference between the waves going along the upper and the lower arms of the ring. This holds for a region of the parameter space (gate potential, Coulomb repulsion, and temperature) irrespective of the dot being in

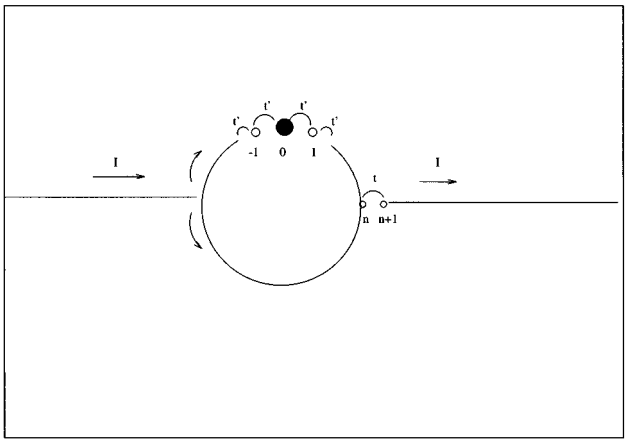

FIG. 1. Schematic representation of the ring connected to two contacts with a three-site cluster inserted in its upper arm. The quantum dot is at site 0. The total current is calculated between sites n and $n+1$.

resonance or not. On the other hand, in the Coulomb blockade regime one observes a strong ϕ dependence only when the level localized at the dot satisfies the resonant tunneling condition.

II. THEORY

The system is described by an Anderson-impurity first-neighbor tight-binding Hamiltonian defined over a ring and two contacts. Although the electron-electron interaction is present in the entire system we assume it to be restricted to the dot where, due to quantum confinement, the electrons interact more strongly. The Hamiltonian is then given by

$$H=H_c+\sum_{ij\sigma} t_{ij}c_{i\sigma}^{\dagger}c_{j\sigma}+t'\sum_{\sigma} (c_{1\sigma}^{\dagger}c_{2\sigma}+c_{-1\sigma}^{\dagger}c_{-2\sigma}+\text{c.c.}), \tag{1}$$

where i,j denote the atomic sites in the ring and contacts, t_{ij} is the first-neighbor hopping matrix element, t' is the hopping connecting the dot to the upper arm of the ring, and H_c represents the dot modeled by a cluster of three sites and is given by

$$H_c=V_0\sum_{\sigma} n_{0\sigma}+Un_{0\uparrow}n_{0\downarrow}$$
$$+t'\sum_{\sigma} [c_{0\sigma}^{\dagger}c_{1\sigma}+c_{1\sigma}^{\dagger}c_{0\sigma}+c_{0\sigma}^{\dagger}c_{-1\sigma}+c_{-1\sigma}^{\dagger}c_{0\sigma}], \tag{2}$$

where U and V_0 correspond, respectively, to the electronic repulsion and gate potential on the dot, which is at site 0. The local energies of the two other sites, 1 and -1, are chosen to be zero and their interaction with the dot is t', as illustrated in Fig. 1. The matrix element t' in Eq. (2) plays the role of the hybridization of the usual Anderson Hamiltonian; in this sense H_c is equivalent to an overscreened Anderson Hamiltonian with a nonlocal hybridization. Therefore, one expects to obtain a Kondo effect in the limit $t'<t$. The applied electric potential is taken to be negligibly small so that its contribution to the site energies can be neglected. The transport is supposed to be ballistic in nature so that the Hamiltonian does not include a dissipative mechanism or other degrees of freedom, but does include electrons. The external magnetic field producing the flux is incorporated in the first-neighbor matrix elements, t_{ij}, of the ring as

$$t_{ij}=te^{-(i\pi/N)(\phi/\phi_0)}, \tag{3}$$

where t is the first-neighbor hopping, ϕ is the quantum flux crossing the ring, $\phi=\oint\vec{A}\cdot\vec{dl}$, where $\vec{A}$ is the vector potential, ϕ_0 is the quantum of flux, and $2N$ is the number of atoms of the ring with lattice parameter a.

The system is considered to be strictly one dimensional (1D), constituted by one line of atoms, which is, evidently, not a realistic situation. Transverse quantum confinement would produce some transverse quantum states for which different 1D electronic channels would be available for electrons to move along the ring. However, if the width of the wire is small enough these states can be well separated in energy and we can restrict ourselves to the study of a one-channel system. The current circulating along the ring is calculated using the Keldysh formalism.[6] In addition to the usual advanced and retarded Green functions, two other correlation functions are required:

$$G_{ij\sigma}^{-+}(\omega)=i\int_{-\infty}^{\infty}\langle c_{j\sigma}^{\dagger}(t)c_{i\sigma}(0)\rangle e^{i\omega t}dt, \tag{4a}$$

$$G_{ij\sigma}^{+-}(\omega)=-i\int_{-\infty}^{\infty}\langle c_{i\sigma}(0)c_{j\sigma}^{\dagger}(t)\rangle e^{i\omega t}dt, \tag{4b}$$

where the mean values are calculated on a nonequilibrium stationary state of the system under the effect of an applied electric potential. $G_{ii}^{-+}(\omega)$ gives the spectral representation of the electronic occupation at site i, corresponding to this current flowing stationary state. To calculate the transport properties the system is partitioned into two semi-infinite supports so that the two subsystems are in thermodynamic equilibrium, the electric current is zero, and the corresponding Green functions can be obtained by standard techniques. The dressed Green functions for the nonequilibrium situation are calculated through a Dyson equation obtained by reestablishing the connection between the two subsystems, according to the Keldysh formalism. Following this idea the total current circulating along the contacts due to the application of an external bias can be obtained from

$$\langle I\rangle=\frac{2et}{h}\sum_{\sigma}\int_{-\infty}^{\infty}[G_{n,n+1\sigma}^{-+}(\omega)-G_{n+1,n\sigma}^{-+}(\omega)]d\omega, \tag{5}$$

where n and $n+1$ are two adjacent sites belonging to the contacts. In our calculation these sites are chosen as shown in Fig. 1.

The cluster Hamiltonian H_c is diagonalized by considering, for simplicity, the electron-electron interaction U to be infinite. The eigenvalues and eigenvectors for all possible numbers of particles are then calculated. To obtain the propagators for the total system we calculate first the Green function for the cluster using the grand-canonical ensemble:

$$g_{ij\sigma}(\omega)=\frac{1}{Z}\sum_{m,n}\left(e^{-\beta E'_m}+e^{-\beta E'_n}\right)\frac{\langle n|c^{\dagger}_{i\sigma}|m\rangle\langle m|c_{j\sigma}|n\rangle}{\omega-(E_n-E_m)},$$

$$i,j=1,0,\overline{1}, \quad (6)$$

with

$$H_c|m\rangle=E_m|m\rangle, \quad E'_m=E_m-\mu N_c, \quad Z=\sum_m e^{-\beta E'_m},$$

where Z is the cluster partition function, $\beta=(k_BT)^{-1}$, N_c is the number of electrons in the cluster, and μ is the chemical potential.

The Green functions appearing in Eq. (5) are calculated using a cumulant diagrammatic expansion where the nondiagonal matrix elements linking the dot with the rest of the system is taken to be the perturbation. The expansion is restricted to the ''chain approximation,''[7] which has shown to be a suitable scheme to describe the Kondo and Coulomb blockade effects.[8]

Within this approximation the propagators for the total system are obtained solving the Dyson equation

$$G_{ij\sigma}(\omega)=g_{ij\sigma}(\omega)+\sum_{m\not{i}} g_{i\not{i}}(\omega)t'_{\not{i}m}G_{mj\sigma}(\omega), \quad (7)$$

where $g_{ij\sigma}(\omega)$ has been extended to represent the undressed Green function of the two noninteracting subsystems, the cluster given by Eq. (6) and the rest of the system. The Kondo regime is attained for values of the gate potential V_0 such that the dot resonant level is below the Fermi level ε_F. As the approximation proposed is exact at the atomic limit it describes the Coulomb blockade in an appropriate way.

III. RESULTS AND DISCUSSIONS

Using the above formalism we study the current circulating along a ring of 2^7 atoms having a quantum dot inserted in one of its arms, under a small applied electric potential of $0.03t$. The dot is subjected to a variable gate potential V_0 and interacts with the rest of the ring with a $t'=0.1t$. This value is justified because there is a barrier that reduces the transmission probability between the dot and the rest of the ring. The ring is connected to two semi-infinite linear chains.

The tunneling current as a function of the magnetic flux encircled by the ring, for different values of the gate potential V_0, is presented in Fig. 2, for low and high temperature (T). By varying the gate potential we can change the energy of the dot resonant level, which does not coincide with V_0 due to the interaction of the dot with the rest of the system. Let us first analyze the behavior at high T, which has been chosen to correspond to $k_BT=0.1t$. For V_0 such that the dot resonant level coincides with the Fermi level, which was taken to be $-0.05t$, the system is in the resonant tunneling condition and the current circulates along the upper arm of the ring, where the dot is located, as well as along the lower arm, producing interference at the right contact. The interference pattern depends on the magnetic flux encircled by the ring since the magnetic field introduces a phase shift between the currents circulating along the two arms. As a result the total current shows a strong dependence on the magnetic flux

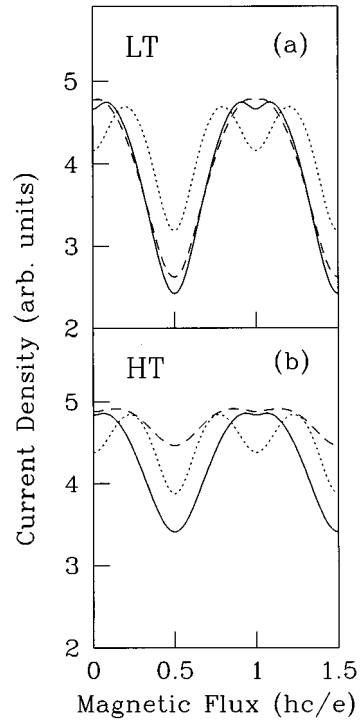

FIG. 2. Current density as a function of magnetic flux at (a) low T and (b) high T, for different values of the gate potential V_0/t: 0.2, dashed line; 0.3, continuous line; 0.5, dotted line.

as shown in Fig. 2(b) for V_0 equal to $0.3t$ (continuous line). On the other hand, when the upper arm is taken out of resonance by increasing or reducing the gate potential, the electrons circulate mainly along the lower arm and the interference is reduced. The dependence of the current on the magnetic flux becomes weaker and the amplitude of the oscillations is smaller, as illustrated in Fig. 2(b) for V_0 equal to $0.5t$ (dotted line) and $0.2t$ (dashed line).

By reducing the temperature below T_K we obtain the curves shown in Fig. 2(a), where the current is depicted as a function of the magnetic flux for $k_BT=0.01t$ with the same values of the gate potential as in Fig. 2(b). One can see that, unlike the high-T case, the current shows large oscillations for $V_0=0.2t$ (dashed curve), in which case the dot level is below the Fermi level and the system is in the Kondo regime. This is a consequence of the appearance of an Abrikosov-Suhl resonance at the Fermi level providing a channel for the electron to go along the upper arm of the ring through the dot, giving rise to a strong interference with the current circulating along the lower arm.

These features are better clarified by analyzing the local density of states (LDOS) at the dot, which is shown in Fig. 3, for the same values of temperature and gate potential as in Fig. 2 and for a small energy range, of the order of the applied potential, around the Fermi level. For $V_0\leqslant 0.2t$ the LDOS shows the Kondo peak approximately pinned at the Fermi level and the resonant level is far lower in energy. This is illustrated by the dashed curves corresponding to $V_0=0.2t$, where the only structure appearing in the energy range considered is the Kondo peak. Notice that at high T this peak is also present but strongly reduced. Increasing V_0 further, the resonant peak moves towards the Fermi level

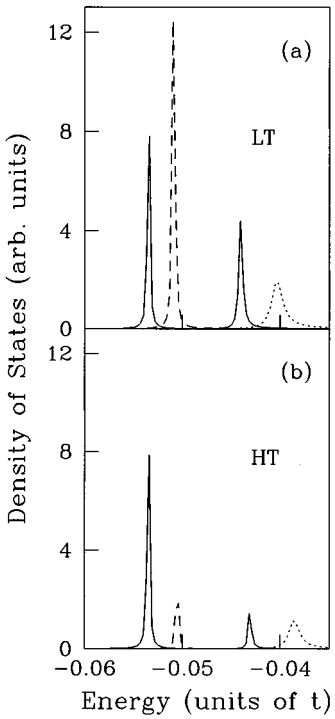

FIG. 3. Local density of states at the dot site at (a) low T and (b) high T, for the same values of the gate potential as in Fig. 2. $V_0/t = 0.2$ (dashed line), 0.3 (continuous line), 0.5 (dotted line).

and as it gets close to the original Kondo peak their interaction results in a double structure in the LDOS that has a weak dependence on temperature. This is shown in Fig. 3 by the continuous curves corresponding to $V_0 = 0.3t$. For greater values of the gate potential these two structures merge into one peak, represented by the dotted curves, which shifts towards higher energies and the Kondo effect disappears.

The distinction between the high-T and low-T behavior is made evident in Fig. 4 where the oscillation amplitude of the current is presented as a function of the gate potential V_0 for the same low (continuous line) and high (dashed line) temperatures as in Figs. 2 and 3. One can see that for the whole range of values of the gate potential for which the system is in the Kondo regime ($V_0 \leqslant 0.2t$) the oscillations of the current are much larger for low T than for high T. On the other hand, for $V_0 > 0.4t$ the behavior of the oscillations for both temperatures is similar. However, the current oscillation amplitude is smaller for high T than for low T, although the LDOS near resonance is approximately temperature independent. At high T, due to the spread of the Fermi distribution there are more channels contributing to the current with different energies and, as a consequence, different phases. At low T the phase dispersion is restricted to the window opened by the applied potential, which is enlarged by increasing the temperature. The smaller phase resolution of the experiment at high T reduces the amplitude of oscillations since there is no magnetic flux for which the electrons going along the different arms of the ring can be totally in phase or out of phase.

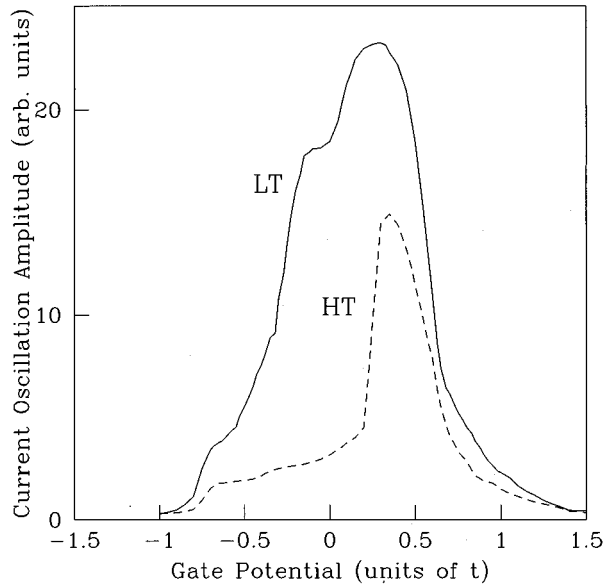

FIG. 4. Current oscillation amplitude as a function of gate potential at low T (continuous line), and at high T (dashed line).

The not completely monotonic behavior of the oscillation amplitude at low T, shown in Fig. 4, is a result of the mesoscopic character of the ring, which is reflected on the LDOS by the existence of several structures that interact slightly with the Kondo peak as a function of the gate potential.

We have shown that an imperfect ring threaded by a magnetic flux is a device very sensitive to distinguish between the low- and high-temperature behavior in the Kondo regime. At low T the Bohm-Aharonov oscillations reflect the presence of the Kondo resonance, which provides a channel by which the electrons can go through the dot, producing interference. At high T the Abrikosov-Suhl resonance disappears and the oscillations are important only when the dot level is at the resonance condition. We hope these results motivate an experimental verification of this effect.

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