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Bistability of persistent currents in mesoscopic rings

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Abstract. We study the persistent currents flowing in a mesoscopic ring threaded by a magnetic flux and connected to a stub of finite length. Multistability processes and Coulomb blockade are demonstrated to be present in this system. These properties are functions of the magnetic flux crossing the ring which plays the role that the external applied potential fulfills in the multistability behaviour of the standard mesoscopic heterostructures.

1. Introduction

The existence of persistent currents in a conducting mesoscopic ring threaded by a magnetic flux was proposed by Büttiker *et al* [1] and experimentally observed in an ensemble of rings and in semiconductor and metallic loops [2]. In a ring, the magnetic flux can be introduced through a boundary condition for the electronic wave function.

$$\Phi(x + 2\pi r) = \Phi(x)\, \mathrm{e}^{2\pi \mathrm{i}\phi/\phi_0} \tag{1}$$

where r is the radius of the ring , $\phi_0 = h/e$ is a quantum of magnetic flux and ϕ is the real magnetic flux encircled by the loop. Equation (1) introduces a periodicity to all the physical properties of the system as a function of ϕ with the period associated with ϕ_0. For a particular energy level the persistent current flowing along the system can be obtained by calculating the derivative of the energy with respect to the magnetic flux. The total current is obtained summing the contributions over all the occupied states below the Fermi level.

Since the original experiment [2] there has been a considerable theoretical effort to understand currents and current fluctuations of non-interacting electrons in open and closed rings [3, 4]. Many works have been devoted to studying the effect of electronic interaction upon the current in closed rings and the interplay between correlation and disorder has been reported in these systems using a number of different methods [4]. From an experimental point of view, works emphasizing different geometries in open and closed systems have been reported and transport through a quantum dot embbeded in the ring has been studied [5].

We study the persistent currents flowing in a mesoscopic ring threaded by a magnetic flux and connected to a stub of finite length. A change in the magnetic field produces level crossings and eventually an interchange of position between the ground state and the first excited level. This crossing gives rise to metastable situations. A metastable state corresponds to a local minimum of the energy in the parameter space separated by an energy barrier from the absolute minimum. So, if this particular state is obtained through

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an adiabatic variation of the magnetic flux, the system is unable to reach its ground state remaining in the relative local minimum.

This multistability can occur in a interacting perfect ring and also in a inhomogeneous one, as is the case of a perfect ring plus a stub of finite length. In this last case the stub acts as a reservoir of particles and the magnetic flux crossing the ring plays the role that the external applied potential fulfills in transport in standard mesoscopic heterostructures. This system has already been studied [6] focusing on other properties, within the context of the electrochemical capacity ideas. The structure is described by a tight-binding Hamiltonian given by

$$\hat{H}_r = -t \sum_{\sigma,i=1}^{N_r} \hat{c}^{\dagger}_{i,\sigma} \hat{c}_{i+1,\sigma} + \sum_{\sigma,\sigma',j,i=1}^{N_r} U^{\sigma,\sigma'}_{i,j} \hat{n}^{c}_{i,\sigma} \hat{n}^{c}_{j,\sigma'} \tag{2}$$

$$\hat{H}_s = -t \sum_{\sigma,i=1}^{N_s-1} \hat{d}^{\dagger}_{i,\sigma} \hat{d}_{i+1,\sigma} + \sum_{\sigma,\sigma',j,i=1}^{N_s} U^{\sigma,\sigma'}_{i,j} \hat{n}^{d}_{i,\sigma} \hat{n}^{d}_{j,\sigma'} + V_o \sum_{\sigma,i=1}^{N_s} \hat{n}^{d}_{i,\sigma} \tag{3}$$

$$\hat{H}_i = -t_0 \sum_{\sigma} \hat{c}^{\dagger}_{1,\sigma} \hat{d}_{1,\sigma} + \mathrm{CC} \tag{4}$$

where $\hat{H}_r$ corresponds to the ring, $\hat{H}_s$ to the stub, which is a wire of finite length connected to the ring through the Hamiltonian $\hat{H}_i$ and N_r and N_s are the numbers of atomic sites belonging to the ring and to the stub respectively. For the ring, it is assumed that $N_r+1 = 1$, and the magnetic flux is incorporated as the boundary condition (1).

We model the gate potential which controls the state of charge of the stub through the diagonal elements of $\hat{H}_s$ given by V_o. For the case of ballistic transport in an isolated ring, we have verified that the properties of the system are weakly dependent upon the spatial range of the e–e interaction. The effects of non-locality in the Coulomb interaction could be restricted to the first-neighbour intersite electronic repulsion U_1 that controls the effects that the charge accumulated in the stub has on the currents circulating along the ring. Restricted to the intrasite and first-neighbour intersite contributions, the Coulomb interaction can be written as $U^{\sigma,\sigma'}_{i,j} = U_0 \delta_{i,j} \delta_{\sigma',-\sigma} + U_1(\delta_{j,i-1} + \delta_{j,1+1})$.

The current is characterized by an energy scale that is given by the energy difference between two successive states below the Fermi level (E_F). For small values of E_F it turns out to be

$$\delta E = 4\pi^2 t^2 (2n+1)/N_r^2 \tag{5}$$

where n is the integer number that defines the state wave vector $k = 2\pi n/N_r a$, where a is the lattice parameter. Although due to numerical limitations we are obliged to take a ring with a small number of atoms, it is possible to obtain an adequate physical representation of the system by scaling the Coulomb parameters U_0 and U_1 to the energy difference δE defined at the neighbourhood of the Fermi level.

The size of a disordered ring is an extremely important parameter in studying the properties of persistent currents because the localization length of the states near the Fermi energy defines a characteristic length in the system. The behaviour is different whether the size of the ring is larger or smaller than this magnitude. However, for an ordered ring, the absence of this length permits us to take an ideal small 1D loop to study a real ring. To be able to solve the problem in an exact numerical way we restrict the study to the one-channel problem. This is not a severe limitation because nowadays it is possible to build up mesoscopic wires thin enough to have sufficent energy separation of the different channels created by the lateral confinement [7].

To find the ground state we use a standard Lanczos algorithm. The knowledge of this permits us to calculate several quantities of interest for the problem: the current in the ring, the charge in the stub and the total spin of the ground state as function of the external magnetic flux and of the gate potential V_o. The current is calculated as the mean value on the ground state of the operator $\hat{J}$:

$$\hat{J} = (4\pi et/h)\,\mathrm{Im}\left(\sum_{\sigma,i=1}^{N_r}\left(\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{i+1,\sigma} - \hat{c}^{\dagger}_{i+1,\sigma}\hat{c}_{o,\sigma}\right)\right). \tag{6}$$

2. Results

We study first an ordered ring by assuming that $t_0 = 0$. The persistent current of the non-interacting ring can be understood if we assume that the one-particle energy levels move along the free particle dispersion relation as the magnetic field increases, reducing the energy difference between the levels that correspond to the wave vector $-2\pi i/N_r a$ and $2\pi(i+1)/N_r a$ for an arbitrary integer i.

When the system possesses $2n$ particles there is an accidental degeneracy between the state with $S = 0$ and $S = 1$, where S is the spin of the many-body state. This occurs for a magnetic flux $\phi_* = \phi_0/2$ for the case in which n is an odd integer, or when $\phi_* = 0$ if n is even. It is important to notice that the state with $S = 1$ is the ground state only for this particular value of flux (ϕ_*). If $\phi = \phi_* + \epsilon$, where ϵ is an arbitrary small number, the ground state is in the $S = 0$ subspace. In this case there is degeneracy but not level crossing.

The Coulomb forces between the electrons shift the accidental degeneracy to other values of ϕ_*: $\phi_* < \phi_0/2$ for n even and $\phi_* > 0$ for n odd as it is shown in figure 1. It is straightforward to realize that it is the Coulomb forces which originate the level crossing.

When the number of particles is odd there is no accidental degeneracy for the non-interacting case. However, for interacting electrons the states with $S = 3/2$ and $S = 1/2$ could coincide in energy for $\phi = \phi_*$, $0 < \phi_* < \phi_0/2$, if the electronic repulsion were greater than the kinetic energy difference between the last two occupied levels.

The two many-body solutions mentioned above interchange their condition of being the ground state and the first excited state at $\phi = \phi_*$. If U is small enough, a perturbative argument can be given as follows. Let us suppose that the system has an even number of electrons and that its ground state has $S = 0$. Increasing the magnetic flux, when $\phi > \phi_*$ the system could reduce its energy by occupying the state with total spin $S = 1$. Here the two electrons next to the Fermi level are unpaired: one has a positive wave vector k and the other a negative one and both the same value of S_z. However, for this process to take place during an adiabatic evolution, the system has to go through an intermediate state in which one of the electrons hops from the state with positive k to another with negative value of k without flipping its spin. Due to the Coulomb interaction, the energy of the intermediate state is greater than the energy of the flipped spin final state $S = 1$, and also is greater than the energy of the initial state $S = 0$ due to its greater kinetic energy, so it defines the top of a potential barrier which separates the two states. Under the hypothesis of thermodynamic equilibrium, at $\phi = \phi_*$ the system changes its current discontinuously from a positive to a negative value only if there is present an external spin flip mechanism capable of overcoming the potential barrier that exists separating the two states in phase space. Although the spin characterizes the two bistable states, the phenomenon is not connected to this incidental fact. The bistability is a result of the level crossing of the two lowest-energy solutions which are relative minima and stable in phase space. As a consequence, an adiabatic increase of the

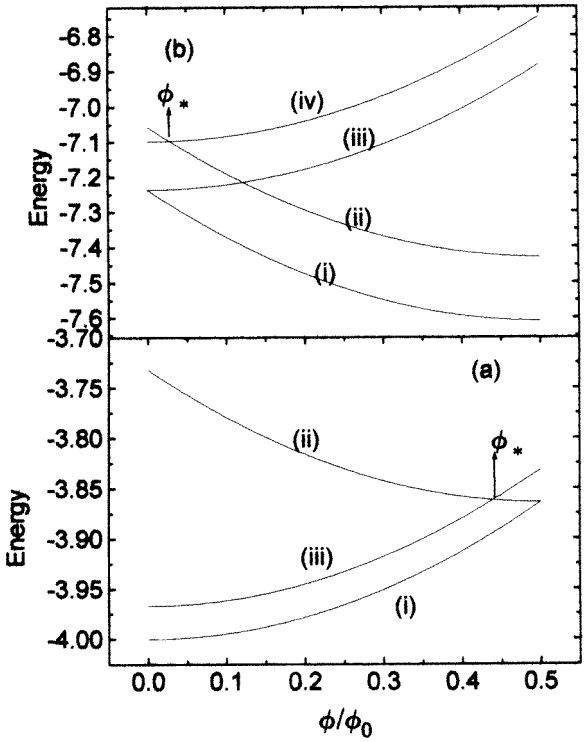

Figure 1. (a) Two particles in a 12-site ring. The energy is measured in units of the parameter t: (i) is the energy of the $S = 0$ state with $U_0 = 0$, (ii) is the energy of the $S = 1$ state and (iii) is the energy of the $S = 0$ state with $U_0 = 0.5t$. (b) Four particles in a ten-sites ring : (i) is the energy of the $S = 0$ state with $U_0 = 0$, (ii) is the energy of the $S = 0$ state with $U_0 = 0.5t$, (iii) is the energy of the $S = 1$ state with $U_0 = 0$ and (iv) is the energy of the $S = 1$ state with $U_0 = 0.5t$.

magnetic field will not always maintain the system in its ground state.

Numerically this adiabatic process can be simulated as follows. It is necessary to obtain the ground state of the system threaded by a flux $\phi_1 = \phi_0 + \delta\phi$ where $\delta\phi$ is an arbitrary small flux. The wave function $|\alpha_0(\phi_0)\rangle$ corresponding to the ground state of the system under the effect of the flux ϕ_0 is taken as the starting state to begin the process. This state has a total spin S_0 and a total wave vector $K(\phi_0)$. It can be written as a linear combination of eigenstates of the Hamiltonian with flux ϕ_1, $|\alpha_n(\phi_1)\rangle$,

$$|\alpha_0(\phi_0)\rangle = \sum_n a_n \big|\alpha_n\big(\phi_1\big)\big\rangle. \tag{7}$$

Note that a change in the magnetic flux produces a spread of the state over the quantum number K but not in the S quantum number. Let us call the state that provides the dominant contribution to equation (7) by $|\alpha_{n_0}(\phi_1)\rangle$, which possesses the total wave vector $K(\phi_1)$ closest to the original $K(\phi_0)$, and the same total spin (S_0) as the $|\alpha_0(\phi_0)\rangle$ state (within the numerical precision).

It is fundamental to know whether in this process the system will remain in a unstable or metastable situation or not. To clarify this point, let us define the three-dimensional space (S, K, E) where S, K and E are the total spin, the total wave vector and the energy

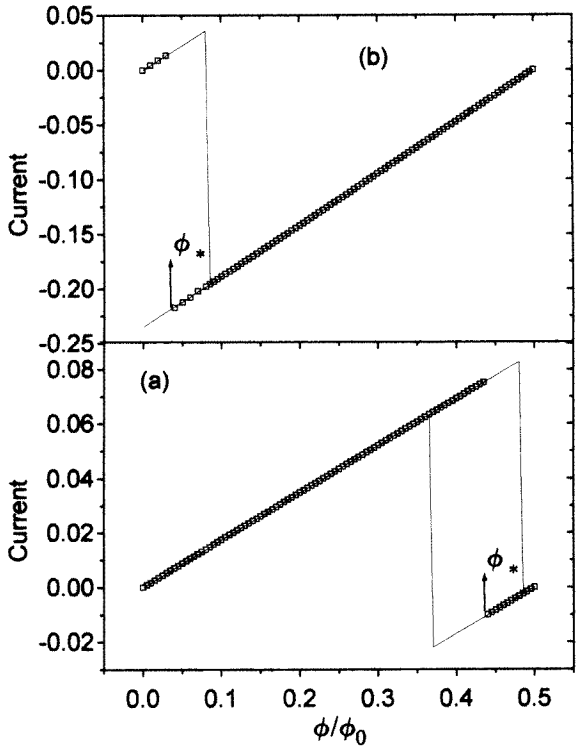

Figure 2. (a) Current versus flux for two particles in a 12-site ring and $U_0 = 0.5t$: the open squares correspond to the ground state; the continuous line corresponds to the current of the metastable states. (b) Current versus flux for four particles in a ten-site ring and $U_0 = 0.5t$: the open squares correspond to the ground state; the continuous line corresponds to the current of the metastable states. The current is measured in units of $4\pi te/h$.

respectively. The behaviour of the system will depend on the topology of this space in the neighbourhood of the starting point defined by the state $|\alpha_0(\phi_0)\rangle$. Suppose that the point corresponding to S_0 and $K(\phi_1)$ is an absolute minimum for the energy. Then, the system evolving from a small region around this point will go always towards it. Now, suppose that there is another minimum, which belongs to a different (S, K) subspace, and that it is the true absolute minimum. The existence of this minimum will modify the topology of the space around the starting point $S_0, K(\phi_0)$. However, if the energy difference between the two minima is not great enough, the topology within a small vicinity of the starting point will remain unchanged. Then, the system evolving adiabatically from this point will continue going toward the $S_0, K(\phi_1)$ state.

An ideal tool to study this problem is the modified Lanczos alghorithm used to find the ground state of the system. Ths method requires the definition of a new state $|\beta\rangle$ by applying the Hamiltonian to the $|\alpha_0(\phi_0)\rangle$ state and subtracting the projection over it. The Hamiltonian represented in the basis $|\alpha_0(\phi_0)\rangle$, $|\beta\rangle$ is diagonalized and the lowest-energy state is taken as the starting new vector (as it is always a better approximation to the real ground state). This procedure is continued until convergence is reached. In the process of diagonalizing the 2×2 matrix at each step the lowest of the two diagonal elements (d_α, d_β) determines the evolution of the initial state. The procedure follows a method in which the

energy obtained at step n is lower than the energy at step $n-1$. If the state $|\alpha_{n_0}(\phi_1)\rangle$ does correspond to a minimum in the parameter space the process goes toward it, reducing the energy at each step. In the opposite situation, at an arbitrary step of the procedure the relation between d_α and d_β is inverted ($d_\beta < d_\alpha$) and the system evolves to the orthogonal state β. The quantum numbers corresponding to this state are in general arbitrarily far from the quantum numbers of the original state even for $\delta\phi$ infinitesimally small. This is a procedure through which we are able to find numerically the frontiers of the bistable region.

Then, when the magnetic flux is changed adiabatically in the neighbourhood of ϕ_*, it is possible for the system to persist in a metastable state above and below ϕ_*, depending on whether the flux is increasing or decreasing. This introduces a hysteresis loop that appears as a bistability in the I–ϕ characteristic curve as shown in figure 2 with a continuous line.

In standard double-barrier heterostructures (DBHs), transport involves non-linear phenomena reflected in the observation of multiple stabilities in the I–V characteristic curve in the region where the device exhibits a negative differential conduction [8]. This property can be thought to be produced by an accumulation of electronic charge in the well at resonance and a rapid leakage of it when the applied voltage has just taken the device out of resonance. This non-linear effect is essentially a result of the interaction between the charges in the well and has been extensively studied theoretically assuming that the potential profile seen by the carriers, as they go along, depends in a self-consistent way upon the charge distribution [9].

For our system, a bistability very similar to the one described above for the DBH can be obtained in the I–ϕ characteristic curve. This is because there is a part of the system, the stub in our case, the well for the standard DBH, which is capable of acting as a reservoir of particles controlled by the external applied potential for the case of the DBH or by the external magnetic field or the gate potential in our case.

Let us focus our attention on the ring weakly coupled to the stub taking a small t_0. In order to discuss conceptually the bistable behaviour, we define the energy per particle E_α such that the total energy of the system is given by

$$E = \sum_\alpha E_\alpha \langle \hat{n}_\alpha \rangle \tag{8}$$

where

$$E_\alpha = e_\alpha + \sum_{i,j,\sigma,\sigma'} U_{i,j}^{\sigma,\sigma'} \langle \hat{n}_{i,\sigma} \hat{n}_{j,\sigma'} \rangle / N_e \tag{9}$$

and $\langle ... \rangle$ corresponds to the mean value on the ground state of the operators involved. e_α refers to the energy of an electron without the Coulomb interaction and N_e is the number of electrons in the system.

In this case the phase space in which the bistability occurs is defined by the number of particles in the stub and the total spin. The starting state to initialize the numerical calculation is assumed to be the solution that corresponds to the previous smaller (greater) magnetic flux or V_o. This procedure simulates the behaviour of the system when the flux or the gate potential is adiabatically increased (decreased). In figure 3 we present the variation of the total energy and the E_α levels of the ring and the stub as a function of the magnetic flux for the case with $U_0 = 0.3$, $U_1 = U_0/2$, $t_0 = 0.0001$ and $V_o = 0$ in units of the parameter t. For such a small value of the Coulomb parameters the pseudo-single-particle description is valid. Also a small value of the t_0 parameter implies that one of the variables in the parameter space (the charge into the stub) becomes quasi-discrete. The pseudo-single-particle description exhibits a flux-insensitive behaviour corresponding to a state localized at the stub, and a flux-dependent state that describes a mobile particle inside the ring. Due

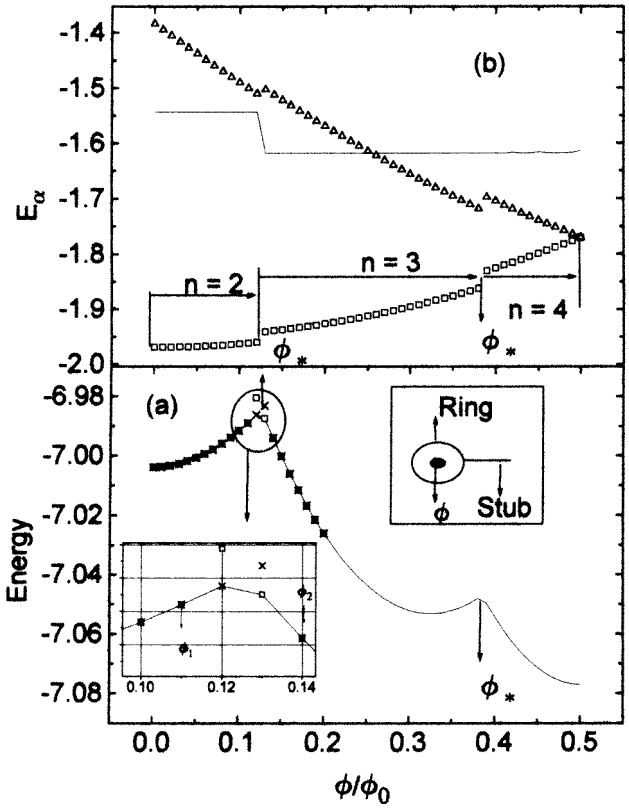

Figure 3. Four particles in an eight-site ring weakly coupled to a four-site stub as shown in the right inset of (a). The number of electrons in the ring is n. (a) The continuous line represents the energy of the ground state. The crosses correspond to the energy obtained raising the flux adiabatically from zero. The open squares represent the energy obtained decreasing the flux adiabatically from the right of ϕ_2. It is also shown in the lower inset of the figure. (b) Pseudo-single-particle levels of the system as a function of the magnetic flux. Open squares and triangles correspond to the first and second levels of the ring respectively and the continuous line to the first level of the stub. The energy is measured in units of the parameter t.

to a change in the magnetic flux, when a charge goes from one part of the system to the other, a finite shift of the levels of each subsystem occurs due to the Coulomb interaction together with a modification of the total spin of the ground state. It is the dependence of these levels with the state of charge, mainly in the stub but also in the ring, which drives the bistability. The system can reduce its onergy at $\phi = \phi_*$ changing its charge distribution, as shown in figure 3. However, along an adiabatic path as analysed above, these two states of charge are separated in phase space by a potential barrier which vanishes for a particular external magnetic flux ϕ_* when the transition occurs. At these values of the flux the energy of the total system changes discontinuously.

In this example, the bistability is unfavoured by small values of the parameters t_0 and U_0. For greater values of U_0, in order to obtain an interchange of charge between the ring and the stub, it is necessary to produce energy variations that go beyond the range allowed by the magnetic flux. So, in this case the gate potential is the relevant variable that controls the phenomenology of the system. In figure 4 the dependence of the current on V_o

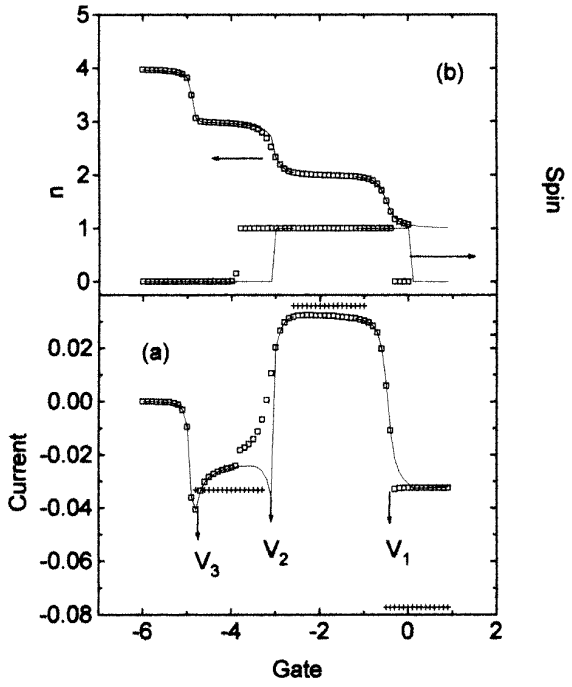

Figure 4. Four particles in an eight-site ring coupled to a four-site stub with $t_0 = 0.5t$,$\phi = 0.4\phi_0$ and $U_0 = 4t$. Open squares correspond to a process where the gate potential is decreasing slowly from zero. The continuous line corresponds to a situation in which the gate potential is increased adiabatically from -6. (a) Current as function of gate potential. From V_2 to the left the open squares correspond to the ground state. From V_2 to the right the ground state corresponds to the continuous line. Crosses represent the current of ($n = 1, 2, 3$) interacting particles in a perfect ring. (b) Charge in the stub (left) and total spin (right axis) as a function of the gate potential. The current is measured in units of $4\pi te/h$.

is presented for $t_0 = 0.5t$.

For this value of t_0 the interchange of charge of the two subsystems permits the existence of regions where the current in the ring is caused by a fractional number of electrons. There are regions in which the charge is almost constant while in others it is highly dependent upon the gate potential. There, the behaviour of the total spin of the ground state can change as it occurs at V_1 and V_2 in figure 4. Associated with it a bistability appears, as discussed above.

For a 1D DBH the Coulomb blockade effect reflects the fact that, as soon as one electron enters the well region, the entrance of a second one is excluded simply because it has to overcome the Coulomb repulsion produced by the first electron already inside it. Here the Coulomb blockade phenomenon is an intra-site effect. An electron cannot flow because another one is already occupying the region through which it has to go to become an electrical carrier. In our case, there is an inter-site Coulomb blockade effect produced by the repulsion that the charge inside the stub exercises over the flowing electrons within the ring in the vicinity of the stub. This is reflected in a reduction of the current in the regions where the charge is stable, independent of V_o, in comparison with the current that corresponds to a perfect ring with the same state of charge.

3. Conclusions

In conclusion we have presented a study of the many-body problem of an inhomogeneous closed ring enclosing a magnetic flux. We have shown that these systems have a bistable behaviour that can be associated with the physics of a non-linear system. We have also studied the effect that the imperfection has upon the persistent current flowing along the ring showing Coulomb blockade effect between the stub and the ring. The development of sub-micrometre physics makes it possible to construct this sort of device. We hope the predicted phenomenology could be a motivation for experimentalists to look for it in real systems.

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