Persistent currents in Möbius strips

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Relation between the geometry of a two-dimensional sample and its equilibrium physical properties is exemplified here for a system of non-interacting electrons on a Möbius strip. Dispersion relation for a clean sample is derived and its persistent current under moderate disorder is elucidated, using statistical analysis pertinent to a single sample experiment. The flux periodicity is found to be distinct from that in a cylindrical sample, and the essential role of disorder in the ability to experimentally identify a Möbius strip is pointed out.

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I. INTRODUCTION

An important theme in quantum mechanics is to find a relation between a global geometry of a sample (*e.g.*, boundary conditions) and its physical properties. We address this issue by comparing flux periodicity of persistent currents in a cylinder and in a Möbius strip. The aim is to determine whether the geometrical (in some sense topological) difference is tangible and experimentally observable. At zero temperature, the persistent current $I(\phi)$ in a ring can be expressed as[1]

$$I(\phi) = -\frac{\partial E(\phi)}{\partial \phi} = \sum_{n=1}^{\infty} I_n \sin(2\pi n\phi), \tag{1}$$

where ϕ is the magnetic flux threading the ring in units of $\Phi_0 = hc/e$, $E(\phi)$ is the ground state energy, and I_n are the current harmonics.

The current $I(\phi)$ is an anti-symmetric and periodic function of ϕ with period 1. Possible occurrence of smaller flux periodicity in mesoscopic physics is one of the cornerstones of weak localization. For the cylinder geometry, conductance measurements[2] and magnetization of 10^7 copper rings[3] indicate the emergence of periodicity 1/2. It is shown to be intimately related to the procedure of *averaging* over disorder realizations and numbers of electrons in the rings[2,4,5,6]. Very recently, a microscopic $NbSe_3$ Möbius strip has been fabricated[7]. Obviously, in this case, attention should be focused on a *single sample* measurement[8] for which there is no self-averaging.

Let us first mention several intuitive points relevant to the flux periodicity in the Möbius strip, based on semiclassical arguments and geometry[9]. First, recall that the periodicity is related to interference between trajectories (such as Aharonov-Bohm interference between different trajectories or weak-localization interference between time-reversed paths). In the cylinder (Möbius) geometry, an electron moving in the *longitudinal direction* along the ring encircles the system once (*twice*) before returning to its initial position. Therefore, we might expect different flux periodicities of the persistent current between the two cases. Second, unlike a cylinder which can be "pressed" into a one-dimensional ring, the Möbius strip cannot be pressed into a one-dimensional structure. This brings in another important factor, namely, the motion of electrons in the *transverse* direction. In a tight-binding model this motion is controlled by the transverse hopping. If it is very weak, the twice-encircling property of the Möbius strip implies the dominance of even harmonics I_{2n}. Contrary, for a strong transverse hopping, the current in the Möbius strip is expected to be effectively similar to that in the cylindrical strip[10]. In the following we are mainly interested in a regime where the transverse hopping is slightly less than with the longitudinal one. Third, the role of disorder should be carefully examined. Weak disorder is not expected to significantly alter interference between semi-classical trajectories discussed above, while strong disorder should result in a reduced sensitivity to the pertinent geometry, due to localization effects. The most intriguing disorder effect might then be expected in a moderate strength of disorder which will be used below. The upshot of the present study is that the periodicity pattern in a Möbius strip is remarkably distinct from that of a cylinder, and that disorder plays a crucial role in making the statistical effect detectable.

II. MODEL

A Möbius strip is modelled by considering a non-interacting particle in a rectangle of length L_x and width L_y, requiring its wave-function $\psi(x, y)$ to satisfy Dirichlet boundary conditions in the y direction, and Möbius boundary conditions[11] in the x direction:

$$\psi(x, -L_y/2) = \psi(x, L_y/2) = 0 \quad \text{(Dirichlet B.C.)}\ , \tag{2}$$

$$\psi(x+L_x, y) = \psi(x, -y) \quad \text{(Möbius B.C.)}\ . \tag{3}$$

The quantized wave-numbers are $k_y = (\pi/L_y)n_y$ and $k_x = (2\pi/L_x)([\frac{1}{2}]_{n_y} + n_x)$, where $n_y = 1, 2, \cdots$ and $n_x = 0, \pm1, \pm2, \cdots$. The notation $[\alpha]_n$ represents α for $n =$ even and 0 for $n =$ odd. In the cylinder geometry, Eq. (3) should be replaced by $\psi(x+L_x, y) = \psi(x, y)$, and gives $k_x = (2\pi/L_x)n_x$. Thus, only the $n_y =$ even eigenstates are affected by the switch from the conventional cylinder (periodic) boundary conditions to the Möbius ones.

In the absence of disorder, the energies of the eigenstates both in the Möbius and cylinder strips are given by the formula

$$E_{n_x n_y} = \epsilon_x\left(k_x - \frac{2\pi\phi}{L_x}\right) + \epsilon_y(k_y), \tag{4}$$

where ϵ_x and ϵ_y provide the dispersion relation. Equation (4) is rather general for clean systems. To be more specific, let us model the Möbius strip by a tight-binding Hamiltonian. The Möbius strip is constructed from a rectangular lattice including $N \times 2M$ sites. The rectangle is twisted by 180°, and its two sides are connected, such that longitudinal wire 1 is attached to wire $2M$, wire 2 is attached to wire $2M-1$ and so on. The Möbius strip so constructed includes M longitudinal wires with $2N$ sites on each one. The Hamiltonian is then

$$H_{\text{Möbius}} = \sum_{n=1}^{2N}\sum_{m=1}^{M}\left[\varepsilon_{nm}c^\dagger_{nm}c_{nm} - t_1 e^{-2\pi i\phi/N}c^\dagger_{nm}c_{n+1m}\right] - t_2\sum_{n=1}^{2N}\sum_{m=1}^{M-1}c^\dagger_{nm+1}c_{nm} - \frac{t_2}{2}\sum_{n=1}^{2N}c^\dagger_{nM}c_{n+NM} + \text{h.c.} \quad (5)$$

where c_{nm} is the fermion operator at the site (n,m) $(n = 1,2,\ldots,2N,\ m = 1,2,\ldots,M)$ and t_1 and t_2 are longitudinal and transverse hopping amplitudes respectively. The quantity ε_{nm} is the site energy. Connecting the two sides of the rectangle without twisting, we obtain a cylindrical strip which includes $2M$ longitudinal wires composed of N sites. The Hamiltonian of the cylinder is

$$H_{\text{cylinder}} = \sum_{n=1}^{N}\sum_{m=1}^{2M}\left[\varepsilon_{nm}c^\dagger_{nm}c_{nm} - t_1 e^{-2\pi i\phi/N}c^\dagger_{nm}c_{n+1m}\right] - t_2\sum_{n=1}^{N}\sum_{m=1}^{2M-1}c^\dagger_{nm+1}c_{nm} + \text{h.c.} \quad (6)$$

Locally the two Hamiltonians (5) and (6) look the same. But there is a couple of essential differences between them: a) The Möbius Hamiltonian (5) includes an extra term which describes long range hopping between distant parts of the Mth wire[11]. b) While the magnetic phase accumulated along the longitudinal direction on each link is the same (that is, $2\pi\phi/N$), the corresponding number of links is different ($2N$ for the Möbius strip and N for the cylinder).

III. THE SPECTRUM

We first consider a system without disorder, namely, $\varepsilon_{nm} = 0$. The dispersion relation for an electron in the Möbius strip reads,

$$E_{n_x n_y} = -\ 2t_1\cos\left[\frac{2\pi}{N}\left(\left[\frac{1}{2}\right]_{n_y} + n_x - \phi\right)\right] -\ 2t_2\cos\left(\frac{\pi}{2M+1}n_y\right)\ , \quad (7)$$

where $n_x = 1,\cdots,N$ and $n_y = 1,\cdots,2M$. Defining new indexes $k = [1]_{n_y} + 2n_x$ and $q = [\frac{1}{2}]_k + n_y/2$, one obtains a more suggestive form,

$$E_{kq} = -\ 2t_1\cos\left[\frac{\pi}{N}(k-2\phi)\right] -\ 2t_2\cos\left[\frac{\pi}{2M+1}\left(2q-[1]_k\right)\right], \quad (8)$$

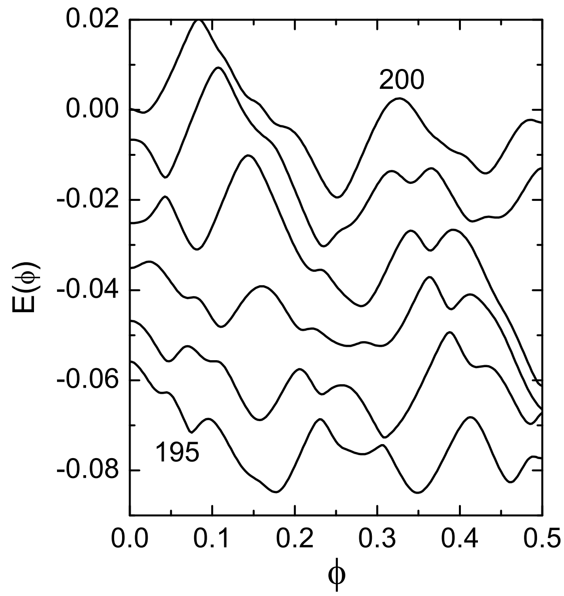

FIG. 1: Single-particle energy spectrum as a function of flux threading the Möbius ring. The 195th-200th energy levels are shown. The parameters are $N = 20$, $M = 10$, $t_2 = 0.5$, and $W = 0.5$. Energies are measured in units of t_1.

where $k = 1,\cdots,2N$ and $q = 1,\cdots,M$. It is instructive to compare it with the energy in the cylinder geometry, $E_{kq} = -2t_1\cos\left[\frac{2\pi}{N}(k-\phi)\right] - 2t_2\cos\left(\frac{\pi}{2M+1}q\right)$, where $k = 1,\cdots,N$ and $q = 1,\cdots,2M$. Despite the apparent similarity between these two spectra, there are at least two important differences. First, the combination of flux and longitudinal momentum is distinct, namely, it is $k-\phi$ for the cylinder and $k-2\phi$ for the Möbius strip. For a small ratio t_2/t_1 this might affect the periodicity of the current[10]. Second, the mini-band structure is different.

We now turn to elucidate the current in disordered Möbius strips. The random numbers ε_{nm} are assumed to be uniformly distributed over the range $-W/2 \le \varepsilon_{nm} \le W/2$, where W represents the strength of disorder. The Hamiltonian Eq. (5) [or Eq. (6)] is treated numerically. As an example, the evolution of single-particle energies with flux in a disordered Möbius strip with $N = 20$ and $M = 10$ is shown in Fig. 1. The parameters are $t_2/t_1 = 0.5$ and $W/t_1 = 0.5$. The pattern of avoided crossing turns out to be remarkably different from that for a cylinder (see ref. 5 figure 1 therein). It must then be reflected in the behavior of persistent currents.

The first stage of the analysis is an inspection of the typical values of I_n, aiming in determination of their dependence on the ratio t_2/t_1. As expected, in the absence of averaging we find typical I_1 dominance in case of the cylinder geometry irrespective of the t_2/t_1 ratio. For the Möbius geometry the emerging picture is quite different. Figure 2 shows the Fourier components of the persistent current for a clean Möbius strip as a function of the ratio

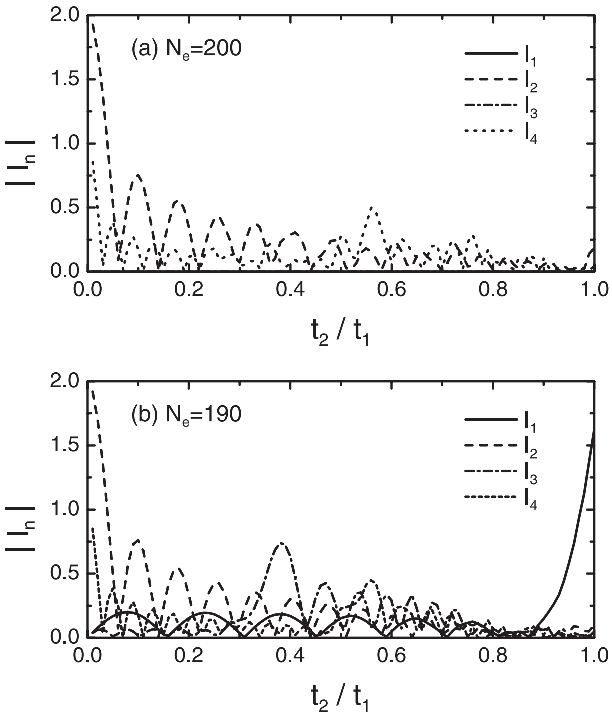

FIG. 2: Fourier components of the persistent current for the clean Möbius strip as a function of the transverse-hopping energy (a) at the half-filling and (b) below the half-filling. The size of the Möbius strip is given by $N = 20$ and $M = 10$.

t_2/t_1 at and below the half-filling ($N_e = 200$). For small ratios ($t_2/t_1 < 0.1$) we find, as can be naively expected, I_2 dominance. The expected effect of averaging in the cylinder case is to emphasize the I_2 contribution, while in the Möbius case the expected effect is to emphasize the I_4 contribution. For clean Möbius strip the I_n with odd n, as a function of the number of electrons N_e, is anti-symmetric around half-filling. Therefore I_1 and I_3 completely vanish [Fig. 2(a)]. See further discussionin Sect. V. To avoid this particularity at the half-filling, we display in Fig. 2(b) also the case where the number of electrons ($N_e = 190$) is below half-filling. For large ratios ($t_2/t_1 > 0.8$) we observe in Fig. 2(b) a cylinder-like regime where there is typically I_1 dominance. This is because the strong transverse hopping changes the periodicity of the Möbius strip to that of the conventional cylinder. The somewhat unexpected observation is that there is a distinct wide intermediate regime ($0.1 < t_2/t_1 < 0.8$) where I_1, I_2, I_3 and I_4 are all comparable. This is the regime which is of experimental relevance. The expected effect of averaging in this regime is to emphasize both the I_2 and the I_4 contributions.

IV. STATISTICAL ANALYSIS

The problem arising in the analysis of persistent currents in disordered Möbius strips is how to characterize the statistics of the calculated data. It was already pointed out that essential properties of observables result from the averaging procedure and the nature of the underlying statistical ensemble[4,5,6]. On the other hand, fabrication of a Möbius strip requires an outstanding effort[7], and hence, anticipated measurements of the persistent current would probably be performed on a single sample. Thus, somewhat unfortunately, the important results reported therein and the powerful calculation methods based on super-symmetry might be less useful for *single-sample* experiments since there is no averaging.

What is then the most efficient way to present our calculated results? The answer is provided by elementary statistics. An experimental result consists of a set of K measurements $I(\phi_i)$, $i = 1, 2, \ldots, K$ performed on a given sample. This sample is taken out of an ensemble of Möbius strips with different disorder realizations, electron numbers N_e, aspect ratios, *etc.* The set $\{I(\phi_i)|i = 1, \ldots, K\}$ can be regarded as an instance of a random vector in a K dimensional space. Alternatively, this instance can be represented by the current harmonics $(I_1, I_2, \ldots)$ defined via Eq. (1). For our purpose it seems adequate to keep only the first 4 harmonics. The relevant statistical ensemble is then a set of "points" (I_1, I_2, I_3, I_4) in four-dimensional probability space, each point corresponds to a possible experimental measurement of the current on the *entire* ϕ interval. Let us denote the number of points within an infinitesimal four-dimensional volume element by $P(I_1, I_2, I_3, I_4)dI_1dI_2dI_3dI_4$. The distribution function P is normalized to $\mathcal{N}$, the total number of members in the ensemble. The most probable (typical) experimental result is then determined by the quadruple I_1, I_2, I_3, I_4 at which P is maximal. Another quantity, which seems more informative and easy to analyze, is the distribution

$$p_n(I_n) = \int_0^{\frac{1}{2}|I_n|} P(I_1, I_2, I_3, I_4) \prod_{m \neq n} d|I_m|. \qquad (9)$$

This corresponds to the possibility of finding a sample whose current $I(\phi)$ is approximately described by $I(\phi) \approx I_n \sin(2\pi n\phi)$. (For a sample counted by $p_n(I_n)$, all the harmonics other than I_n are at most half of I_n in magnitude). The number of members in the ensemble that exhibit I_n dominance is therefore $\mathcal{N}_n = \int_0^\infty p_n(I_n)d|I_n|$. If $\mathcal{N}_n > \mathcal{N}_m$ for any $m \neq n$, the typical periodicity of $I(\phi)$ is dominantly $1/n$. In actual calculations, we assume that the lattice structure, the aspect ratio, and the strength of disorder are fixed, and that the temperature is very low. Then, two quantities are still fluctuating, namely, the filling factor (or the electron number N_e) and the specific realization of disorder. We generate an ensemble of $\mathcal{N} = \mathcal{N}^a\mathcal{N}^b$ members corresponding to $\mathcal{N}^a$ consecutive values of N_e, usually around half filling, and $\mathcal{N}^b$ realizations of disorder for each one of them. Actually, for our systems of size $N = 20$, $M = 10$ with $t_1 = 1$, $t_2 = 0.5$, and $W = 0.5$, we take $150 \leq N_e \leq 250$, hence $\mathcal{N}^a = 101$ and $\mathcal{N}^b = 250$, so that $\mathcal{N} = 25250$. The distributions $p_n(I_n)$ for the cylinder and Möbius ensembles are shown in Fig. 3.

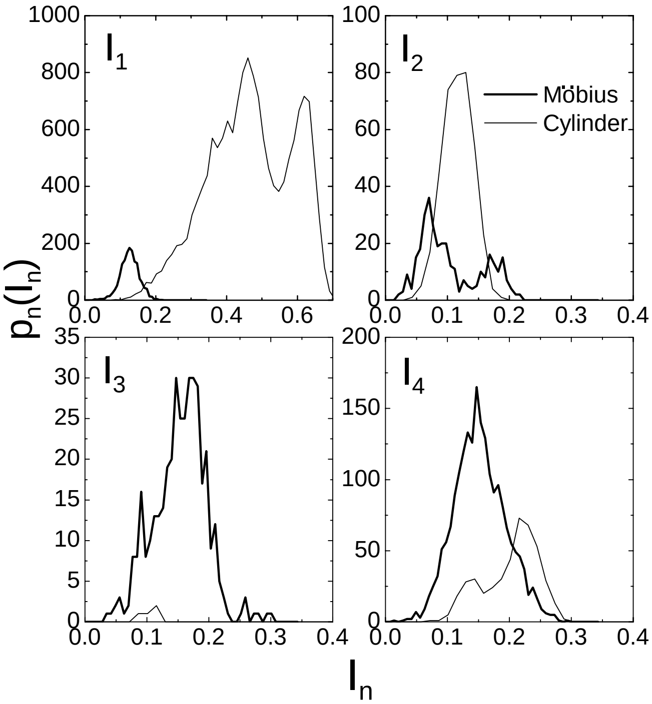

FIG. 3: The distributions $p_n(I_n)$ ($n = 1, 2, 3, 4$) defined by Eq. (9) for the cylinder and Möbius ensembles. The numbers of members with I_n dominance are $\mathcal{N}_1 = 15,829$, $\mathcal{N}_2 = 382$, $\mathcal{N}_3 = 4$, and $\mathcal{N}_4 = 439$ for the cylinder ensemble, and $\mathcal{N}_1 = 1,562$, $\mathcal{N}_2 = 336$, $\mathcal{N}_3 = 384$, and $\mathcal{N}_4 = 1,992$ for the Möbius ensemble.

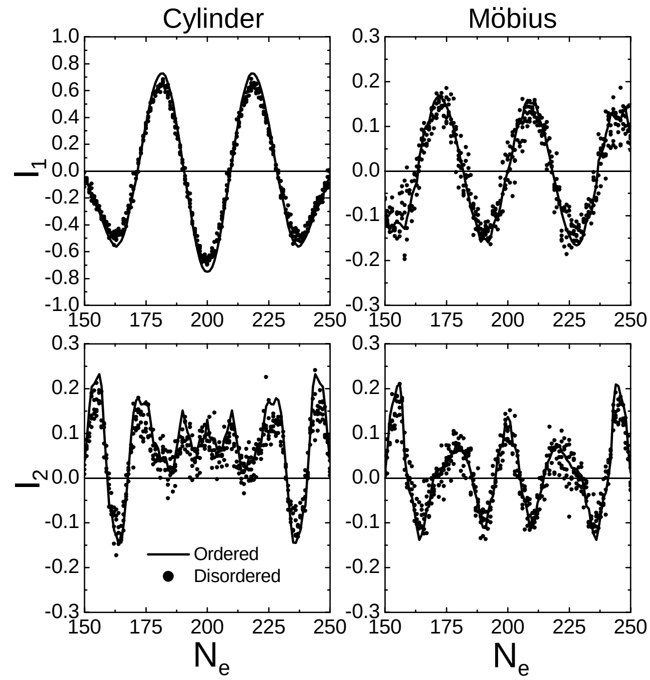

FIG. 4: I_1 and I_2 as a function of N_e for the ordered (solid line) and disordered (dots) systems. Parameters describing the systems are the same with those for Fig. 3.

V. MAIN OBSERVATIONS

The most striking result that can be deduced from Fig. 3 is the essential reduction of $\mathcal{N}_1$ for the Möbius ensemble compared with the cylinder one. For the present ratio $N/2M = 1$, there is also a strong tendency towards $\Phi_0/4$ periodicity, since $\mathcal{N}_4 > \mathcal{N}_{m\neq 4}$ for the Möbius ensemble. This result is intriguing, because here we have no averaging procedure which is crucial to get the 1/2 periodicity in cylindrical strips. However, this 1/4 periodicity emerges only for the specific ratio $N/2M = 1$. We have calculated the distributions $p_n(I_n)$ for Möbius strips with several aspect ratios. The value of $\mathcal{N}_n$ depends on the aspect ratio. No specific n gives prominent $\mathcal{N}_n$ independently of the aspect ratio. On the other hand, the collapse of I_1 dominance in the Möbius ensemble is robust and persists in systems with different ratios $N/2M$ as well. We can safely say that $\mathcal{N}_1$, $\mathcal{N}_2$, $\mathcal{N}_3$, and $\mathcal{N}_4$ become all comparable in the Möbius ensemble.

The natural question that comes to mind is whether this result is a consequence of the Möbius geometry or, rather, it is due to the presence of disorder. In order to answer this question, we have performed the calculation of $P^0(I_1, I_2, I_3, I_4)$ for a "clean" Möbius ensemble (without disorder, only N_e is being changed). We found out that the probability to find any I_n dominance is extremely small. The immediate conclusion is that disorder is essential for the identification of Möbius strips via $I_{n>1}$ dominance. Does this mean that interference or weak-localization effects due to the presence of disorder is important? To clarify this point, we should understand how $P^0(I_1, I_2, I_3, I_4)$ is modified by disorder. The distribution $P^0(I_1, I_2, I_3, I_4)$ is, in fact, a function defined on a one dimensional curve $[I_1(N_e), I_2(N_e), I_3(N_e), I_4(N_e)]$ in (I_1, I_2, I_3, I_4) space. For this reason, it is unlikely to find a sample where one of the I_n is dominant. The effect of disorder is to give some "thickness" to this curve (see Fig. 4). Taking into account that the amplitudes of $I_n(N_e)$ for Möbius strips are all comparable, the thickness gives a finite probability to find samples where one of the I_n is dominant. On the contrary, in the case of cylindrical strips, the amplitude of $I_1(N_e)$ is overwhelmingly larger than those of $I_{n\neq 1}(N_e)$, which makes it unlikely to find $I_{n\neq 1}(N_e)$ dominated samples even if we take the statistical effect of disorder into account. We should note here that the function I_n with odd n for the clean Möbius strip is an even function around the half-filling ($N_e = 200$) and an odd function for odd n, while the function I_n for arbitrary n is an even function in the cylinder case.

Our findings regarding $\mathcal{N}_n$ for the Möbius ensemble are based on the fact that the amplitudes of $I_n(N_e)$ are all comparable for Möbius strips. As we have observed in Fig. 2, this is a robust statistical property in the intermediate regime $0.1 < t_2/t_1 < 0.8$. The choice $t_2/t_1 = 0.5$ above, provides typical results for $p_n(I_n)$ and $\mathcal{N}_n$ in case that t_2/t_1 is within this distinct regime.

VI. CONCLUSIONS

We have studied the persistent currents of non-interacting electrons in Möbius strips. The spectral properties for a clean system were found analytically, and the effect of disorder on the currents was analyzed numerically. We have found that disorder is quite essential for the identification of Möbius strips. The issue of disorder averaging is not relevant for single sample experiments, and hence, special care is required for statistical analysis of the current harmonics. The fingerprint of the Möbius geometry is an enhanced probability to find samples in which I_n, with $n > 1$ dominates. This should be contrasted with the case of cylinder geometry, where there is a clear I_1 dominance. The above assertion regarding the fingerprint of the Möbius geometry is correct provided the effect of disorder is properly taken into account.

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

[2] B. L. Altshuler, A. G. Aronov, B. Z. Spivak, D. Yu. Sharvin and Yu. V. Sharvin, Pis'ma Zh. Eksp. Teor. Fiz. **35**, 484 (1982) [JETP Lett. **35**, 589 (1982)].

[3] L. Lévy, G. Dolan, J. Dunsmir and H. Bouchiat, Phys. Rev. Lett. **64**, 2074 (1990).

[4] H. F. Cheung, E. K. Riedel and Y. Gefen, Phys. Rev. Lett. **62**, 587 (1989).

[5] Hélène Bouchiat and Gilles Montambaux, J. Phys. France **50**, 2695 (1989).

[6] B. L. Altshuler, Y. Gefen and Y. Imry, Phys. Rev. Lett. **66**, 88 (1991).

[7] S. Tanda, T. Tsuneta, Y. Okajima, K. Inagaki, K. Yamaya, and N. Hatakenaka, Nature **417**, 397 (2002).

[8] V. Chandrasekhar, R. A. Webb, M. J. Brady, M. B. Ketchen, W. J. Galager, and A. Kleinsasser, Phys. Rev. Lett. **67**, 3578 (1991).

[9] It has been theoretically predicted that a novel state appears in a superconducting Möbius strip under a magnetic field: M. Hayashi and H. Ebisawa, J. Phys. Soc. Jpn. **70**, 3495 (2001).

[10] Fredric Mila, C. A. Stafford and Sylvian Capponi, Phys. Rev. **B57**, 1457 (1998).

[11] If, instead of Eq. (2), we assume the periodic B.C. in the y direction, the Möbius B.C. of Eq. (3) are modified as $\psi(x + L_x, y) = \psi(x, y + L_y)$. This leads to a long-range hopping term in Eq. (5), that does not "discriminate" the Mth wire. Yet another possibility is to *keep* Eq. (3). This possibility is of *academic* interest, since it corresponds to an geometry that cannot be embedded in a 3D Euclidean space. In the latter case, there is a symmetry breaking that prevents having a stationary current in the y direction.