Period halving of Persistent Currents in Mesoscopic Möbius ladders

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We investigate the period halving of persistent currents (PCs) of non-interacting electrons in isolated mesoscopic Möbius ladders without disorder, pierced by Aharonov-Bohm flux. The mechanisms of the period halving effect depend on the parity of the number of electrons as well as on the interchain hopping. Although the data of PCs in mesoscopic systems are sample-specific, some simple rules are found in the canonical ensemble average, such as all the odd harmonics of the PCs disappear, and the signals of even harmonics are non-negative.

The persistent currents (PCs) in mesoscopic rings has been explored for many years [1]. Early in 1983, the effect of elastic scattering was first understood by Büttiker et al., and thus the possibility of observing nano-amper PCs in nano-scale normal metal rings with disorder was revealed [2]. Since then the problem of PCs has been studied in many distinct aspects [3–21]. Among the interesting characters of PCs, the period halving phenomenon is particular simple but significant. In the early works about the ring systems with Aharonov-Bohm (AB) flux [22,23], it has been shown generally that all relevant physical properties of this “ring” are periodic in Φ with period halving [2]. Since then the problem of PCs has been studied in many distinct aspects [3–21]. Among the interesting characters of PCs, the period halving phenomenon is particular simple but significant. In the early works about the ring systems with Aharonov-Bohm (AB) flux [22,23], it has been shown generally that all relevant physical properties of this “ring” are periodic in Φ with period halving [2].

The schematic drawing of a Möbius ladder with N rungs is shown in Fig.1. The two chains on the opposite sides of the rectangle are connected as the unique edge of the Möbius ladder. If all the rungs are Broken off, the ladder will become a double-ring structure [19]. For the sake of simplicity, we take the energy integral between two nearest-neighbor sites along the edge as the energy unit, then the Hamiltonian for electrons with spin σ (up or down) in such a lattice can be written as

$$\hat{H}_\sigma = -\sum_{n=1}^{2N} \left( e^{i\theta} \hat{a}_n^\dagger \hat{a}_{n+\sigma} + e^{-i\theta} \hat{a}_{n+\sigma}^\dagger \hat{a}_n \right) - t_\perp \sum_{n=1}^{N} \left( \hat{a}_{n+N\sigma}^\dagger \hat{a}_n + \hat{a}_n^\dagger \hat{a}_{n+N\sigma} \right)$$

where $\hat{a}_n$ ($\hat{a}_n^\dagger$) is an annihilation (creation) operator for an electron with spin σ at site n, the phase $\theta \equiv 2\pi \Phi / \Phi_0$ arises from the path integral of vector potential $\int \vec{A} \cdot d\vec{r}$ between corresponding two nearest-neighbor sites along the edge of Möbius ladder, and $\Phi$ is the AB flux through the Möbius structure. In addition, the on-site energy for each site is set to be zero, but the matrix element $t_\perp$ for interchain hopping, i.e., hopping perpendicular to the edge is an important tunable parameter of the systems. The two kinds of electrons with spin-up and spin-down will contribute to the total Hamiltonian in a simple way that $\hat{H} = \hat{H}_\uparrow + \hat{H}_\downarrow$.

Such a Hamiltonian is readily diagonalized as

$$\hat{H} = \sum_{k,\sigma} \varepsilon_k \hat{b}_k^\dagger \hat{b}_k$$

with eigen-energy values

$$\varepsilon_k = -2\cos \frac{\pi}{N} \left( k + \frac{2\Phi}{\Phi_0} \right) - t_\perp (-1)^k$$

by introducing an unitary transformation

$$\hat{b}_k \equiv \frac{1}{\sqrt{2N}} \sum_{n=1}^{2N} e^{i\kappa n} \hat{a}_n, \quad \hat{a}_n = \frac{1}{\sqrt{2N}} \sum_k e^{-i\kappa n} \hat{b}_k$$

here $k = 0, 1, 2, \ldots, 2N - 1$ so that the wave vectors $k\pi / N$ is limited in the first Brillouin zone and the periodic condition $a_{n+2N} = a_n$ is satisfied. If $t_\perp > 2$, then Eq.(3) depicts a two-band spectrum with band gap $\Delta E = 2(t_\perp - 2)$. 

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At first glance, any single eigen-energy given by Eq.(3) is a periodic function of \( \Phi \) with period \( N\Phi_0 \), but in fact the PCs vary with the AB flux with period \( \Phi_0 \) because thermodynamic properties are determined by the whole eigen-energy spectrum. The periodicity of \( \{ \varepsilon_k \} \) is easy to see by using an equality \( \varepsilon_k(\Phi + \Phi_0) = \varepsilon_{k+2}(\Phi) \). This is very the reason why all the calculations of PCs can be limited in the flux range \( \Phi \in [0, \Phi_0) \).

However, a Möbius ladder with \( t_\perp = 0 \) becomes a double-ring structure [19], and the dispersion relation Eq.(3) will be reduced as

\[
\varepsilon_k = -2\cos \frac{\pi}{N} \left( k + \frac{\Phi^*}{\Phi_0} \right) \tag{5}
\]

here \( \Phi^* \equiv 2\Phi \) is defined as the flux-linkage through the double-ring structure. The flux-linkage is two times of the AB flux because the electrons have to travel along the full edge of the Möbius ladder, thus encircling the flux twice. Therefore the PCs in a double-ring system must be a periodic function of AB flux with period half a flux quantum \( \Phi_0/2 \) because of \( \varepsilon_k(\Phi^* + \Phi_0) = \varepsilon_{k+1}(\Phi^*) \).

In Ref. [19], this simple result is referred as “Entire periodic halving” effect.

There is no obvious reason to ensure that the well-known formula of PCs in one-dimensional ring systems is still held for some subtle cases such as the Möbius ladders. Therefore we try to prove it based upon some basic concept of quantum mechanics. It is obvious that the current at \( n \)th rungs involve two parts: the current from \( n \) to \( n + 1 \) in one chain and the current from \( n + N \) to \( n + N + 1 \) in another chain. So we have

\[
\hat{J} = \hat{j}_n + \hat{j}_{n+N} = \frac{1}{N} \sum_{n=1}^{N} (\hat{j}_n + \hat{j}_{n+N}) = \frac{1}{N} \sum_{n=1}^{2N} \hat{j}_n \tag{6}
\]

in the second step of above derivation, the conservation condition of current has been used. Applying the concept of probability current in Hilbert space [24]

\[
\hat{j}_n = \hat{j}_{n \rightarrow n+1} - \hat{j}_{n+1 \rightarrow n} = \frac{1}{\hbar} \sum_{\sigma} \left( e^{i\theta_{n+1a}a_n^\dagger a_{n+1}^\dagger - e^{-i\theta_{n+1a}}a_{n+1a}a_n^\dagger} \right) \tag{7}
\]

to above equation (6), then we prove that the charge current operator for the Hamiltonian system defined in Eq.(1) can still be re-obtained as \( I(\Phi) = -\partial \mathcal{H}(\Phi) / \partial \Phi \). Simple calcualtion yields the formula of PCs in a Möbius ladder

\[
I(\Phi) = -e \left\langle \hat{J} \right\rangle = -I_0 \sum_{k,\sigma} \bar{n}_{k,\sigma} \sin \frac{\pi}{N} \left( k + \frac{2\Phi}{\Phi_0} \right) \tag{8}
\]

where \( I_0 \equiv 4\pi/\Phi_0 \), and \( \bar{n}_{k,\sigma} = \langle \hat{b}_k^\dagger \hat{b}_{k,\sigma} \rangle \) stands for the thermodynamic averaged number of electrons in quantum state \((k, \sigma)\).

The formula Eq.(8) provide us a base to study the PCs in Möbius ladders. For the sake of clarity, we will in the present paper focus on the systems with fixed number of electrons at absolute zero temperature. In this case, all the \( N_e \) electrons will fill into single-electron quantum states \((k, \sigma)\) according to their eigen-energy values from ground state to higher energy states one by one. It means that \( \bar{n}_{k,\sigma} = 1 \) for occupied states and otherwise \( \bar{n}_{k,\sigma} = 0 \).

The conventional way for analyzing the periodic behavior of PCs is to calculate the Fourier harmonics of the data of currents at \( K \) discrete values of AB flux \( \Phi_\ell = \ell \Phi_0/N, \ell = 0, \cdots, K - 1 \), thus Eq.(9a) can be re-written as

\[
I_\ell = \frac{1}{\sqrt{K}} \sum_{m=0}^{K-1} F_m \exp(i\omega_m \ell/K), \tag{9a}
\]

\[
F_m = \frac{1}{\sqrt{K}} \sum_{\ell=0}^{K-1} I_\ell \exp(-i\omega_m \ell/K) \tag{9b}
\]

for \( m, \ell = 0, 1, \cdots, K - 1 \), and the spectra theorem is written as \( \sum_{m=0}^{K-1} |F_m| = \sum_{\ell=0}^{K-1} |I_\ell|^2 \). In fact, the real part of \( F_m \) keeps to be zero and \( F_{K-m} = F_m^* \) because \( I(\Phi_0 - \Phi) = -I(\Phi) \) for \( 0 \leq \Phi < \Phi_0 \). Thus Eq.(9a) can be re-written as

\[
I_\ell = \frac{1}{\sqrt{K}} \sum_{m=1}^{K-1} S_m \sin(\ell \omega_m / K), \tag{10}
\]

where \( S_m = -Im(F_m) \) and \( Im(\cdots) \) denotes the imaginary part of a complex number. In practical experiments [6–10], \( S_m \) will be detected as the amplitude of signals of harmonics \( \omega_m = 2m\pi \) with period \( \Phi_0/m \). In what follows, we will present only first twenty harmonics [25].

The plots in Fig.2 are some typical results selected from our numerical simulations on PCs in double-ring systems. We find that the PCs in any single double-ring system with odd number of electrons is a period function of \( \Phi \) with period \( \Phi_0/4 \), halving of the period \( \Phi_0/2 \) as discussed in the paragraph below eq.(5) and shown in Fig.2(a), and that the second harmonic with period \( \Phi_0/2 \) of even number electrons in single double-ring system does not appear as shown in Fig.2(b); but however we find also that the second harmonic will be strongly suppressed in summation of PCs in two systems with adjacent even numbers of electrons, such as shown Fig.2(c). Note that a double-ring system is equivalent to a 1D ring pierced by a AB flux \( \Phi^* = 2\Phi \), we suppose that the parity effect of electron number exists in the PCs of mesoscopic
rings. We hope that this observation will shed light on the mechanism of period behaving of PCs.

Some other interesting properties of PCs in canonical ensemble average are shown in Fig.3. It is well-known that the PCs in mesoscopic systems are sample-specific, but simple rules always appear in some kinds of averages. We calculate the PCs and relevant Fourier harmonics varying with the AB flux for different Möbius ladders with different fixed numbers of electrons. The data of single system show that the PCs can be paramagnetic or diamagnetic, the first harmonic can exist or vanish. Following the works of Bouchiat and Montambaux [5], we take the arithmetic mean values of PCs on the number of electrons. The averaged PCs and corresponding harmonics manifest some surprising characters. All the odd harmonics disappear, and the even harmonics keeps to be non-negative. In addition, very small probability amplitude of inter-chain hopping, as small as to be non-negative. In addition, very small probability amplitude of inter-chain hopping, as small as $t_\perp = 0.01$ shown in Fig.3(b), can result in a considerable harmonic of period $\Phi_0/2$.

In conclusion we study the problem of PCs in Möbius ladder systems of non-interacting electrons with a tunable parameter $t_\perp$. It is proven exactly that the well-known formula for PCs in 1D rings still holds for the complicated new structures. A series of simulation results manifest that the perpendicular hopping elements and the parity of the number of total electrons influence the periodic behaviors of PCs dramatically. As proposed by Mila et al [18], a Möbius structure with controllable inter-chain hopping could be fabricated in GaAs heterostructure using a wide quantum wire. Our present study provides a base for further investigations on the disorder effect, temperature effect, and the effect of electron interaction. Then we can expect that these relevant theoretical results are testable in experiment.

This work is supported by National Key Program for Basic Research, 2001-03500, and partly by the Guangdong Provincial Natural Science Foundation of China.

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Strictly speaking, $S_m$ is not the amplitude of $m$th harmonic; but for the low order harmonics, it is a very good approximation.

FIG. 1. Schematic drawing of a Möbius ladder with $N$ rungs. The AB flux $\Phi$ pierces through the center of the structure.

FIG. 2. Typical curves of PCs (left column) and first twenty harmonics of Fourier transformation (right column) for $N = 100$ double-ring systems. (a) odd number of electrons $N_e = 281$; (b) even number of electrons $N_e = 280$; (c) summation of the PCs and corresponding harmonics of two systems with adjacent even numbers of electrons, i.e., $N_e = 280$ and $N_e = 282$.

FIG. 3. Typical curves of canonical ensemble averaged PCs (left column) and first twenty harmonics(right column). (a) $t_\perp = 0$; (b) $t_{\text{tot}} = 0.01$; (c) $t_\perp = 1.0$. 3
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Fig. 3 Wenji Deng et al (02/03/17)