On the way to meet the experimental observation of persistent current in a mesoscopic cylinder: A mean field study

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The behavior of persistent current in a mesoscopic cylinder threaded by an Aharonov–Bohm flux \( \phi \) is carefully investigated within a Hartree–Fock mean field approach. We examine the combined effect of second-neighbor hopping integral and Hubbard correlation on the enhancement of persistent current in presence of disorder. A significant change in current amplitude is observed compared to the traditional nearest-neighbor hopping model and the current amplitude becomes quite comparable to experimental realizations. Our analysis is found to exhibit several interesting results which have so far remained unaddressed.

1 Introduction

Over the last many years appearance of persistent current in metallic single-channel rings and multi-channel cylinders has drawn much attention in theoretical as well as in experimental research. In mesoscopic regime where dimensions of a system are comparable to mean free path of an electron the phase coherence of electronic states is of fundamental importance and the existence of dissipationless current in a mesoscopic conducting ring threaded by an Aharonov–Bohm (AB) flux \( \phi \) is a direct consequence of quantum phase coherence. In this new quantum regime, two important aspects appear at low temperatures and they are as follows.

(i) The phase coherence length \( L_\phi \) i.e., the length scale for which an electron maintains its phase memory, increases significantly with the lowering of temperature and becomes comparable to the system size \( L \).
(ii) The energy levels of these small finite size systems are discrete.

These two are the most essential criteria for the existence of persistent current in a small metallic ring/cylinder due to the application of an external magnetic flux \( \phi \). In the pioneering work of Büttiker, Imry and Landauer [1], the appearance of persistent current in metallic rings has been explored. Later, many excellent experiments [2–7] have been carried out in several ring and cylindrical geometries to reveal the actual mechanisms of persistent current. Though much efforts have been paid to study persistent current both theoretically [8–29] as well as experimentally [2–7], yet several drawbacks still exist between the theory and experiment, and the full knowledge about it in this scale is not well established even today.

The results of the single loop experiments are significantly different from those for the ensemble of isolated loops. Persistent currents with expected \( \phi_0 \) periodicity have been observed in isolated single Au rings [3] and in a GaAs-AlGaAs ring [4]. Levy et al. [2] found oscillations with period \( \phi_0/2 \) rather than \( \phi_0 \) in an ensemble of \( 10^7 \) independent Cu rings. Similar \( \phi_0/2 \) oscillations were also reported for an ensemble of disconnected \( 10^3 \) independent Ag rings [6] as well as for an array of \( 10^5 \) isolated GaAs-AlGaAs rings [7]. In a recent experiment, Jariwala et al. [5] obtained both \( \phi_0 \) and \( \phi_0/2 \) periodic persistent currents in an array of 30 diffusive mesoscopic Au rings. Except for the case of the nearly ballistic GaAs-AlGaAs ring [4], all the measured currents are in general one or two orders of magnitude larger than those expected from the theory.
Free electron theory predicts that at $T = 0$, an ordered one-dimensional metallic ring threaded by magnetic flux $\phi$ supports persistent current with maximum amplitude $I_0 = ev_F/L$, where $v_F$ is the Fermi velocity and $L$ is the circumference of the ring. Metals are intrinsically disordered which tends to decrease the persistent current, and the calculations show that the disorder-averaged current $(\langle I \rangle)$ crucially depends on the choice of the ensemble [9, 13, 14]. The magnitude of the current $(\langle I^2 \rangle)^{1/2}$ is however insensitive to the averaging issues, and is of the order of $I_0/L$, $I_0$ being the elastic mean free path of the electrons. This expression remains valid even if one takes into account the finite width of the ring by adding contributions from the transverse channels, since disorder leads to a compensation between the channels [9, 13]. However, the measurements on an ensemble of $10^7$ Cu rings [2] reported a diamagnetic persistent current of average amplitude $3 \times 10^{-3} ev_F/L$ with half a flux-quantum periodicity. Such $\phi_0/2$ oscillations with diamagnetic response were also found in other persistent current experiments consisting of ensemble of isolated rings [6, 7].

Measurements on single isolated mesoscopic rings on the other hand detected $\phi_0$-periodic persistent currents with amplitudes of the order of $I_0 \sim ev_F/L$, (closed to the value for an ordered ring). Theory and experiment [4] seem to agree only when disorder is weak. In another recent nice experiment Bluhm et al. [30] have measured the magnetic response of 33 individual cold mesoscopic gold rings, one ring at a time, using a scanning SQUID technique. They have measured the plane component and predicted that the measured current amplitude agrees quite well with theory [8] in a single ballistic ring [4] and an ensemble of 16 nearly ballistic rings [31]. However, the amplitudes of the currents in single-isolated-diffusive gold rings [3] were two orders of magnitude larger than the theoretical estimates. This discrepancy initiated intense theoretical activity, and it is generally believed that the electron–electron correlation plays an important role in the disordered diffusive rings [19–21]. An explanation based on the perturbative calculation in presence of interaction and disorder has been proposed and it seems to give a quantitative estimate closer to the experimental results, but still it is less than the measured currents by an order of magnitude, and the interaction parameter used in the theory is not well understood physically. Most of these theoretical results have been obtained based on a tight-binding framework within the nearest-neighbor hopping (NNH) approximation. This is an important approximation and it has been shown that within the NNH model electronic correlation provides a small enhancement of current amplitude in disordered materials i.e., a weak delocalizing effect is observed in presence of electron–electron (e–e) interaction. As an attempt in the present work we modify the traditional NNH model by incorporating the effects of higher order hopping integrals, at least second-neighbor hopping (SNH), in addition to the NNH integral. It is also quite physical since electrons have some finite probabilities to hop from one site to other sites apart from nearest-neighbor with reduced strengths. We will show that the inclusion of higher order hopping integrals gives significant enhancement of current amplitude and it reaches quite closer to the current amplitude of ordered systems.

The other important controversy comes for the determination of the sign of low-field currents and still it is an unresolved issue between theoretical and experimental results. In an experiment on persistent current Levy et al. [2] have shown diamagnetic nature for the measured currents at low-field limit. While, in other experiment Chandrasekhar et al. [3] have obtained paramagnetic response near zero field limit. Jariwala et al. [5] have predicted diamagnetic persistent current in their experiment and similar diamagnetic response in the vicinity of zero field limit were also supported in an experiment done by Debloock [6] et al. on Ag rings. Yu and Fowler [22] have shown both diamagnetic and paramagnetic responses in mesoscopic Hubbard rings. Though in a theoretical work Cheung et al. [9] have predicted that the direction of current is random depending on the total number of electrons in the system and the specific realization of the random potentials. Hence, prediction of the sign of low-field currents is still an open challenge and further studies on persistent current in mesoscopic systems are needed to remove the existing controversies.

In the present paper we address the behavior of persistent current in an interacting mesoscopic ring with finite width threaded by an Aharonov–Bohm flux $\phi$. A simple tight-binding Hamiltonian is used to illustrate the system and all the calculations are performed within a mean field approach. Using a generalized Hartree–Fock (HF) approximation [32, 33], we compute numerically persistent current $(I)$ as functions of AB flux $\phi$, total number of electrons $N_e$, e–e interaction strength $U$, SNH integral, disorder strength $W$, and system size $N$. The main motivation of the present work is to illustrate the effects of higher order hopping integrals on the enhancement of persistent current in disordered mesoscopic cylinders. Our results can be utilized to study magnetic response in any interacting mesoscopic system.

In what follows, we present the results. In Section 2, we describe the geometric model and generalized Hartree–Fock theory to study magnetic response in the model quantum system. Section 3 contains the numerical results. Finally, in Section 4 we draw our conclusions.

2 Model and synopsis of the theoretical formulation Let us start by referring to Fig. 1, where a small metallic cylinder is threaded by a magnetic flux $\phi$. The filled black circles correspond to the positions of the atomic sites in the cylinder. To predict the size of a cylinder we use two parameters $N$ and $M$, where the 1st one ($N$) represents total number of atomic sites in each circular ring and the other one ($M$) gives total number of identical circular rings. For the description of our model quantum system we use a tight-binding (T-B) framework and in order to incorporate the effect of higher order hopping integrals to the Hamiltonian here we consider SNH (shown by the red
dashed line in Fig. 1) in addition to the NNH of electrons. Considering both NNH and SNH integrals the T-B Hamiltonian for the cylindrical system in Wannier basis looks in the form

\[ H_c = \sum_{i,j} \varepsilon_{ij,\sigma} c_{ij,\sigma}^\dagger c_{ij,\sigma} + \sum_{i,j} t_{ij} \left[ e^{i\theta_i} c_{ij,\sigma}^\dagger c_{i+1,j,\sigma} + \text{h.c.} \right] + \sum_{ij} t_d^{ij} \left[ e^{i\theta_d} c_{ij,\sigma}^\dagger c_{i+1,j+1,\sigma} + \text{h.c.} \right] + \sum_{ij} U_{ij} c_{ij,\uparrow}^\dagger c_{ij,\downarrow}^\dagger c_{ij,\downarrow} c_{ij,\uparrow} + \text{h.c.} \right] \]  

(1)

where \((i, j)\) represent the co-ordinate of a lattice site. The index \(i\) runs from 1 to \(M\), while the integer \(j\) goes from 1 to \(N\). \(\varepsilon_{ij,\sigma}\) is the on-site energy of an electron at the site \((i, j)\) of spin \(\sigma\) (\(\uparrow, \downarrow\)). \(t_{ij}\) and \(t_d^{ij}\) are the NNH and SNH integrals, respectively. Due to the presence of magnetic flux \(\Phi\) (measured in unit of the elementary flux quantum \(\Phi_0 = \hbar c/4e\)), a phase factor \(\theta_i = 2\pi\Phi_i/\Phi_0\) appears in the Hamiltonian when an electron hops longitudinally from one site to its neighboring site, and accordingly, a negative sign comes when the electron hops in the reverse direction. \(\theta_d\) is the associated phase factor for the diagonal motion of an electron between two neighboring concentric rings. No phase factor appears when an electron moves along the vertical direction which is set by proper choice of the gauge for the vector potential \(\mathbf{A}\) associated with the magnetic field \(\mathbf{B}\), and this choice makes the phase factors \((\theta_i, \theta_d)\) identical to each other for the longitudinal and diagonal motions. Since the magnetic field corresponding to the AB flux \(\Phi\) does not penetrate anywhere of the surface of the cylinder, we ignore Zeeman term in the above tight-binding Hamiltonian (Eq. (1)). \(c_{ij,\sigma}\) and \(c_{ij,\sigma}^\dagger\) are the creation and annihilation operators, respectively, of an electron at the site \((i, j)\) with spin \(\sigma\). \(U\) is the on-site Hubbard interaction term.

2.1 Decoupling of the interacting Hamiltonian

To get the energy eigenvalues of the interacting model quantum system described by the above tight-binding Hamiltonian given in Eq. (1), first we decouple the interacting Hamiltonian using generalized Hartree–Fock approach, the so-called mean field approximation. In this procedure, the full Hamiltonian is completely decoupled into two parts. One is associated with the up-spin electrons, while the other is related to the down-spin electrons with their modified site energies. For up and down spin Hamiltonians, the modified site energies are expressed in the form

\[ \varepsilon'_{i,j,\sigma} = \varepsilon_{i,j,\sigma} + U\langle n_{i,j,\sigma} \rangle, \]  

(2)

\[ \varepsilon'_{i,j,\sigma} = \varepsilon_{i,j,\sigma} + U\langle n_{i,j,\sigma} \rangle, \]  

(3)

where \(n_{i,j,\sigma} = c_{i,j,\sigma}^\dagger c_{i,j,\sigma}\) is the number operator. With these site energies, the full Hamiltonian (Eq. (1)) can be written in the decoupled form as

\[ H_c = \sum_{ij} \varepsilon'_{ij,\sigma} n_{ij,\sigma} + \sum_{ij} t_{ij} \left[ e^{i\theta_i} n_{ij,\uparrow} + \text{h.c.} \right] + \sum_{ij} t_d^{ij} \left[ e^{i\theta_d} n_{ij,\downarrow} + \text{h.c.} \right] + \sum_{ij} U_{ij} N_{ij} + \text{h.c.} \]  

(4)

where \(H_1\) and \(H_d\) correspond to the effective tight-binding Hamiltonians for the up and down spin electrons, respectively. The last term is a constant term which provides an energy shift in the total energy.

2.2 Self consistent procedure

With these decoupled Hamiltonians \((H_1\) and \(H_d)\) of up and down spin electrons, now we start our self consistent procedure considering initial guess values of \(\langle n_{ij,\uparrow} \rangle\) and \(\langle n_{ij,\downarrow} \rangle\). For these initial set of values of \(\langle n_{ij,\uparrow} \rangle\) and \(\langle n_{ij,\downarrow} \rangle\), we numerically diagonalize the up and down spin Hamiltonians. Then we calculate a new set of values of \(\langle n_{ij,\uparrow} \rangle\) and \(\langle n_{ij,\downarrow} \rangle\). These steps are repeated until a self consistent solution is achieved.

2.3 Calculation of ground state energy

After achieving the self consistent solution, the ground state energy \(E_0\) for a particular filling at absolute zero temperature \((T = 0\ \text{K})\) can be determined by taking the sum of individual states up to Fermi energy \((E_F)\) for both up and down spins. Thus, we can write the final form of ground state energy as

\[ E_0 = \sum_p E_{p,\uparrow} + \sum_p E_{p,\downarrow} - \sum_{ij} U\langle n_{ij,\uparrow} \rangle\langle n_{ij,\downarrow} \rangle, \]  

(5)

where the index \(p\) runs for the states up to the Fermi level. \(E_{p,\uparrow} (E_{p,\downarrow})\) is the single particle energy eigenvalue for \(p\)-th eigenstate obtained by diagonalizing the Hamiltonian \(H_1\) \((H_d)\).
2.4 Calculation of persistent current

At absolute zero temperature, total persistent current of the system is obtained from the expression

\[ I(\phi) = -e \frac{\partial E_0(\phi)}{\partial \phi}, \]  

(6)

where \( E_0(\phi) \) is the ground state energy for a particular filling.

In the present work we perform all the essential features of persistent current at absolute zero temperature and use the units where \( c = h = e = 1 \). Throughout our numerical calculations we set the NNH strength \( t_l = -1 \) and fix \( M = 2 \) i.e., cylinders with two identical rings. Energy scale is measured in unit of \( t_l \).

3 Numerical results and discussion

Following the above theoretical prescription now we start to analyze our numerical results. We describe the results in three different parts. In the first part, we consider perfect cylinders with only NNH integral. In the second part, disordered cylinders described with only NNH integral are considered. Finally, in the third part we discuss the effect of SNH integral on the enhancement of persistent current in disordered cylinders.

3.1 Perfect cylinders with NNH integral

For perfect cylinders we choose \( a_{i,j} = a_{j,i} = 0 \) for all \((i, j)\). Since here we consider the cylinders described with NNH integral only, the SNH strength \( t_d \) is fixed to zero.

3.1.1 Energy-flux characteristics

As illustrative in examples, in Fig. 2 we show the variation of ground state energy levels as a function of magnetic flux \( \phi \) for some typical mesoscopic cylinders where \( N \) is fixed at 5 (odd \( N \)). In (a) the results are given for the quarterly-filled \((N_e = 5)\) cylinders, while in (b) the curves correspond to the results for the half-filled \((N_e = 10)\) cylinders. The red, green, and blue lines represent the ground state energy levels for \( U = 0, 0.5, \) and 1, respectively. It is observed that the ground state energy shows oscillatory behavior as a function of \( \phi \) and the energy increases as the electronic correlation strength \( U \) gets increased. Most significantly we see that the ground state energy levels give two different types of periodicities depending on the electron filling. At quarter-filling, ground state energy level gives \( \phi_0 = 1 \), since \( c = h = e = 1 \) in our chosen unit system, flux-quantum periodicity. On the other hand, at half-filling it shows \( \phi_0/2 \) flux-quantum periodicity. The situation becomes quite different when the total number of atomic sites \( N \) in individual rings is even. For our illustrative purposes in Fig. 3 we plot the lowest energy levels as a function of \( \phi \) for some typical mesoscopic cylinders considering \( N = 8 \) (even \( N \)). The curves of different colors correspond to the identical meaning as in Fig. 2. From the spectra given in Figs. 3(a) (quarter-filled case) and (b) (half-filled case) it is clearly observed that the ground state energy levels vary periodically with AB flux \( \phi \) exhibiting only \( \phi_0 \) flux-quantum periodicity. Thus, it can be emphasized.

Figure 2 (online color at: www.pss-b.com) Ground state energy levels as a function of flux \( \phi \) for some perfect cylinders with \( N = 5 \) and \( M = 2 \). The red, green, and blue curves correspond to \( U = 0, 0.5, \) and 1, respectively. (a) Quarter-filled case and (b) half-filled case.

Figure 3 (online color at: www.pss-b.com) Ground state energy levels as a function of flux \( \phi \) for some perfect cylinders considering \( N = 8 \) and \( M = 2 \). The red, green, and blue curves correspond to \( U = 0, 0.5, \) and 1, respectively. (a) Quarter-filled case and (b) half-filled case.
that the appearance of half flux-quantum periodicity strongly depends on the electron filling as well as on the oddness and evenness of the total number of atomic sites $N$ in individual rings. Only for the half-filled cylinders with odd $N$, the lowest energy level gets $\phi_0/2$ periodicity with flux $\phi$. Now it is important to note that this half flux-quantum periodicity does not depend on the width ($M$) of the cylinder and also it is independent of the Hubbard correlation strength $U$. Hence, depending on the system size and filling of electrons variable periodicities are observed in the variation of lowest energy level. It may provide an important signature in studying magnetic response in nano-scale loop geometries.

### 3.1.2 Current-flux characteristics

In Fig. 4 we display the current–flux characteristics for some impurity free mesoscopic cylinders considering $M = 2$. In (a) the results are given for the half-filled case where we set $N = 15$. The red line corresponds to the current for the non-interacting ($U = 0$) case, while the green and blue lines represent the currents when $U = 1.5$ and $2$, respectively. From the curves we notice that the current amplitude gradually decreases with the increase of electronic correlation strength $U$. The reason is that at half-filling each site is occupied by at least one electron of up spin or down spin, and the placing of a second electron of opposite spin needs more energy due to the repulsive effect of $U$. Thus conduction becomes difficult as it requires more energy when an electron hops from its own site and situates at the neighboring site. Now both for the non-interacting and interacting cases, current shows half flux-quantum periodicity as a function of $\phi$ obeying the energy–flux characteristics since here we choose odd $N$ ($N = 15$). The behavior of the persistent currents for even $N$ is shown in (b) where we set $N = 20$. The currents are drawn for the quarter-filled case i.e., $N = 20$, where the red, green, and blue curves correspond to $U = 0$, 2, and 3, respectively. The reduction of current amplitude with the increase of Hubbard interaction strength is also observed for this quarter-filled case, similar to the case of half-filled as described earlier. But the point is that at quarter-filling, the reduction of current amplitude is much smaller compared to the half-filled situation. This is quite obvious in the sense that at less than half-filling “empty” lattice sites are available where electrons can hop easily without any cost of extra energy and the conduction becomes much easier than the half-filled situation. In this quarter-filled case, persistent currents provide only $\phi_0$ flux-quantum periodicity following the $E-\phi$ diagram. From these current–flux characteristics it can be concluded that for “ordered” cylinders current amplitude always decreases with the enhancement in Hubbard correlation strength $U$.

![Figure 4](online color at: www.pss-b.com) Persistent current as a function of flux $\phi$ for some ordered mesoscopic cylinders considering $M = 2$. (a) Half-filled case with $N = 15$. The red, green, and blue curves correspond to $U = 0$, 1.5, and 2, respectively. (b) Quarter-filled case with $N = 20$. The red, green, and blue curves correspond to $U = 0$, 2, and 3, respectively.

### 3.2 Disordered cylinders with NNH integral

In order to describe the effect of impurities on electron transport now we focus our attention on the results of some typical disordered cylinders described with NNH integral. Here we consider the diagonal disordered cylinders i.e., impurities are introduced only at the site energies without disturbing the hopping integrals. The site energies in each concentric ring are chosen from a correlated distribution function which looks in the form

$$ e_{j,\dagger} = e_{j,\downarrow} = W \cos(j\lambda\pi), $$

where $W$ is the impurity strength, $\lambda$ an irrational number and we choose $\lambda = (1 + \sqrt{5})/2$, for the sake of our illustration. Setting $\lambda = 0$, we get back the pure system with uniform site energy $W$. Now, instead of considering site energies from a correlated distribution function, as mentioned above in Eq. 7, we can also take them randomly from a “Box” distribution function of width $W$. But in the later case we have to take the average over a large number of disordered configurations (from the stand point of statistical average) and since it is really a difficult task in the aspect of numerical computation we select the other option. Not only that in the averaging process several mesoscopic phenomena may disappear. Therefore, the averaging process is an important issue in low-dimensional systems.

In presence of disorder, energy levels get modified significantly. For our illustrative purposes in Fig. 5 we plot ground state energy levels as a function of magnetic flux $\phi$ for some disordered mesoscopic cylinders when they are half-filled. The Hubbard interaction strength $U$ is set at 1 and the impurity strength $W$ is fixed to 2. In (a) the ground state...
energy level is shown for a cylinder with $N = 5$ (odd), while in (b) it is presented for a cylinder taking $N = 8$ (even). Quite interestingly we see that for the cylinder with odd $N$, the half flux-quantum periodicity of the lowest energy level disappears in the presence of impurity and it provides conventional $\phi_0$ periodicity. Hence, for cylinders with odd $N$, $\phi_0/2$ flux-quantum periodicity will be observed only when they are free from any impurity. For the disordered cylinder with even $N$ ($N = 8$), the lowest energy level as usual provides $\phi_0$ periodicity similar to the impurity free cylinders containing even $N$. Apart from this periodic nature, impurities play another significant role in the determination of the slope of the energy levels. The slope of the lowest energy level decreases significantly compared to the perfect case, and therefore, a prominent change in current amplitude also takes place.

To justify the above facts, in Fig. 6 we present the variations of persistent currents with AB flux $\phi$ for a half-filled mesoscopic cylinder, described in the framework of NNH model, considering $N = 15$ and $M = 2$. The red curve represents the current for the ordered ($W = 0$) non-interacting ($U = 0$) cylinder. It shows saw-tooth like nature with flux $\phi$ providing $\phi_0/2$ flux-quantum periodicity. The situation becomes completely different when impurities are introduced in the cylinder as seen by the other two curves. The green curve represents the current for the case only when impurities are considered but the effect of electronic correlation is not taken into account. It shows a continuous like nature with $\phi_0$ flux-quantum periodicity. The most important observation is that the current amplitude gets reduced enormously, even an order of magnitude, compared to the perfect cylinder. This is due to the localization of the energy eigenstates in the presence of impurity, which is the so-called Anderson localization. Hence, a large difference exists in the current amplitudes of an ordered and disordered non-interacting cylinders and it was the main controversial issue among the theoretical and experimental predictions. Experimental verifications suggest that the measured current amplitude is quite comparable to the theoretical current amplitude obtained in a perfect system. To remove this controversy, as a first attempt, we include the effect of e–e correlation in the disordered cylinder described by the NNH model. The result is shown by the blue curve where $U$ is fixed at 1.5. It is observed that the current amplitude gets increased compared to the non-interacting disordered cylinder, though the increment is too small. Not only that the enhancement can take place only for small values of $U$, while for large enough $U$ the current amplitude rather decreases. This phenomenon can be implemented as follows. For the non-interacting disordered cylinder the probability of getting two opposite spin electrons becomes higher at the atomic sites where the site energies are lower than the other sites since the electrons get pinned at the lower site energies to minimize the ground state energy, and this pinning of electrons becomes increased with the rise of impurity strength $W$. As a result the mobility of electrons and hence the current amplitude gets reduced with the increase of impurity strength $W$. Now, if we introduce electronic correlation in the system then it tries to depin two opposite spin electrons those are situated together due to the Coulomb repulsion. Therefore, the electronic mobility is enhanced which provides larger current amplitude. But, for large enough interaction strength, no electron can able to hop from one site to other at the half-filling since then each site is occupied either by an up or down spin electron which does not allow other electron of opposite spin due to the repulsive term $U$. Accordingly, the current
amplitude gradually decreases with \( U \). On the other hand, at less than half-filling though there is some finite probability to hop an electron from one site to the other available “empty” site but still it is very small. So, in brief, we can say that within the NNH approximation electron–electron interaction does not provide any significant contribution to enhance the current amplitude, and hence the controversy regarding the current amplitude still persists.

3.3 Disordered cylinders with NNH and SNH integrals

To overcome the existing situation regarding the current amplitude, in this sub-section, finally we make an attempt by incorporating the effect of SNH integral in addition to the NNH integral.

A significant change in current amplitude takes place when we include the contribution of SNH integral in addition to the NNH integral. As representative examples, in Fig. 7 we plot the current–flux characteristics for a half-filled mesoscopic cylinder considering \( N = 15 \) and \( M = 2 \). The black, magenta, and gold lines correspond to the results in the presence of NNH integral, while the other three colored curves (red, green, and blue) represent the currents in the absence of SNH integral. Here we choose \( t_d = -0.6 \). The black curve refers to the persistent current for the perfect (\( W = 0 \)) non-interacting (\( U = 0 \)) cylinder and it achieves much higher amplitude compared to the NNH model (red curve). This additional contribution comes from the SNH integral since it allows electrons to hop further. In addition it is also noticed that the current varies periodically with \( \phi \) providing \( \phi_0/2 \) flux-quantum periodicity, instead of \( \phi_0/2 \) as in the case of NNH integral model (red curve). Thus, it can be emphasized that \( \phi_0/2 \) periodicity will be observed only when the cylinder is (a) free from impurity, (b) half-filled, (c) made with odd \( N \), and (d) described by the NNH model. The main focus of this sub-section is to interpret the combined effect of SNH integral and electron–electron correlation on the enhancement of persistent current amplitude in disordered cylinder. To do this we narrate the effect of SNH integral in disordered non-interacting cylinder. The nature of the current for this particular case is shown by the magenta curve of Fig. 7. It shows that the current amplitude gets reduced compared to the perfect case (black line), which is expected, but the reduction of the current amplitude is quite small than the NNH integral model. This is due the fact that the SNH integral tries to delocalize the electronic states, and therefore, the mobility of the electrons is enriched. The situation becomes more interesting when we include the effect of Hubbard interaction. The behavior of the current in the presence of interaction is plotted by the gold curve of Fig. 7 where we fix \( U = 1.5 \). Very interestingly, we see that the current amplitude is enhanced significantly and quite comparable to that of the perfect cylinder.

For better clarity of the results discussed above, in Fig. 8 we also present the similar feature of persistent current for other hopping strength of SNH integral. Here we set \( t_d = -0.8 \). From these curves we see that the current amplitude gets enhanced more as we increase the SNH strength.

Thus, it can be predicted that the presence of SNH integral and Hubbard interaction can provide a persistent current which may be comparable to the measured current amplitudes. In this presentation we consider the effect of only SNH integral as a higher order hopping integral in addition to the NNH model, and, illustrate how such a higher order hopping integral leads an important role on the enhancement of current amplitude in presence of Hubbard correlation for disordered cylinders. Instead of considering only the SNH integral we can also take the contributions

**Figure 7** (online color at: www.pss-b.com) Persistent current as a function of flux \( \phi \) for a half-filled mesoscopic cylinder taking \( N = 15 \) and \( M = 2 \) in the presence of NNH and SNH integrals. The black line corresponds to the ordered case when \( U = 0 \), whereas the magenta and gold lines correspond to the disordered case (\( W = 2 \)) when \( U = 0 \) and 1.5, respectively. Here SNH integral is fixed at \(-0.6\). The currents shown by the red, green, and blue lines for the ring described with NNH model (identical to Fig. 6) are re-plotted to judge the effect of SNH integral over NNH model much clearly.

**Figure 8** (online color at: www.pss-b.com) Persistent current as a function of flux \( \phi \) for a half-filled mesoscopic cylinder taking \( N = 15 \) and \( M = 2 \) in the presence of NNH and SNH integrals. The black line corresponds to the ordered case when \( U = 0 \), whereas the magenta and gold lines correspond to the disordered case (\( W = 2 \)) when \( U = 0 \) and 1.5, respectively. Here SNH integral is fixed at \(-0.8\). The currents shown by the red, green, and blue lines for the ring described with NNH model (identical to Fig. 6) are re-plotted to judge the effect of SNH integral over NNH model much clearly.
from all possible higher order hopping integrals with reduced hopping strengths. Since the strengths of other higher order hopping integrals are too small, the contributions from these factors are reasonably small and they will not provide any significant change in the current amplitude. Finally, we can say that further studies are needed by incorporating all these factors.

4 Conclusion To summarize, in the present work we have addressed the behavior of persistent current in an interacting mesoscopic cylinder threaded by an Aharonov–Bohm flux $\phi$. We have adopted a tight-binding Hamiltonian to describe the model quantum system and all the numerical calculations have been done within a mean field approximation. Using the generalized Hartree–Fock (HF) approximation, we have computed persistent current as functions of SNH integral, impurity strength $W$, AB flux $\phi$, electron filling $N/N$, and system size $N$. Our numerical results have provided several interesting features and the present study may be helpful in understanding magnetic response in nano-scale loop geometries.

The essential features observed from our analysis are as follows.

(i) In the determination of the lowest energy level we see that the energy level varies periodically with $\phi$ exhibiting both $\phi_{0}/2$ and $\phi_{0}$ flux-quantum periodicities depending on the choices of the parameters describing the tight-binding Hamiltonian.

(ii) In the NNH model, current amplitude gets significantly reduced when impurities are introduced in the system. With the inclusion of Hubbard interaction ($U$), the current amplitude can be enhanced, though the enhancement becomes too small compared to the experimental verifications.

(iii) A significant change in the current amplitude takes place when the effect of SNH integral is taken into account. The combined effect of SNH and Hubbard interaction can provide the current which is quite comparable to the experimental realizations. So in short we can say that the conventional NNH model can be modified by incorporating the higher order hopping integrals.

Throughout the analysis we have kept the width of the cylinders at a fixed value ($M = 2$), for the sake of our illustration. All these results are also valid for cylinders of larger widths. Here we have considered several important approximations by ignoring the effects of temperature, electron-phonon interaction, etc. Due to these factors, any scattering process that appears in the cylinder would have influence on electronic phases. At the end, we would like to say that we need further study in such systems by incorporating all these effects.

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References

[1] M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. 96A, 365 (1983).
[2] L. P. Levy, G. Dolan, J. Dunsmuir, and H. Bouchiat, Phys. Rev. Lett. 64, 2074 (1990).
[3] V. Chandrasekhar, R. A. Webb, M. J. Brady, M. B. Ketchen, W. J. Gallagher, and A. Kleinsasser, Phys. Rev. Lett. 67, 3578 (1991).
[4] D. Mailly, C. Chapelier, and A. Benoist, Phys. Rev. Lett. 70, 2020 (1993).
[5] E. M. Q. Jariwala, P. Mohanty, M. B. Ketchen, and R. A. Webb, Phys. Rev. Lett. 86, 1594 (2001).
[6] R. Debloch, R. Bel, B. Reulet, H. Bouchiat, and D. Mailly, Phys. Rev. Lett. 89, 206803 (2002).
[7] B. Reulet, M. Ramin, H. Bouchiat, and D. Mailly, Phys. Rev. Lett. 75, 124 (1995).
[8] H. F. Cheung, Y. Gefen, E. K. Riedel, and W. H. Shih, Phys. Rev. B 37, 6050 (1988).
[9] H. F. Cheung and E. K. Riedel, Phys. Rev. Lett. 62, 587 (1989).
[10] L. K. Castelano, G.-Q. Bai, B. Partoens, and F. M. Peeters, Phys. Rev. B 78, 195315 (2008).
[11] M. Zarenia, M. J. Pereira, F. M. Peeters, and G. de Farias, Phys. Rev. B 81, 045431 (2010).
[12] D. Y. Vodolazov, F. M. Peeters, T. T. Hongisto, and K. Yu. Arutyunov, Europhys. Lett. 75, 315 (2006).
[13] G. Montambaux, H. Bouchiat, D. Sigeti, and R. Friesner, Phys. Rev. B 42, 7647 (1990).
[14] M. Abraham and R. Berkovits, Phys. Rev. Lett. 70, 1509 (1993).
[15] F. von Oppen and E. K. Riedel, Phys. Rev. Lett. 66, 84 (1991).
[16] G. Schmid, Phys. Rev. Lett. 66, 80 (1991).
[17] V. Ambegaokar and U. Eckern, Phys. Rev. Lett. 65, 381 (1990).
[18] B. L. Altshuler, Y. Gefen, and Y. Imry, Phys. Rev. Lett. 66, 88 (1991).
[19] B. Reulet, M. Ramin, H. Bouchiat, and D. Mailly, Phys. Rev. Lett. 75, 124 (1995).
[20] T. Giamarchi and B. S. Shastry, Phys. Rev. B 39, 6050 (1989).
[21] V. Chandrasekhar and P. Onorato, Physica E 45, 8258 (1994).
[22] M. Abraham and R. Berkovits, Phys. Rev. Lett. 70, 1509 (1993).
[23] G. Bouzerar, D. Poilblanc, and G. Montambaux, Phys. Rev. B 94, 9258 (2014).
[24] G. Montambaux, H. Bouchiat, D. Sigeti, and R. Friesner, Europhys. Lett. 75, 315 (2006).
[25] H. Bouchiat and G. Montambaux, J. Phys. (Paris) 50, 2695 (1999).
[26] L. A. Kastelano, G.-Q. Hai, B. Partoens, and F. M. Peeters, Phys. Rev. B 78, 195315 (2008).
[27] M. Zarenia, M. J. Pereira, F. M. Peeters, and G. de Farias, Phys. Rev. B 81, 045431 (2010).
[28] D. Y. Vodolazov, F. M. Peeters, T. T. Hongisto, and K. Yu. Arutyunov, Europhys. Lett. 75, 315 (2006).
[29] G. Montambaux, H. Bouchiat, D. Sigeti, and R. Friesner, Phys. Rev. B 42, 7647 (1990).
[30] H. Bouchiat and G. Montambaux, J. Phys. (Paris) 50, 2695 (1999).
[31] L. A. Kastelano, G.-Q. Hai, B. Partoens, and F. M. Peeters, Phys. Rev. B 78, 195315 (2008).
[32] M. Zarenia, M. J. Pereira, F. M. Peeters, and G. de Farias, Phys. Rev. B 81, 045431 (2010).
[33] D. Y. Vodolazov, F. M. Peeters, T. T. Hongisto, and K. Yu. Arutyunov, Europhys. Lett. 75, 315 (2006).
[34] G. Montambaux, H. Bouchiat, D. Sigeti, and R. Friesner, Phys. Rev. B 42, 7647 (1990).
[35] H. Bouchiat and G. Montambaux, J. Phys. (Paris) 50, 2695 (1999).
[36] L. A. Kastelano, G.-Q. Hai, B. Partoens, and F. M. Peeters, Phys. Rev. B 78, 195315 (2008).
[37] M. Zarenia, M. J. Pereira, F. M. Peeters, and G. de Farias, Phys. Rev. B 81, 045431 (2010).
[38] D. Y. Vodolazov, F. M. Peeters, T. T. Hongisto, and K. Yu. Arutyunov, Europhys. Lett. 75, 315 (2006).
[39] G. Montambaux, H. Bouchiat, D. Sigeti, and R. Friesner, Phys. Rev. B 42, 7647 (1990).
[40] H. Bouchiat and G. Montambaux, J. Phys. (Paris) 50, 2695 (1999).