Persistent currents in mesoscopic cavities with surface roughness

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We consider a bidimensional discrete annular cavity with surface roughness (SR) threaded by a magnetic flux. In the ballistic regime and at half filling, localized border-states show up. These border states contribute coherently to the persistent current and the magnitude of the typical current $I_{typ}$ is enhanced with respect to their value in the absence of confinement. This result is robust with respect to changes in the relevant lengths of the sample.

In recent years, advances in nanotechnology made possible to design mesoscopic samples in which the carriers are mainly scattered by the boundaries of the system [1]. In this situation, where the elastic mean free path is much larger than the system size, the sample can be considered in the ballistic regime in order to compute the relevant transport quantities. In addition, the potential used to confine the carriers into the mesoscopic device has a symmetry quite different from that of the lattice of the sample. Therefore, even when the bulk disorder is absent, surface roughness (SR) is present with the consequence of the irregular scattering of the carriers at the borders of the sample.

In this article we present a model of SR which emerges naturally when the topology of the discrete lattice and the confining potential are different. The relevant feature of our model is that the effect of the SR on the eigenstates depends on the energy of these states. As the energy spectrum is bounded, the lattice parameter $a$ is a cut off for the allowed wavelengths and the wavelengths close to $a$ will be the most sensitives to the SR. Therefore, the SR that we model will be relevant near half filling, i.e in the metallic regime.

When the sample is threaded by a magnetic flux persistent currents are originated [2,3]. Although much work has been done concerning the influence of bulk disorder on persistent currents [4], less is known about the ballistic regime.

Our goal is to characterize the effect of the confinement and the SR on the magnitude of the persistent current in that regime.

The total current can be calculated at zero temperature as $I \sim \partial E / \partial \phi$, with $E$ the total energy of the system and $\phi$ the magnetic flux. The value of $I_{typ} \equiv \sqrt{\int I^2 \, d\phi}$ depends on the number of open channels present in the system $M$. For discrete systems with cylindrical geometry and away from half filling, $I_{typ} \sim \sqrt{M}$ [5,6]. This behavior can be understood taking into account the properties of the crossings (or quasicrossings) that appear in the spectrum when the flux is varied [7]. They occur mainly between levels belonging to different channels and frustrate the coherent increased of the current [8]. Although very particular geometric configurations can give rise to coherent contributions of all the channels [9,10], those sharp configurations are very difficult to obtain experimentally.

We consider a $N \times N$ cluster on a square lattice. In the following all the lengths will be given in units of $a$. Taking a single atomic level per lattice site the Hamiltonian is,

$$H = \sum_{m,n} \epsilon_{m,n} |m,n><m,n| + \sum_{m,n,m',n'} t_{m,n;m',n'} |m,n><m',n'|,$$

where $(m,n) \equiv m$ labels the coordinates of the sites in the lattice. The hopping integrals $t_{m,m'}$ are restricted to nearest neighbours. Assuming that the vector potential $A$ has only azimutal component we take $t_{m,m+1} = t \exp(i \int_{m}^{m+1} A \cdot dl)$, in units of the quantum flux $\phi_o$, where $l$ is a vector that points from the site $m$ to any of its four nearest neighbours.

With the on-site energies, $\epsilon_m$, we simulate the confining potential in order to obtain the required profile of the sample. In particular for an annular cavity with internal radius $r$ and external radius $R$, we define

$$\epsilon_m = \begin{cases} 
0 & \text{if } r \leq |m| \leq R \\
V & \text{otherwise ,}
\end{cases}$$

where $V$ is large enough to confine the carriers within the annulus. For the present geometry the two relevant length scales can be chosen as the internal radius $r$ and the mean width of the sample $W$. While the second determines
For a given value of the Fermi energy $E_F$, the ratio $s = W/r$ controls the strength of SR. For $s \gg 1$ and for carriers with a wavelength of the order of $a$, two successive scattering events by the inner and outer boundaries of the sample are uncorrelated. On the other hand, for $s \ll 1$ and the same wavelengths those events are strongly correlated. Therefore the eigenstates corresponding to these particular wavelengths will evolve from generic extended ones to strongly localized as the value of $s$ is reduced.

In order to describe our results we will focus in two representative samples: S1, with $W = 40$ and $r = 20$ and S2, with $W = 16$ and $r = 90$. The values are given in units of $a$. In both samples the averaged area of the sample is $A$ and equal to the total number of sites.

In Fig. 2, we show for sample S1 the bottom (Fig. 2(a)) and the quarter filling (Fig. 2(b)) regions of the energy spectrum as a function of the normalized flux $\phi/\phi_0$ together with a generic charge distribution for each region. Fig. 2(a) corresponds to the large wavelength numbers, that are the less sensitive ones to the effect of the SR. This region of the spectrum looks qualitatively similar to the spectrum of an integrable Aharonov-Bohm annular billiard [3]. That is, crossings between levels belonging to the same channel at $\alpha = 0$ and $\alpha = 1/2$ and crossings between levels belonging to different channels for $0 < \alpha < 1/2$. Moreover, a generic charge distribution corresponds to eigenstates with well defined value of the angular quantum number.

In the quarter filling region of the spectrum the typical wavelengths are greater than $a$ but small enough to make the states sensitive to the global polygonal shape of the sample. Therefore, as the energy increases, avoided crossings are showed up as a function of $\alpha$. The corresponding charge distributions are quite similar to those of a continuous polygonal billiard and are extended states in general (see Fig. 1(b)). In both energy regions, when an occupied level crosses (or quasicrosses) an empty one, the total current $I$ exhibits a discontinuity (or abrupt oscillation). The magnitude of $I_{typ}$ will be reduced with respect to the situation with no crossings in the interval $(0, \alpha/2)$ [3]. As it is shown in Fig. 2, below half filling, $I_{typ}$ is a highly fluctuating function of the number of particles $N_p$. This is a consequence of the randomness in the distribution of crossings (or quasicrossings) present in these regions of the spectrum [8]. For sample S2 a qualitative similar behavior is found.

The upper region of the spectrum, close to half filling, is shown in Fig. 2(a) for S1. As we have already mentioned, in this region the states are sensitive to the fine structure of the boundaries of the sample. A bunching of quasi-degenerated eigenenergies appears at zero flux corresponding to two different types of localized states. One type are the angular localized states whose characteristic charge distribution is depicted in the left side of Fig. 2(b). These states are trapped in regions where the sample has more steps on the boundaries. They are unsensitive to the magnetic flux and are the origin of the flat lines in the spectrum. The other type of states are mostly radially localized and look like whispering gallery modes. These states are sensitive to the magnetic flux and therefore will carry a finite current. The right side of Fig. 2(b) displays the characteristic charge distributions for these states. We remark that qualitatively the same description holds for sample S2. Nevertheless, as the fraction of angular localized states decreases with the width $W$ of the sample, the number of quasi-degenerated flat levels in the spectrum of S2 at half filling will be greater than in S1.

Opposite to what happens for models with diagonal disorder, for the present system the localization is obtained without introducing an additional scale of energy. Only remains the scale defined by the kinetic energy. Therefore, at zero flux, the energy of the localized states will be very close to zero. This is a consequence of the finite character of the spectrum and its symmetry.

In order to quantify the described effect we have to consider two energy scales. One is the mean level spacing $\Delta$ near half filling between levels of a given channel and in the absence of confinement, $\Delta = \hbar^2/\rho$, where $\rho$ is the mean density of states near half filling [3]. The other relevant energy scale, $\Delta_q$, is a measure of the effect of the confinement on the eigenstates and eigenvalues of the system without borders. To obtain a generic quantitative relation between $\Delta_q$ and $\Delta$ is not a simple task. However we present the following argument: for $W \rightarrow \infty$ the effect of the confinement tends to zero, and then $\Delta_q < \Delta/M$. On the other hand, for $W \rightarrow 0$ the effect of the SR is maximized and $\Delta_q > \Delta$. In this regime the eigenstates become angular localized, i.e. are not current carrying. By increasing $W$ we can go from one limit to the other one. Therefore in a wide intermediate regime it should be satisfied that $\Delta_q < \Delta < \Delta$.

When this condition is accomplished the interaction with the borders mixes states belonging almost all to different channels (i.e. mainly with similar angular momentum), making radially localized eigenfunctions, which corresponds to the quasidegenerated levels bunching at zero energy that are current carrying. Therefore even in the presence of SR, typical states like the whispering gallery modes survive in the discrete system close to half filling. This have an important consequence on the values of $I_{typ}$ close to half filling, as it is shown in Fig. 2 for both samples S1 and S2. As there are not crossings between occupied and empty levels in all the region of variation of the flux, $I_{typ}$ increases monotonically with $N_p$. A plateau occurs at the maximum value of $I_{typ}$ and appears when the flat levels (angular localized states) begin to be filled. As we have already mentioned the width of the plateau for S1 (Fig. 2(a)) is smaller than for S2 (Fig. 2(b)).

As far as we know the enhancement of the persistent currents due to confinement effects in discrete systems has

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not been addressed in previous theoretical works. We believe that the present work could help to understand early experimental results in Au rings [13] which have shown big discrepancies with the existing theories.

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FIG. 1. (a) Energy levels at the bottom of the spectrum as a function of the rescaled magnetic flux $\alpha$ for sample S1 together with a typical charge distribution. (b) Idem as (a) but for the quarter filling region of the spectrum.
FIG. 2. (a) Energy levels close to half filling as a function of the rescaled magnetic flux $\alpha$ for $S1$. (b) Typical charge distributions for angular localized states (left side) and radially localized states (right side).
FIG. 3. (a) Typical current as a function of $N_p$ for sample $S1$. (b) Idem as (a) for sample $S2$. 