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.
I. INTRODUCTION

The existence of persistent currents in a conducting mesoscopic ring threaded by a magnetic flux was proposed for the first time by Büttiker, Imry and Landauer [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.

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

where $r$ is the radius of the ring, $\phi_0 = h/e$ is a quantum of magnetic flux and $\phi$ 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 $\phi$ with the period associated to $\phi_0$. 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 was devoted to study the effect of electronic interaction upon the current in closed rings and the interplay between correlation and disorder has been reported in this systems using a number of different methods [4]. From an experimental point of view, works emphasizing on different geometries in open and closed systems has been reported and transport through a quantum dot embedded in the ring has been studied [3].

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
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 an inhomogeneous one, as it is the case of a perfect ring plus a stub of finite length. In this 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 focusing other properties, within the context of the electrochemical capacity ideas. The structure is described by a tight-binding Hamiltonian given by:

$$\hat{H}_r = -t \sum_{\sigma,j=1}^{N_r} \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,j,\sigma} + \sum_{\sigma,\sigma',j,i=1}^{N_r} U_{i,j}^{\sigma,\sigma'} \hat{n}^c_{i,\sigma} \hat{n}^c_{j,\sigma'}$$

$$\hat{H}_s = -t \sum_{\sigma,i=1}^{N_s-1} \hat{d}^\dagger_{i,\sigma} \hat{d}_{i+1,\sigma} + \sum_{\sigma,\sigma',j,i=1}^{N_s} U_{i,j}^{\sigma,\sigma'} \hat{n}^d_{i,\sigma} \hat{n}^d_{j,\sigma'} + V_o \sum_{\sigma,i=1}^{N_s} \hat{n}^d_{i,\sigma}$$

$$\hat{H}_i = -t_0 \sum_{\sigma} \hat{c}^\dagger_{1,\sigma} \hat{d}_{1,\sigma} + c.c.$$

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 neighbor 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 $U_{i,j}^{\sigma,\sigma'} = U_0 \delta_{i,j} \delta_{\sigma',-\sigma} + U_1 (\delta_{j,i-1} + \delta_{j,i+1})$. 

3
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 results to be:

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

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 small number of atoms, it is possible to get an adequate physical representation of the system by scaling the Coulomb parameters $U_0$ and $U_1$ to the energy difference $\delta E$ defined at the neighbourhood of the Fermi level.

The size of a disordered ring is an extremely important parameter to study 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 bigger or smaller than this magnitude. However, for an ordered ring, the absence of this length permits to take an ideal small 1-D loop to study a real ring. Also it is necessary to suppose that it is thin enough as to produce a sufficient energy separation of the different channels created by the lateral confinement.

To find the ground state we use a standard Lanczos algorithm. The knowledge of it permits 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 $\hat{J}$

$$\hat{J} = (4\pi et/h) \text{Im} \left( \sum_{\sigma,i=1}^{N_e} (\hat{c}_i^{\dagger,\sigma} \hat{c}_{i+1,\sigma} - \hat{c}_{i+1,\sigma}^{\dagger} \hat{c}_{i,\sigma}) \right).$$

\(II.\ \text{RESULTS}\)

We study first an ordered ring just 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 \((\phi_*)\). If \(\phi = \phi_* + \epsilon\), where \(\epsilon\) 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 \(\phi_*; \phi_* < \phi_0/2\) for \(n\) even and \(\phi_* > 0\) for \(n\) odd as it is shown in Fig. 1. It is straightforward to realize that are the Coulomb forces which originates 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 both states. Under the hypothesis of thermodynamic equilibrium, at \( \phi = \phi_x \) the system changes its current discontinuously from a positive to a negative value only if it is present an external spin flip mechanism capable of overcoming the potential barrier that exists separating both states in phase space.

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 \( \phi_0 \) 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 \( \phi_1 \),

\[
|\alpha_0(\phi_0)\rangle = \sum_n a_n |\alpha_n(\phi_1)\rangle 
\]

Note that a change in the magnetic flux produce an 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 if in this process the system will remain in an unstable or metastable situation or not. To clarify this point, let us define the three dimensional space \((S, K, E)\) where \( S, K, E \) are the total spin, the total wave vector and the energy respectively. The behavior 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 around 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 algorithm used to find the ground state of the system. This method requires the definition of a new state $|\beta>$ by applying the Hamiltonian to the $|\alpha_0(\phi_0)>$ state and subtracting the projection over it. The Hamiltonian represented in the basis $|\alpha_0(\phi_0)>$, $|\beta>$ 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 2x2 matrix at each step the lowest of the two diagonal elements $(d_\alpha, d_\beta)$ determines the evolution of the initial state. The procedure follows a way in which the energy obtained at the $n$ step is lower than the energy at the step $n - 1$. If the state $|\alpha_{n0}(\phi_1)>$ 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 $d_\alpha$ and $d_\beta$ is inverted ($d_\beta < d_\alpha$) and the system evolves to the orthogonal state $\beta$. The quantum numbers corresponding to this state are in general arbitrary far apart 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 neighborhood of $\phi_*$, it is possible for the system to persist in a metastable state above and below $\phi_*$, depending whether the flux is increasing or decreasing. This introduces a hysteresis loop that appears as a bistability in the $I-\phi$ characteristic curve as shown in Fig. 2 with a continuous line.

In standard double-barrier heterostructures (DBH), 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 [7]. 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 is 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.

For our system, a bistability very similar to the one described above for the DBH can be obtained in the $I - \phi$ 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 reservoirs 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 to 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 $E_\alpha$ such that the total energy of the system is given by

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

where

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

and $\langle ... \rangle$ corresponds to the mean value on the ground state of the operators involved. $e_\alpha$ 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 takes place 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 $V_0$. This procedure simulates the behaviour of the system when the flux or the gate potential is adiabatically increased (decreased). In Fig. 3 we present the variation of the total energy and the $E_\alpha$ 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 $V_0 = 0$ 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 discret. The pseudo single particle description exhibits a flux-nsensitive behaviour corresponding to a state localized at the stub, and a flux depending state that describes a mobile particle inside the ring. Due to a change in the magnetic flux, when a charge goes from one part of the system to the other, a finit 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 Fig.3. However, along an adiabatic path as analyzed above, these two states of charge are separated in phase space by a potential barrier which vanishes for a particular external magnetic flux $\phi_*$ 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 the small value of the parameters $t_0, U_0$. 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 Fig.4 the dependence of the current on $V_0$ 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 the total spin of the ground state can change as it occurs at $V_1$ and $V_2$ in Fig. 4. Associated with it a bistability appears, as discussed above.

For a 1-D DBH the Coulomb blockade effect reflects 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 nearby of the stub. This is reflected in a reduction of the current in the regions where the charge is stable, independent of $V_0$, in comparison with the current that corresponds to a perfect ring with the same state of charge.

**III. 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 to 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-micrometer physics makes it possible to construct this sort of devices. We hope the predicted phenomenology could be a motivation for experimentalists to look for it in real systems.

**IV. ACKNOWLEDGMENTS**

One of us (E.V.A.) would like to acknowledge very interesting discussions related to the subject of this work with M. Buttiker. We would like to acknowledge the hospitality of the Department of Physics of UFF, Brazil, and the Department of Physics of UBA, Argentina. This work was partially supported by the Brazilian financial agencies CNPq and FINEP and by the grant B-11487/4B005 of the Andes-Vitae-Antorchas Foundation. Also, G. Ch. would like to acknowledge to UBA for a partial grant.
REFERENCES

[1] M. Büttiker, Y. Imry and R. Landauer, Phys. Lett. 96A, 365 (1983)

[2] L.P. Levy et al., Phys. Rev. Lett. 64, 2064 (1990); V. Chandrasekhar et al., Phys. Rev. Lett. 67, 3578 (1991); D. Mailly, C. Chapelieer, Phys. Rev. Lett. 70, 2020 (1993)

[3] M. A. Davidovich and E.V. Anda, Phys. Rev. B 50, 8559 (1994)

[4] F. von Oppen, E. K. Riedel, Phys. Rev. Lett. 66 84 (1991); B.L Altshuler, Y. Gefen, Y. Imry, Phys. Rev. Lett. 66, 88 (1991); Daniel Loss, Phys. Rev. Lett. 69, 343 (1992); M. Abraham et al, Phys. Rev. Lett. 70, 1509 (1993); G. Vignale, Phys. Rev. Lett. 72, 433 (1994); G. Bouzerar et al. Phys. Rev. B 49, 8258 (1994); F. V. Kusmartsev et al., Phys. Rev. B 49, 16234 (1994); H. Kato et al. Phys. Rev. B 50, 4943 (1994); W. Deng et al. Phys. Rev. B 50, 7655 (1994); G. Chiappe, E. Louis y J.A. Verges, unpublished

[5] Bertrand Reulet et al., Phys. Rev. Lett. 75, 124 (1995); A. Yacoby et al., Phys. Rev. Lett. 74, 4047 (1995)

[6] M. Büttiker, 16th Nordic Semiconductor Meeting, Laugarvatn, Iceland (to be published); P. Singha Deo, Phys. Rev. B 51, 5441 (1995); M. Büttiker and C.A. Stafford (unpublished).

[7] V. J. Goldman, D. C. Tsui and J. E. Cunningham, Phys. Rev. Lett. 58, 1256 (1987)

[8] P. Pernas, F. Flores and E. V. Anda Phys. Rev. B 47, 4779 (1993); O. Sofo and C. Balseiro, Phys. Rev. B 42, 11 (1992)
FIGURES

Fig.1: (a) Two particles in a twelve sites ring. The energy is measured in unit Fo:he
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 $U_0 = 0.5t$.

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

Fig.3: Four particles in a eight sites ring weakly coupled to a four sites 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 0. The open squares represent the energy obtained decreasing the
flux adiabatically from the right of $\phi_2$. 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 level of the ring respectively. The continuous
line to the first level of the stub. The energy is measured in units of the parameter $t$. 

12
Fig. 4: Four particles in an eight sites ring coupled to a four sites 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 0. 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 axis) and total spin (right axis) as a function of the gate potential. The current is measured in units of \( 4\pi te/h \). 