Persistent currents with long-range hopping in 1D single-isolated-diffusive rings

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Abstract

We show from exact calculations that a simple tight-binding Hamiltonian with diagonal disorder and long-range hopping integrals, falling off as a power \( \mu \) of the inter-site separation, correctly describes the experimentally observed amplitude (close to the value of an ordered ring) and flux-periodicity \( (hc/e) \) of persistent currents in single-isolated-diffusive normal metal rings of mesoscopic size. Long-range hopping integrals tend to delocalize the electrons even in the presence of disorder resulting orders of magnitude enhancement of persistent current relative to earlier predictions.

Keywords: Model Calculations, Magnetotransport

The phenomenon of persistent current in mesoscopic normal metal rings has generated a lot of excitement as well as controversy over the past years. In a pioneering work, Büttiker, Imry and Landauer predicted that, even in the presence of disorder, an isolated 1D metallic ring threaded by magnetic flux \( \phi \) can support an equilibrium persistent current with periodicity \( \phi_0 = ch/e \), the flux quantum. Later, experimental observations confirm the existence of persistent currents in isolated mesoscopic rings. However, these experiments yield many results that are not well-understood theoretically even today.

The calculations show that the disorder-averaged current \( \langle I \rangle \) crucially depends on the choice of the ensemble of isolated loops. Persistent currents with expected \( \phi_0 \) periodicity have been observed in isolated single Au rings \( \phi_0 \) and in a GaAs-AlGaAs ring \( \phi_0 \). Levy et al. 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 \( 10^5 \) Ag rings \( \phi_0 \) as well as for an array of \( 10^5 \) isolated GaAs-AlGaAs rings \( \phi_0 \). In a recent experiment, Jariwala et al. obtained both \( \phi_0 \) and \( \phi_0/2 \) periodic persistent currents in an array of thirty diffusive mesoscopic Au rings. Except for the case of the nearly ballistic GaAs-AlGaAs ring \( \phi_0 \), all the measured currents are in general one or two orders of magnitude larger than those expected from the theory \( \phi_0 \). The diamagnetic response of the measured \( \phi_0/2 \) oscillations of ensemble-averaged persistent currents near zero magnetic field also contrasts with most predictions \( \phi_0 \).

Free electron theory predicts that at \( T = 0 \), an ordered 1D 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 \( \phi_0 \). The magnitude of the current \( \langle I \rangle \) is however insensitive to the averaging issues, and is of the order of \( I_0/L \), \( L \) 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 \( \phi_0 \). However, the measurements on an ensemble of \( 10^7 \) Cu rings \( \phi_0 \) 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 \( \phi_0 \).

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 \( \phi_0 \) seem to agree only when disorder is weak. However, the amplitudes of the currents in single-isolated-diffusive gold rings \( \phi_0 \) 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 \( \phi_0 \), though the physical origin behind this enhancement of persistent current is still unclear.

In this letter we will address the problem of enhancement of persistent current in single-isolated-diffusive...
(SID) mesoscopic rings. The large amplitude of the observed currents in SID mesoscopic rings strongly challenges the conventional theories of persistent current. It indicates that in all the previous models some fundamental mechanism is missing which could compensate the effect of impurities, and thus prevents reduction of the current due to disorder. The existing theories are basically within the framework of the Anderson model where the transport properties of the electrons are dominated by the localization phenomenon that essentially reduces the persistent current. In a recent work, Balagurov et al. have shown that the electrons become delocalized if one includes long-range hopping (LRH) integrals in the Anderson model.

We describe a \( N \)-site ring enclosing a magnetic flux \( \phi \) (in units of the elementary flux quantum \( \phi_0 \)) by the following Hamiltonian in the Wannier basis

\[
H = \sum_i \epsilon_i c_i^\dagger c_i + \sum_{i \neq j} v_{i,j} \left[ e^{-i\theta} c_i^\dagger c_j + h.c. \right]
\]

where \( \epsilon_i \)'s are the site energies, \( v_{i,j} \)'s are the hopping integrals, and \( \theta = \frac{2\pi}{|i-j|} \). The \( \epsilon_i \)'s are uncorrelated random variables drawn from some distributive function \( P(\epsilon) \), and, the non-random LRH integrals are taken as \( v_{i,j} = v/|i-j|^\mu \), \( v \) being a constant representing the nearest-neighbor hopping (NNH) integrals. It should be noted that the physical domain of the exponent \( \mu \) is determined by the boundness of the spectrum [20]. The choice of the distribution function \( P(\epsilon) \) which we shall use are the “box” distribution

\[
P(\epsilon) = \frac{\Theta(W - |\epsilon|)}{W}
\]

of width \( W \), and the “binary-alloy” distribution

\[
P(\epsilon) = c\delta(\epsilon - \epsilon_A) + (1-c)\delta(\epsilon - \epsilon_B)
\]

where \( c \) and \( 1-c \) are respectively the concentrations of two types of atoms with site energies \( \epsilon_A \) and \( \epsilon_B \). In the following we use the units \( h = e = 1 \).

For an ordered ring, setting \( \epsilon_i = 0 \) for all \( i \), the energy of the \( n \)th eigenstate can be expressed as

\[
E_n(\phi) = \frac{2\nu}{m^\mu} \cos \left[ \frac{2\pi m}{N} (n + \phi) \right]
\]

where \( m \) is an integer. The current carried by this eigenstate is given by

\[
I_n(\phi) = \left( \frac{4\pi v}{N} \right) \sum_{m=1}^{N-1} m^{(1-\mu)} \sin \left[ \frac{2\pi m}{N} (n + \phi) \right].
\]

FIG. 1: \( I - \phi \) characteristics of ordered spinless fermionic rings with \( \mu = 1.6, \ v = -1, \ N = 50 \), and, a) \( N_e = 20 \) and b) \( N_e = 23 \). The solid and dashed lines are respectively for the rings with all LRH and only NNH integrals.

For spinless electrons, we can express the total current at \( T = 0 \) in the following form

\[
I(\phi) = \sum_n I_n(\phi)
\]

where \( N_e \) is the number of electrons and \( -\lfloor N_e/2 \rfloor \leq n < \lfloor N_e/2 \rfloor \) (\( \lfloor z \rfloor \) denotes the integer part of \( z \)). In the above expression we restrict \( \phi \) in the domains \(-0.5 \leq \phi < 0.5 \) and \( 0 \leq \phi < 1 \) for the systems respectively with odd and even number of electrons. The \( I(\phi) \) versus \( \phi \) curves for some representative impurity-free systems are plotted in Fig. 1. The persistent current as a function of \( \phi \) always exhibits discontinuity at certain points as long as there is no impurity in the system. The ground states are degenerate at these points of discontinuity due to the crossing of the energy levels. In the presence of all LRH integrals it is found that the amplitude of the current initially increases as we increase the system size, but eventually it falls when the system becomes larger. This is due to the fact that as we increase the number of sites, the Hamiltonian Eq. 11 includes some additional higher order hopping integrals which causes an increase in the net velocity of the electrons, but after certain system size this increment in velocity drops to zero because the
additional hopping integrals are then between far enough sites giving negligible contributions.

If we take into account the spin of the electrons, then the total persistent current in an ordered ring with even number of electrons is given by

\[ I(\phi) = 2 \sum_n I_n(\phi) \quad (7) \]

where \(-[N_e/4] \leq n < [N_e/4]\), and here we restrict \(\phi\) in the domain \(0 \leq \phi < 1\) if \(N_e/2\) is even while in the domain \(-0.5 \leq \phi < 0.5\) if \(N_e/2\) is odd. If the system contains odd number of electrons, we have

\[ I(\phi) = 2 \sum_n I_n(\phi) + I_n'(\phi) \quad (8) \]

where \(-[(N_e - 1)/4] \leq n < [(N_e - 1)/4]\). The quantum number \(n'\) has to be determined in the following way. Any odd value of \(N_e\) can be expressed into the form \((4p \pm 1)\) where \(p = 1, 2, 3, \ldots\), and the quantum number \(n'\) becomes equal to \(\pm p\) corresponding to these two forms of \(N_e\). In the above expression we restrict \(\phi\) in the range \(0 \leq \phi < 1\) when \(N_e\) is of the form \((4p - 1)\), whereas \(\phi\) is to be bounded between \(-0.5 \leq \phi < 0.5\) when \(N_e\) has the form \((4p + 1)\). We do not display the \(I - \phi\) characteristics for spin fermionic systems as in the absence of electron-electron interaction, the electron spin cannot alter the characteristic features of the persistent currents from those presented in Fig. 1.

![FIG. 2: \(I - \phi\) curves of spinless fermionic rings with all LRH integrals. \(\epsilon_i\)’s are chosen randomly from Eq. (2) and the parameters are \(\mu = 1.4, v = -1, N = 50\), and, a) \(N_e = 20\) and b) \(N_e = 23\). The dotted curve and the three solid curves in each of these figures are respectively for the ordered and three microscopic disordered configurations of the ring.](image)

![FIG. 3: \(I - \phi\) curves for the same systems as those in Fig. 2 excepting that the \(\epsilon_i\)’s are chosen randomly from Eq. (3).](image)

Now we address the problem of persistent current in SID mesoscopic rings using the Hamiltonian Eq. (1), and, in this study we do not consider the spin of the electrons as it will not change the qualitative behavior of the currents within the one-electron picture. We present exact calculation of the currents in the presence of all LRH integrals in the tight-binding Hamiltonian with diagonal disorder, and it involves exact numerical diagonalization of the Hamiltonian matrices. The results for some representative examples are given in Fig. 2 and Fig. 3. In Fig. 3 we plot \(I(\phi)\) versus \(\phi\) curves for the systems with \(v = -1, \mu = 1.4, N = 50\), and, \(N_e = 20\) and 23, where disorder is introduced by random choice of \(\epsilon_i\)’s from the “box” distribution Eq. (3) setting \(W = 1\). The solid lines correspond to three microscopic configurations of disorder, while the dotted lines are for the ordered cases obtained by setting all \(\epsilon_i\)’s equal to zero. Fig. 3 is the \(I - \phi\) characteristics of the systems with the same set of parameters as those in Fig. 4 where site energies are cho-
sen randomly from the “binary-alloy” distribution given by Eq. 3 with $c = 0.5$ and $\delta = |\epsilon_A - \epsilon_B| = 1$. We consider three typical disordered configurations of the ring compatible with the “binary-alloy” distribution, and the $I - \phi$ curves for these configurations are represented by solid lines in Fig. 3. The dotted lines in this figure are identical to those in Fig. 2.

Let us now analyze the results presented in Fig. 2 and Fig. 3. We see that for the present model of SID mesoscopic ring, the persistent currents are always periodic in $\phi$ with periodicity $\phi_0$. Fig. 2 and Fig. 3 clearly show that the $I - \phi$ characteristics of a given SID mesoscopic ring are almost insensitive to the microscopic configuration of disorder of the ring, and, we have checked considering 100 distinct configurations of the given system that all the $I - \phi$ curves nearly collapse to a single curve. These figures are self-explanatory to reveal the fact that as we vary the microscopic configurations of the ring, the persistent currents do not fluctuate in sign and the fluctuation in magnitude becomes exceedingly small. The most interesting result is that in the present model persistent current is not reduced by disorder, and it is apparent from Fig. 2 and Fig. 3 that the currents in the disordered rings are of the same order of magnitude as the current in the ordered ring. We have also noticed certain interesting features of the $I - \phi$ curves that are characteristics of any disordered ring. The discontinuity in $I(\phi)$ as a function of $\phi$ are characteristics of the ordered systems which disappears due to disorder, and the current in the disordered rings are always zero at these points of discontinuity. This result can be easily understood on a very general ground. We can treat disorder as a perturbation over the ordered situation that lifts the degeneracy at the crossing points of the unperturbed energy levels. So gaps open up at the ground level in the presence of disorder making $I(\phi)$ a continuous function of $\phi$, and, also $I(\phi)$ becomes exactly equal to zero at these points of discontinuity.

In conclusion, we have investigated the behavior of persistent currents in SID mesoscopic rings by a simple model including all LRH integrals in the usual Anderson model. Our exact calculations show that both the sign and magnitude of the experimentally observed currents can be explained from the present model. In this work we have convincingly established that the essential physical mechanisms are the LRH integrals that accounts for the observed behavior of persistent currents in SID mesoscopic rings.

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