# Persistent currents in small one-dimensional metal rings

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We have performed analytical calculations and computer simulations to study the persistent current I in small isolated one-dimensional metal rings enclosing a magnetic flux  $\phi$ . We have calculated I as a function of flux  $\phi$ , ring circumference L, temperature T, chemical potential  $\mu$ , and randomness W. We find that I decreases exponentially with T, that I decreases as  $W^2$  for weak W and as  $\exp(-L/\xi)$  for strong W, where  $\xi$  denotes the localization length, and that I is periodic in  $\phi$  with period  $\phi_0 = hc/e$ . For certain averaging procedures the periodicity may change to  $\phi_0/2$ .

# I. INTRODUCTION

With the advance in technology, the fabrication of submicrometer devices has become possible. For such "mesoscopic" systems, <sup>1,2</sup> at sufficiently low temperatures, the semiclassical theory of electronic transport breaks down. Two aspects of the new quantum regime that appears at low temperatures are of particular importance. First, the phase coherence length of the electron  $L_{\phi}$  (the length scale over which the electron can be considered to be in a pure state) increases significantly at low temperatures. When  $L_{\phi}$  becomes comparable to some relevant length scale (e.g., the system size), interference effects become important. An apt example is the Aharonov-Bohm oscillations in the magnetoresistance of small conducting rings. Second, the energy levels of closed systems are discrete. For mesoscopic systems this discreteness will be felt at low temperatures that are experimentally accessible. The discreteness plays a major role in the appearance of persistent currents in small normal metal rings discussed below.

The physics of small metallic rings in an excellent testing ground for many ideas in the field of mesoscopic physics. The resistance of such one-, two-, and fourterminal structures, its dependence on the enclosed magnetic flux, fluctuations, and various averaging procedures have been discussed extensively in the literature. $^{1-11}$  On the other hand, the problem of persistent currents, pertinent to isolated conducting loops or cylinders threaded by a magnetic flux, is less well understood. Here the term "persistent current" refers to the circulating current in isolated rings, which is a periodic function of the enclosed flux with period  $\phi_0$ ,  $\phi_0 = hc/e$  being the elementary flux quantum. That effect, directly related to the nature of the eigenfunctions of isolated rings and their flux sensitivity, has been the subject of recent theoretical studies.<sup>12,13</sup> Earlier work in the 1960s, e.g., Refs. 14-18, dealing with flux quantization in superconducting rings contain results pertinent to normal metal rings. Bloch,<sup>15</sup> Schick,<sup>16</sup> and Gunther and Imry<sup>17</sup> mention that one can have circulating currents for free electrons in sufficiently small rings or cylinders. The idea of persistent currents that are flux periodic in real normal-metal rings is more recent and based on the observation that the electron wave function may even then coherently extend over the whole circumference of the ring. It was first proposed for one-dimensional systems by Büttiker, Imry, and Landauer<sup>12</sup> in 1983 and by Büttiker<sup>13</sup> in 1985. These authors discuss that elastic scattering as well as finite temperature and weak inelastic scattering do not destroy the effect (cf. also Refs. 10 and 11). Recent reviews by Imry<sup>1</sup> and Washburn and Webb<sup>2</sup> place the persistent-current problem into a broader context and point out many open questions, some of which are addressed below. Until now such currents have not been observed experimentally.

In this paper we study persistent currents in strictly one-dimensional normal-metal rings.<sup>19</sup> We extend the earlier studies to include the dependences on randomness and chemical potential as well as temperature, flux, and ring size, using both analytical and numerical techniques. This is preliminary to the analysis of the experimentally more relevant multichannel systems. The results of the latter will be published in a separate paper.<sup>20</sup>

Specifically, in the present paper we derive and summarize results for the persistent current in one-channel systems of ring geometry threaded by an external magnetic flux  $\phi$ . The self-inductance of the loops is assumed to be small, so that corrections to the flux due to selfinductance may be neglected. Our calculations are for noninteracting systems of electrons. Results for the freeelectron model and the tight-binding model do not differ in their basic character. In Sec. II, we review the calculation of the persistent current in perfect single-channel rings with no impurities, and evaluate the temperature effects in various rings. In Sec. III, we discuss the effects of disorder on the persistent current in one-channel rings at zero temperature. We discuss both the limits of weak and strong disorder. The sensitivity of the currents to disorder is in certain ways analogous to that to temperature. We find that the current amplitude is of the order of the absolute value of the total transmission coefficient

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of the ring (thought to be bent open and connected by leads to reservoirs). In Sec. IV, we discuss the flux dependence of the persistent current upon averaging. This is partly motivated by the results for the magnetoresistance of one-dimensional rings, whose flux dependence changes from  $\phi_0$  to  $\phi_0/2$  periodicity upon averaging (ensemble averaging, energy averaging due to a finite temperature, etc.).<sup>7-9</sup> Our conclusion is that for persistent currents in one dimension "period halving" occurs if one averages over separate isolated rings with the number of electrons varying randomly from ring to ring. A summary of our results and a discussion are presented in Sec. V. In the Appendix, we derive formulas for the persistent current at temperatures large compared to the relevant level spacing.

Throughout our work we assume that the magnetic flux  $\phi$  threads the rings axially but that the electrons always move in a field-free space. The  $\phi_0$  periodicty of the electron wave function is then strictly of the Aharonov-Bohm<sup>21</sup> type. In the one-channel case (see Fig. 1) the spatial degree of freedom of the electron is the azimuthal angle  $\theta$ , and the vector potential A may be chosen to have the form  $\mathbf{A} = 2\pi \hat{\theta} \phi / L^2$ , where r is the radial distance, L the circumference of the loop, and  $\hat{\theta}$  the unit vector in the  $\theta$  direction. We will use as the spatial variable  $x = L\theta/2\pi$  instead of  $\theta$ , so that x varies between 0 and L. For the ring geometry, periodic boundary conditions apply, which lead to the usual quantization of energy levels. The current carried by each eigenstate can be calculated using the current operator. The total current is the sum over the individual contributions from each state, weighted with the appropriate occupation number. Following Byers and Yang<sup>14</sup> and Bloch,<sup>18</sup> we work in a gauge for the vector potential in which the field does not appear explicitly in the Hamiltonian and the current operators, but enters the calculation via the flux-modified boundary conditions.

$$\psi(L) = \exp\left[\frac{i2\pi\phi}{\phi_0}\right]\psi(0) ,$$

$$\frac{d\psi}{dx}\Big|_{x=L} = \exp\left[\frac{i2\pi\phi}{\phi_0}\right]\frac{d\psi}{dx}\Big|_{x=0} ,$$
(1.1)

where

$$\phi_0 = \frac{hc}{e} \quad . \tag{1.2}$$



FIG. 1. One-dimensional ring of circumference L threaded by a magnetic flux  $\phi$ .

These equations imply that the eigenstates and energies and hence all equilibrium physical properties of the ring are periodic in  $\phi$  with period  $\phi_0$ . This is true also in the presence of disorder. A flux  $\phi \neq \phi_0 \times (\text{integer})$  is mathematically equivalent to a change in the boundary conditions of the system. This observation is the key to all our discussions of the sensitivity of the persistent current to changes in temperature, chemical potential, degree of disorder, and other parameters.

There is a close connection between the states of an electron in a loop and the one-dimensional Bloch problem, as seen by identifying  $2\pi\phi/\phi_0$  and kL.<sup>12,14,18</sup> The energy levels of the ring form microbands as a function of  $\phi$  with period  $\phi_0$  analogous to the Bloch electron bands in the extended k-zone picture (Fig. 2). The current carried by level  $E_n$  at T = 0 is

$$I_n = -\frac{ev_n}{L}, \quad v_n = \frac{1}{\hbar} \frac{\partial E_n}{\partial k_n} , \qquad (1.3)$$

or, using the above analogy,

$$I_n = -c \frac{\partial E_n}{\partial \phi} . \tag{1.4}$$

At finite temperatures, instead of summing the currents  $I_n$  over all levels with weight  $f(E_n)$ , one can calculate the current from the thermodynamic potential of the system, <sup>14,18</sup>

$$I(\phi) = -c \frac{\partial F}{\partial \phi} . \tag{1.5}$$

Figure 2 shows schematically the energies of the eigenstates as a function of flux. In the absence of disorder in the ring, the curves form intersecting parabolas. In the presence of disorder, gaps open at the points of intersection, in the same way as band gaps form in the bandstructure problem. Since the band is symmetric in k for the one-dimensional lattice problem, the eigenenergies of the closed ring are symmetric in the flux. From Eq. (1.4), the current carried by an eigenstate is proportional to the



FIG. 2. Schematic diagram of the electron energy levels as a function of the flux  $\phi/\phi_0$  in a one-dimensional ring with and without impurities (solid and dashed curves, respectively).

slope of the energy versus flux curve. Therefore, the current is antisymmetric in the flux. At an integer or half-integer flux quantum, the energy is maximum or minimum; hence, at these values of  $\phi$  the current is zero.

## **II. EFFECTS OF TEMPERATURE**

In this section, the I- $\phi$  characteristics of ideal rings without impurities are determined for zero and nonzero temperature within the free-electron and tight-binding models. It is assumed that at the temperatures considered the phase coherence length of the electron is large compared to the ring circumference,  $L_{\phi} \gg L$ .

A. T = 0

For later reference, we review within the free-electron and tight-binding models the I- $\phi$  characteristics at zero temperature for ideal one-dimensional rings of circumference L threaded by the magnetic flux  $\phi$ , Fig. 1. The results for the two models are similar: The persistent current as function of  $\phi$  is periodic with period  $\phi_0 = hc/e$ and exhibits discontinuous steps at  $\phi$  values for which single electron levels cross the Fermi surface, cf. Eq. (2.4) and Fig. 3 below. Throughout the calculation we assume that the electrons move in a magnetic-field-free space. The electron spin is ignored.

The free-electron model of the ring is defined by

$$H = -\frac{\hbar}{2m}\frac{d^2}{dx^2} + V(x) , \qquad (2.1)$$

with the boundary conditions (1.1). In the absence of impurities,  $V \equiv 0$ , the energy  $E_n$  and current  $I_n = -ev_n/L$ of the *n*th eigenstate are

$$E_{n} = \frac{\hbar^{2}}{2m} \left[ \frac{2\pi}{L} \left[ n + \frac{\phi}{\phi_{0}} \right] \right]^{2},$$

$$I_{n} = -\frac{2\pi e \hbar}{mL^{2}} \left[ n + \frac{\phi}{\phi_{0}} \right],$$
(2.2)

with  $n = 0, \pm 1, \pm 2, \ldots$ . The level spacing at the Fermi surface for zero flux will be denoted by  $\Delta$ . For free electrons,

$$\Delta = \frac{2\pi \hbar v_F}{L} , \qquad (2.3)$$

and there are two eigenstates per energy interval  $\Delta$ .

Here instead of specifying the number of electrons  $N_e$ , we shall specify the chemical potential  $\mu$  or Fermi momentum  $k_F$  at T=0. For certain choices of  $\mu$  or  $k_F$ (both are  $\phi$  independent) the system will have a fixed number of electrons (i.e.,  $k_F = N_e \pi / L$  for free electrons), while for all others the number of electron will vary with the magnetic flux  $\phi$ . The reason is that, at T=0, a state is not occupied if its energy is larger than  $\mu$  and, as seen from Fig. 1, the energy of a particular state may cross the Fermi energy as a function of  $\phi$ .

The total current at T=0 is obtained by adding all contributions from levels with energies less than  $\mu$ . For  $\mu$  characterizing isolated rings with a fixed number of elec-

trons [i.e.,  $\mu = \hbar^2 (N_e \pi)^2 / 2mL^2$ ], the total persistent current is

$$I(\phi) = \begin{cases} -I_0 \frac{2\phi}{\phi_0} & \text{for } N_e \text{ odd, } -0.5 \le \frac{\phi}{\phi_0} < 0.5 \\ -I_0 \left[ \frac{2\phi}{\phi_0} - 1 \right] & \text{for } N_e \text{ even, } 0.0 \le \frac{\phi}{\phi_0} < 1.0 , \end{cases}$$
(2.4)

where  $I_0 = ev_F/L$ . For general  $\mu$ , for which  $N_e$  may vary between even and odd as a function of  $\phi$ , the current assumes one of the above values corresponding to the number of electrons at the particular value of the flux. The results for the various cases are shown in Fig. 3. The current-flux characteristics exhibit sawtooth shapes.

The total persistent current is periodic in  $\phi/\phi_0$  with period 1. It can be expressed as a Fourier sum in  $\phi/\phi_0$ . Neglecting the small difference between the Fermi velocities of systems with  $N_e$  and  $N_e + 1$ , electrons, one obtains



FIG. 3. Persistent current over one period of the magnetic flux from Eq. (2.5). The chemical potential is fixed such that the number of electrons in the ring is (a) even, (b) odd, and (c) changes between even and odd as function of the flux.  $I_0$  and  $\phi_0$  are defined in the text.

$$I(\phi) = \sum_{l=1}^{\infty} \frac{2I_0}{l\pi} \cos(lk_F L) \sin\left[\frac{2l\pi\phi}{\phi_0}\right].$$
 (2.5)

The dependence on the chemical potential becomes simple when the current is expressed in this way.

The tight-binding model for a ring with L = Na is defined by

$$H = -V \sum_{j=1}^{N} (a_{j}^{\dagger}a_{j-1} + a_{j}^{\dagger}a_{j+1}) + \sum_{j=1}^{N} \varepsilon_{j}a_{j}^{\dagger}a_{j} , \quad (2.6)$$

and the boundary conditions (1.1). Here  $a_j^{\dagger}$  and  $a_j$  denote the creation and annihilation operators at site j, V the hopping matrix element,  $\varepsilon_j$  the on-site energy, and a the lattice constant. For the perfect case,  $\varepsilon_j \equiv 0$ , the energy

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$$E_n$$
 and current  $I_n$  of the *n*th eigenstate are

$$E_{n} = -2V \cos \left[ \frac{2\pi}{N} \left[ n + \frac{\phi}{\phi_{0}} \right] \right] ,$$

$$I_{n} = -\frac{2eV}{N\hbar} \sin \left[ \frac{2\pi}{N} \left[ n + \frac{\phi}{\phi_{0}} \right] \right] ,$$
(2.7)

with  $n = 0, \pm 1, \pm 2, \ldots$ . The level spacing at zero flux at the Fermi surface is

$$\Delta = \frac{4\pi V}{N} \sin(k_F a) , \qquad (2.8)$$

which has the same form as Eq. (2.3). The total current at T = 0 for  $\mu = -2V \cos(N_e \pi/N)$ , for which the ring has a fixed number of electrons  $N_e$ , is

$$I(\phi) = \begin{cases} -I_0 \frac{\sin(2\pi\phi/N\phi_0)}{\sin(\pi/N)} & \text{for } N_e \text{ odd, } -0.5 \le \frac{\phi}{\phi_0} < 0.5 \\ -I_0 \frac{\sin[(\pi/N)(2\phi/\phi_0 - 1)]}{\sin(\pi/N)} & \text{for } N_e \text{ even, } 0.0 \le \frac{\phi}{\phi_0} < 1.0 . \end{cases}$$
(2.9)

For large N, the above expressions approach rapidly the free-electron formulas (2.4); the differences are already insignificant for N > 5. For general  $\mu$ , for which  $N_e$  varies between even and odd as a function of  $\phi$ , the current assumes one of the above values accordingly. The total persistent current expressed as a Fourier sum equals the free-electron result (2.5), when N and  $N_e$  are not too small.

### **B.** T > 0

With increasing temperature, the probability that electrons occupy higher levels, which may carry larger currents, increases. However, at higher temperatures, the occupation probabilities of levels close in energy (which encompass levels having currents of opposite sign) are not very different. The net result is significant cancellations of positive and negative contributions to the current. For metals a characteristic temperature  $T^*$  is set by the level spacing  $\Delta$ , Eq. (2.3) or (2.8). We find that the Fourier coefficients of the persistent current [compare Eq. (2.5)] decrease exponentially with temperature,  $exp(-lT/T^*)$  at  $T > T^*$ , however, are not sensitive to temperature at  $T < T^*$  (for low harmonics l). For  $T >> T^*$ , the first harmonic (l = 1) gives a good approximation to the current. The results are summarized in Figs. 4 and 5. Similar behavior holds for systems with a low density of carriers. Note that the persistent current pertains to time averages of the current.<sup>12</sup> A decrease of the current amplitude with temperature was also observed by Büttiker.<sup>13</sup>

Finite temperature affects the system in another important way. At nonzero temperature, thermal excitations, such as phonons, will be present. Such excitations interact with the electrons inelastically, giving rise to phase randomization of the electron wave function (besides some level shifting). Hence such interactions wash out quantum effects. We will assume that some electronphonon coupling exists by which thermal equilibrium is established, but that this coupling is sufficiently weak so that it does not lead to substantial level shifting and broadening (on the scale of  $\Delta$ ). Hence, we assume implicitly that we work at sufficiently low temperatures and small system sizes such that  $I_{\phi}$ , the phase coherence length of the electron, is large compared to L, the circumference of the ring.<sup>22</sup>

To calculate the persistent current we need to know the eigenstates of the system and the thermal distribution function. Typical to mesoscopic systems is the fact that the energy levels form a discrete spectrum. Since the systems are not in the thermodynamic limit, the canonical



FIG. 4. Persistent current vs flux at temperatures  $T/T^*=0$ , 0.5, 1, 2, and 3 for a ring with an odd number of electrons.  $k_B T^* = \Delta/2\pi^2$  is a measure of the level spacing at the Fermi surface.

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FIG. 5. Persistent current vs temperature for a ring with an odd number of electrons at  $\phi/\phi_0 = -0.25$ . The dashed curve represents the high-temperature expansion, Eq. (2.11) with l = 1. The crossover temperature is given by  $T^*$ .

and grand-canonical ensembles give rise to different single-level probability distributions. For a ring that can exchange only energy with a reservoir, a description in terms of a canonical ensemble with fixed number of particles  $N_e$  is appropriate. However, it is more convenient to consider a system that also weakly couples to a particle reservoir, since the distribution function is the wellknown Fermi-Dirac distribution. We expect that the two approaches give similar results for the persistent current. Adapting the latter approach, we characterize the system by a Fermi-Dirac distribution with the chemical potential  $\mu$ , and compute the persistent current at finite temperatures starting from

$$I(\phi) = -\frac{e}{L} \sum_{n=-\infty}^{\infty} \frac{v_n}{e^{\beta(E_n - \mu)} + 1} , \qquad (2.10)$$

where  $\beta = 1/k_B T$ . Details of the calculation are presented in the Appendix. In the following we summarize the principal results for temperatures large compared to the relevant level spacing.

(i) Metals. In the limit  $\mu \gg k_B T$ , Eq. (A13) yields for the persistent current

$$I = \sum_{l=1}^{\infty} \frac{4I_0 T}{\pi T^*} \times \frac{\exp(-lT/T^*)}{1 - \exp(-2lT/T^*)} \cos(lk_F L_x) \sin\left[\frac{2l\pi\phi}{\phi_0}\right],$$
(2.11)

with  $I_0 = ev_F/L$  and

$$k_B T^* = \frac{\Delta}{2\pi^2} = \frac{\hbar v_F}{\pi L} \ . \tag{2.12}$$

 $T^*$  is the characteristic temperature that separates highand low-temperature regimes. The above result derived for the free-electron model holds also for metals with a general band structure provided that near the Fermi surface  $E - E_F \approx \hbar v_F (k - k_F)$ . That includes the tightbinding model. For  $T > T^*$ , the first harmonic (l = 1) in Eq. (2.11) gives a good approximation to the current. The numerical results in Fig. 4 exhibit the feature of the current approaching sinusoidal behavior with increasing temperature. Figure 5 shows that the first harmonic at  $\phi/\phi_0 = -0.25$  fits well the corresponding numerical results for  $T > T^*$ .

(ii) Semiconductors. When  $\mu$  is very small  $(|\mu| \ll k_B T)$  and  $T \gg \tilde{T}/\pi$ , Eq. (A12) yields for the persistent current

$$I(\phi) = \sum_{l=1}^{\infty} \frac{4ek_B T}{\hbar} \cos\left[\left(\frac{\pi l^2 T}{\tilde{T}}\right)^{1/2}\right] \times \exp\left[-\left(\frac{\pi l^2 T}{\tilde{T}}\right)^{1/2}\right] \sin\left(\frac{2l\pi\phi}{\phi_0}\right), \quad (2.13)$$

with the characteristic temperature

$$k_B \tilde{T} \equiv \frac{\tilde{\Delta}}{2\pi^2} = \hbar^2 / mL^2 , \qquad (2.14)$$

where  $\tilde{\Delta}$  denotes the level spacing at the bottom of the band at zero flux. For  $T \gtrsim \tilde{T}/\pi$ , the first harmonic (l=1) in Eq. (2.13) gives a good approximation to the current. This case may apply to semiconductors with small  $\mu$ .

(iii) Insulators. When  $\mu$  is large and negative, and  $T \gg \tilde{T}$ , Eq. (A7) yields for the persistent current

$$I(\phi) = \sum_{l=1}^{\infty} -\frac{elk_BT}{\hbar} \left[ \frac{2T}{\pi \tilde{T}} \right]^{1/2} \exp\left[ \frac{\mu}{k_BT} - \frac{l^2}{2\tilde{T}} \right] \\ \times \sin\left[ \frac{2l\pi\phi}{\phi_0} \right].$$
(2.15)

A more precise condition under which (2.15) is valid is given in (A8).

## C. Conclusion

Nonzero temperature has the two main effects that all discontinuities in the I- $\phi$  characteristic become rounded and that the maximum amplitude of the current decreases. The effects are exhibited in Figs. 4 and 5. The characteristic temperature  $T^*$  (or  $\tilde{T}$ ) is set, for metals, by the level spacing at the Fermi surface,  $\Delta = 2\pi \hbar v_F/L$ , and for systems with a low density of carriers, by the level spacing at the bottom of the band,  $\tilde{\Delta} = \hbar^2 (2\pi)^2 / 2mL^2$ . At  $T > T^*$  (or  $\tilde{T}$ ) the persistent current is proportional to  $\sin(2\pi\phi/\phi_0)$  with an amplitude that decreases exponentially with temperature. For  $T < T^*$  (or  $\tilde{T}$ ) higher harmonics contribute and the maximum amplitude of the total current depends only weakly on temperature.

### **III. EFFECTS OF ELASTIC SCATTERING**

In this section, the  $I-\phi$  characteristics of rings with impurities are expressed in terms of the total transmission coefficient of the rings and discussed both in the weakand strong-scattering regimes. The calculations are for independent electrons at zero temperature.

### A. Transfer-matrix method

We derive the persistent current in disordered onedimensional rings within the tight-binding model using the transfer-matrix method. The model is defined in Eq. (2.6). The  $I-\phi$  characteristics of the ordered tight-binding model were discussed in Sec. II and found to be analogous to those of the free-electron model. Now we include the random potential energy term; in numerical calculations we choose random on-site potentials  $\varepsilon_j$  with independent square distributions of strength -W/2 to +W/2. The hopping matrix element V is set constant so that the disorder parameter is W/V. The transfer-matrix method is well known,  $^{23-25}$  our results for the persistent current are new.

The transfer matrix  $\underline{T}_{j}$  connects the wave function across site x = ja, where a is the lattice constant. It is obtained by requiring that the general wave function,

$$\psi_k(x) = \begin{cases} Ae^{ik[x-(j-1/2)a]} + Be^{-ik[x-(j-1/2)a]} & \text{when } x = (j-1)a, ja \\ Ce^{ik[x-(j+1/2)a]} + De^{-ik[x-(j+1/2)a]} & \text{when } x = ja, (j+1)a \end{cases},$$
(3.1)

satisfy the continuity condition and the tight-binding Schrödinger equation,  $H\psi(x) = E\psi(x)$ , at site *j*. Note that the wave function is defined at discrete x = ja, j = 1, 2, ..., N. We parametrize the solution in term of the energy *E* which is related to the wave vector *k* via<sup>26</sup>

$$E(k) = -2V\cos(ka) . \qquad (3.2)$$

The result is

with the transmission and reflection coefficients

$$t_{j} = \frac{2iV\sin(ka)}{2iV\sin(ka) - \varepsilon_{j}},$$
  

$$r_{j} = t_{j} - 1 = \frac{\varepsilon_{j}}{2iV\sin(ka) - \varepsilon_{j}}.$$
(3.4)

The wave functions at sites  $j + 2, j + 3, \ldots$  are then obtained by multiplying the wave functions at the preceding sites with  $\underline{T}_{j+1}, \underline{T}_{j+2}, \ldots$ , respectively. After having gone through the whole ring one will arrive back at the original site. For the wave function to be an eigenstate of the ring problem it must satisfy the boundary condition (1.1). Writing the total transfer matrix in the form

$$\underline{T} = \begin{bmatrix} 1/t^* & r/t \\ r^*/t^* & 1/t \end{bmatrix} \equiv \prod_{j=0}^{N} \underline{T}_j , \qquad (3.5)$$

the boundary condition can be written

$$\underline{T} \begin{bmatrix} A \\ B \end{bmatrix} = \exp \left[ \frac{i2\pi\phi}{\phi_0} \right] \begin{bmatrix} A \\ B \end{bmatrix}, \qquad (3.6)$$

which, using the relation  $|r|^2 + |t|^2 = 1$ , can be simplified to<sup>25</sup>

$$\cos\left[\frac{2\pi\phi}{\phi_0}\right] = \operatorname{Re}\left[\frac{1}{t}\right] \equiv f(E) . \tag{3.7}$$

Equation (3.7) determines the allowed values of the quantum number k and, therefore, the eigenenergies (3.2). It can be expressed in terms of either k or E. For the current carried by the *n*th eigenstate, we obtain

$$I_{n}(\phi) \equiv -c \frac{\partial E_{n}}{\partial \phi} = \frac{e}{\hbar} \frac{\sin \left[\frac{2\pi\phi}{\phi_{0}}\right]}{\frac{\partial}{\partial E} \operatorname{Re}(1/t)}, \qquad (3.8)$$

where the denominator is calculated at the solutions  $E = E_n$  of (3.7). For the ordered ring,  $t_j = 1$ , i.e.,  $1/t = \exp(-ikL)$ , we recover for the spectrum  $E_n$  and current  $I_n$  the results of Eq. (2.7).

This very simple expression (3.8) for the persistent current is the starting point of our numerical work and analytical analysis. The advantage of this approach is that it allows us to treat large systems without serious computing-time problems. For large L one simply needs to multiply a larger number of matrices  $T_j$  to obtain the total transmission coefficient t. It is also possible to study the large-W limit, in which the then very small persistent current is calculated from the very large slope of Re(1/t). Numerical differentiation allows us to obtain this large slope accurately.

Much information can be deduced from Eqs. (3.7) and (3.8). One important result is that the amplitude of the persistent current is roughly proportional to the modulus of the total transmission coefficient. The current at  $\phi/\phi_0=0.25$  is a good measure of the current amplitude, cf. Eqs. (2.4) and (2.5). [Without impurities, this is the flux at which the energy spectrum is maximally asymmetric, see Eq. (2.2) or (2.7).] We concentrate on the current at this flux in the following discussion.

The matching condition (3.7) involves  $\operatorname{Re}(1/t)$ , which we express as  $\operatorname{Re}(1/t) = |1/t| \cos \alpha$ . [Figure 6 shows  $\operatorname{Re}(1/t)$  versus *E* for four values of *W*.] The two factors vary with energy *E* on very different scales. |1/t| is a slowly varying envelope, whereas  $\cos \alpha$  is a rapidly oscillating factor. For the ordered ring,  $\cos \alpha \equiv \cos(kL)$  is well approximated by  $\cos(2\pi E/\Delta)$ , where  $\Delta$  is the energy range containing two states. For the disordered ring, it is

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FIG. 6. The function  $f(E) \equiv \operatorname{Re}(1/t)$  in the matching equation (3.7), for a ring with L/a = 10, as a function of the energy for different degrees of disorder, W/V = 0, 2, 4, and 16.

appropriate to presume that on average  $\cos \alpha$  has the same form, with an energy range  $\Delta$  that contains on average two levels. Studies of the spectrum of random Hamiltonians show that the level spacing possesses a large de-gree of regularity.<sup>27,28</sup> Except in the limit of extremely strong disorder and away from the band edges, the average level spacing is approximately equal to the unperturbed value. Therefore, for the tight-binding model the level spacing is  $\Delta \approx (4\pi V/N)\sin(k_F a)$  of Eq. (2.8), when  $W \ll 2\pi V$ . When  $W \gg 2\pi V$ , then  $\Delta \approx 2W/N$ . This latter estimate is obtained as follows. For large W the electrons are tightly bound with energies close to their on-site energies  $\varepsilon_i$ . By assumption the  $\varepsilon_i$  have a square distribution, therefore on average there are two levels within the energy range 2W/N. When  $W > 2\pi V$ ,  $\xi$  is less than five lattice constants. Such extremely strong localization does not seem relevant for persistent-current experiments.

The current amplitude can then be estimated from Eq. (3.8). Consider a level  $E_n$  close to the Fermi energy. We assume that  $\cos(2\pi E/\Delta)$  is the major varying factor in  $f(E) \equiv \operatorname{Re}(1/t)$ . When  $W \ll 2\pi V$ ,  $\Delta \approx (4\pi V/N) \sin(k_F a) = 2\pi \hbar v_F/N_a$ , and one obtains  $f'(E) \approx (L/\hbar v_F) |1/t| \sin(2\pi E/\Delta)$ . Replacing  $\sin(2\pi E/\Delta)$  by 1, which is justified at  $\phi/\phi_0 = 0.25$  where the energy levels are given by  $\cos(2\pi E/\Delta) = 0$ , one finds

$$I_n \approx I_0 \mid t \mid , \tag{3.9}$$

where  $I_0 = ev_F / Na$ . When  $W >> 2\pi V$ ,  $\Delta$  is 2W/N. One then obtains in the half-filled-band case

$$I_n \approx \frac{W}{2\pi V} I_0 \mid t \mid \quad . \tag{3.10}$$

The total current at zero temperature is obtained by summing the currents of all states with energies smaller than the Fermi energy. For ordered rings, the total currents at  $\phi/\phi_0=0.25$  is approximately equal to onehalf the current of the last occupied level below the Fermi energy. We expect the same to be true for the average current in the presence of disorder. Using Eq. (3.9), we obtain for the total current amplitude the estimate

$$I \approx \frac{1}{2}I_0 \mid t \mid , \qquad (3.11)$$

where |t| is measured at the Fermi surface. We have checked this result for the special cases of rings with single impurities characterized by  $\delta$ -function and squarebarrier potentials as well as rings with random sets of impurities. The above expression gives good agreement with numerical results for the current amplitude at  $\phi/\phi_0 = 0.25$ .

Further information can be inferred for the case of strong disorder. As a function of  $\phi/\phi_0$ , the left-hand side of the matching equation (3.7) varies between -1 and +1. For strong disorder, |t| is very small, therefore  $f(E) = |1/t| \cos \alpha$  has a very large slope at  $E \approx E_n$ . Hence, the energy range within which f(E) changes from -1 to +1 is very small. Within that energy range, f(E) and f'(E) can be represented accurately by a Taylor series including the f'' term. Substituting this expansion into Eqs. (3.7) and (3.8), one obtains the first and second harmonics of the current,

$$I_n(\phi) = \frac{e}{\hbar} \left[ \frac{1}{f'} \sin\left[\frac{2\pi\phi}{\phi_0}\right] - \frac{f''}{2f'^3} \sin\left[\frac{4\pi\phi}{\phi_0}\right] + \cdots \right] .$$
(3.12)

For  $W \ll 2\pi V$ , one estimates for levels close to the Fermi energy that  $f' = (L/\hbar v_F) |1/t|$  and  $f'' \ll (L/\hbar v_F)^2 |1/t|$ , using the earlier approximations. That means the coefficients of the first two harmonics are

$$\frac{e}{\hbar} \frac{1}{f'} \approx I_0 \mid t \mid ,$$

$$\frac{e}{\hbar} \frac{f''}{2f'^3} \ll \frac{I_0}{2} \mid t \mid^2 .$$
(3.13)

When the transmission amplitude |t| is small, the current is sinusoidal in the flux and has an amplitude proportional to |t|. The amplitudes of higher harmonics are smaller by at least a factor of |t|. We do not show the signs of the coefficients in Eq. (3.13). We know that for any disorder the sign of the first term alternates from level to level since the slope of f(E) alternates. However, the above argument is too crude for statements about the sign of the second term. Numerically there is evidence that the second harmonic of the average total current does not change sign.

Another numerical approach to the disordered tightbinding model is to write the Hamiltonian (2.6) in the form of a matrix, to diagonalize the matrix numerically, and to determine the current of the *n*th level,  $I_n = -c \partial E_n / \partial \phi$ , by numerical differentiation (or to use the current operator on the wave function). We have also worked with this approach. However, we cannot study large disorder with this approach because the very small currents cannot be obtained numerically with sufficient accuracy from  $-c\partial E_n/\partial \phi$  or from applying the current operator.

If the disorder is very weak, perturbation theory is adequate. We will state only two results from perturbation theory that hold for arbitrary impurity potentials in the weak-coupling limit. First, since the correction to the wave function is first order in the impurity potential, the leading correction to the current is second order in the impurity potential. The cross terms do not contribute since they are orthogonal. Second, the corrections to the total current approach zero for large Fermi velocities. The physical reason is that impurities do not appreciably slow down fast-moving particles. For states representing those particles, |t| = 1. Hence the total current (3.11) is approximately equal to the unperturbed one.

#### **B.** Single scatterer

The effects of impurity scattering are easily observed for a ring with a single impurity. For simplicity, we consider the free-electron model with an impurity characterized by a  $\delta$ -function potential,  $V(x) = \epsilon \delta(x)$ , in Eq. (2.1). The case of a square-well potential barrier leads to similar conclusions.

The persistent current  $I_n(\phi)$  is obtained by replacing in Eqs. (3.7) and (3.8) 1/t by  $\exp(-ikL)/t$  with

$$t = \frac{i\hbar^2 k/m}{i\hbar^2 k/m - \varepsilon} , \qquad (3.14)$$

and

$$E(k) = \frac{\hbar^2 k^2}{2m} .$$
 (3.15)

The weak- and strong-coupling regimes are defined by  $\varepsilon \ll \varepsilon^*$  and  $\varepsilon \gg \varepsilon^*$ , respectively, where  $\varepsilon^*$  is determined from  $|V_{kk'}| = (\Delta/2\pi^2)$  with  $|V_{kk'}| = \varepsilon/L$ , which yields

$$\varepsilon^* = \frac{\hbar v_F}{\pi} = \frac{\hbar^2 N_e}{mL} \ . \tag{3.16}$$



FIG. 7. Effect on the persistent current vs flux of a single  $\delta$ -function impurity of strength  $\epsilon/\epsilon^* = 0$ , 0.5, 1, 2, 4, and 8 in a ring with an odd number of electrons. The scale factor is  $\epsilon^* = LT^*$ . The curves resemble those of Fig. 4.

[The factor  $2\pi^2$  is included so that  $\varepsilon^*/L = k_B T^*$ , cf. Eq. (2.12).] Since  $N_e \sim L$ ,  $\varepsilon^*$  like  $v_F$  is "intensive." Figure 7 exhibits the results for the *I*- $\phi$  characteristics at T = 0 for a system with  $N_e$  odd; the results can be generalized to nonzero temperatures by weighting the states with a Fermi distribution function as in Eq. (2.10). Comparing Figs. 5 and 7 is instructive. It shows that the effects of temperature and elastic scattering on the *I*- $\phi$  characteristics are very similar. In the latter case, the curves approach sinusoidal behavior at  $\varepsilon/\varepsilon^* \gg 1$ .

In the weak- and strong-coupling limits, analytical results for the persistent current are obtained by solving Eq. (3.8) in those limits. The persistent current is well approximated, for  $\epsilon/\epsilon^* < \pi$  when  $\phi/\phi_0 \le 0.25$  and for  $\epsilon/\epsilon^* < \pi^2(1-2\phi/\phi_0)$  when  $\phi/\phi_0 \ge 0.25$  (and  $N_e$  odd), by

$$I(\phi) = -I_0 \frac{2\phi}{\phi_0} \left[ 1 - \frac{1}{2\pi^2} \left[ \frac{\varepsilon}{\varepsilon^*} \right]^2 \left[ \frac{1}{\sin^2 \left[ \frac{2\pi\phi}{\phi_0} \right]} - \frac{\cos \left[ \frac{2\pi\phi}{\phi_0} \right]}{\frac{2\pi\phi}{\phi_0} \sin \left[ \frac{2\pi\phi}{\phi_0} \right]} \right] + \cdots \right], \qquad (3.17)$$

and for  $\varepsilon / \varepsilon^* > \pi$ ,

$$I(\phi) = I_0 \frac{\pi}{2} \left[ \left(-1\right)^{N_e} \frac{\varepsilon^*}{\varepsilon} \sin\left(\frac{2\pi\phi}{\phi_0}\right) + \left(\frac{\varepsilon^*}{\varepsilon}\right)^2 \sin\left(\frac{4\pi\phi}{\phi_0}\right) + \cdots \right].$$
(3.18)

In both formulas corrections of order  $1/N_e$  and higher to the terms shown have been dropped. In Eq. (3.17), the first nonvanishing correction is order  $\varepsilon^2$  as expected from perturbation theory. In Eq. (3.18), the amplitudes of the odd harmonics include factors  $(-1)^{N_e}$ , i.e., differ in sign for  $N_e$  even and odd. In magnitude the first harmonic dominates. Its amplitude agrees with Eq. (3.11) with t given by Eq. (3.14). In the form given, Eq. (3.18) holds also for  $\varepsilon$  large and negative.

#### C. Random set of impurities

All electron eigenstates are exponentially localized in one-dimensional disordered systems. We will speak of weakly or strongly disordered rings depending on whether the localization length  $\xi$  is larger or smaller than the circumference L on the ring. In the strongly disordered regime the amplitude of the persistent current is found to decrease exponentially with  $L/\xi$ .

decrease exponentially with  $\hat{L}/\xi$ . In localization theory<sup>29,30</sup> one defines the localization length  $\xi$  in terms of the resistance R (R in units of  $h/e^2$ ) of long one-dimensional wires,

$$\frac{\langle \ln R \rangle}{L} = \frac{2}{\xi} \quad . \tag{3.19}$$

 $\langle \rangle$  denotes an average over the impurity distribution. On the other hand, the Landauer formula gives<sup>31</sup>

$$R = \frac{|r|^2}{|t|^2} = \frac{1 - |t|^2}{|t|^2} .$$
(3.20)

For strong disorder, i.e.,  $|r| \approx 1$ , one obtains from Eqs. (3.19) and (3.20)

$$\langle \ln | 1/t | \rangle \approx \frac{L}{\xi}$$
 (3.21)

Using  $R = \exp(2L/\xi) - 1$  in conjunction with Eq. (3.20) and appropriate averages, <sup>32</sup> one concluded that Eq. (3.21) holds over the full range of disorder.

For the tight-binding model in the half-filled-band case, the localization length has been calculated for long wires in two limits, <sup>33,24</sup>

$$\xi = \frac{105.0aV^2}{W^2} \quad \text{when } W << 2\pi V , \qquad (3.22)$$

and<sup>34,24</sup>

$$\xi = \frac{a}{\ln(W/2eV)} \quad \text{when } W >> 2\pi V \ . \tag{3.23}$$

These results hold for energies close to the Fermi energy  $(\mu = 0)$ .

For the ring geometry we define the crossover from weak to strong disorder by  $L \approx \xi$ . The energy parameter



FIG. 8. Effect of disorder on the average current,  $\overline{I}/I_0 = \exp(\ln(I/I_0))$ , for a ring of N = 20 at  $\phi/\phi_0 = 0.25$  in the half-filled-band case. The dashed curve is the prediction from (3.25) and (3.22). The curves resemble those of Fig. 5.

that determines the sensitivity of the persistent current to disorder is the level spacing  $\Delta$ , Eq. (2.8). In units of  $\Delta$  the degree of disorder (apart from a numerical factor) is measured by

$$U_R = \frac{W}{\sqrt{12L}} \frac{1}{\Delta} , \qquad (3.24)$$

where the first factor is the average of the modulus of the random potential energy in Eq. (2.6). Using  $\Delta = 4\pi a V/L$  and Eq. (3.22), one finds that for sufficiently large L the condition  $L \approx \xi$  implies the crossover value  $U_R^* \approx 0.235$ .

In Fig. 8 we show the average persistent current  $\bar{I}/I_0$ versus  $U_R$  at  $\phi/\phi_0=0.25$  for a small ring of L=20 with ten electrons. The data is obtained from numerical diagonalization of the Hamiltonian (2.6). [Each point represents the exponential of the ensemble average of  $\ln(I/I_0)$  over 100 impurity configurations.] The decay of the amplitude as a function of disorder is very similar to the one as a function of temperature in Fig. 5. The current amplitude, at  $\phi/\phi_0=0.25$ , can also be estimated by using Eqs. (3.11) and (3.21), which yields for  $W \ll 2\pi V$ 

$$I = \frac{1}{2}I_0 \exp\left[-\frac{L}{\xi}\right] . \tag{3.25}$$

The dashed curve in Fig. 8 represents the estimate (3.25) with  $1/\xi$  given by Eq. (3.22). The deviations for  $U_R \gtrsim 0.25$  are due to the fact that there W becomes larger than  $2\pi V$ , so that Eqs. (3.11) and (3.22) no longer apply. For larger L the deviations will occur at larger values of  $U_R$ .

We now consider the half-filled-band case, for which the Fermi energy  $\mu = 0$ . The localization length is given by Eq. (3.22) or (3.23) depending on whether W is smaller or larger than  $2\pi V$ . Approximating the total current by one-half of the current of the highest occupied level, we conjecture from Eqs. (3.12) and (3.13) that for strongly disordered rings ( $W \ll 2\pi V$ ) to leading order,

$$I(\phi) \approx \frac{I_0}{2} \exp\left[-\frac{LW^2}{105.0aV^2}\right] \sin\left[\frac{2\pi\phi}{\phi_0}\right]$$
$$\approx \frac{I_0}{2} \exp(-18.05U_R^2) \sin\left[\frac{2\pi\phi}{\phi_0}\right]. \quad (3.26)$$

For very strong disorder ( $W >> 2\pi V$ ), where  $\Delta \approx 2W/N$ , one obtains as generalization of Eq. (3.10),

$$I(\phi) \approx \frac{I_0}{2} \frac{W}{2\pi V} \left[ \frac{W}{2eV} \right]^{-L/a} \sin\left[ \frac{2\pi\phi}{\phi_0} \right] . \qquad (3.27)$$

However, note that this latter formula is presumably not relevant to persistent-current experiments. The coefficients of the second harmonics are smaller by approximately a factor of  $\exp(-LW^2/105.0aV^2)$  and  $(W/2eV)^{-L/a}$ , respectively.

In Fig. 9 we compare numerical results for  $-(a/L)\ln(I/I_{(W=0)})$  at  $\phi/\phi_0=0.25$  with the asymptotic forms for the inverse localization length from Eqs. (3.22) and (3.23) as functions of the degree of disorder. Accord-



FIG. 9. The inverse localization length in units of the lattice constant a as calculated from (3.25) vs disorder. The dashed curves are the limiting behaviors for small and large W as obtained from Eqs. (3.22) and (3.23), respectively.

ing to Eq. (3.25), the expression  $-(a/L)\ln(I/I_{(W=0)})$ should be equal to the inverse localization length when  $W << 2\pi V$ , and also for large L when  $W >> 2\pi V$ . We find that the data agree very well with the prediction for  $W < 2\pi V$ . For  $W > 2\pi V$ , the agreement is not as good because the current is not precisely of the form  $I_{(W=0)}\exp(-L/\xi)$  [compare the different prefactor in the expression for the current (3.10)]. However, for large L that difference becomes less important and  $-(a/L)\ln(I/I_{(W=0)})$  approaches the asymptotic form of the inverse localization length corresponding to Eq. (3.23).

### **D.** Conclusion

The effects of disorder on the  $I-\phi$  characteristics were discussed for rings with single impurities and random sets of impurities. Like temperature, impurity scattering "mixes" electron states with positive and negative velocities. The effects of impurities are to round off discontinuities in the  $I_n-\phi$  characteristics (gaps appear in the microbands at the band edges, see Fig. 2) and to reduce the amplitude of the current. This is similar to the effects of temperature described in Sec. II. We used the transfer-matrix formalism to study analytically the weakand strong-coupling regimes by making contact with localization theory, and investigated numerically the whole range of disorder.

### **IV. EFFECTS OF AVERAGING**

The resistance of mesoscopic normal-metal ring with two leads connecting it to an external source has been extensively studied as a function of the enclosed magnetic flux.<sup>1,2</sup> It is now understood that the  $\phi_0$  periodicity of the resistance is halved and becomes  $\phi_0/2$  upon the appropriate averaging (ensemble averaging, effective energy averaging occurring at finite temperatures, etc.).<sup>7-9</sup> Here we shall be interested in studying the flux dependence of the persistent current, and in particular we shall examine whether similar "period halving" of the current may take place as a result of various averaging procedures.

First we consider the free-electron problem at T=0. From Eq. (2.5) we see that the *l*th Fourier coefficient is proportional to  $\cos(lk_F L)$ . This means that if we average the persistent current over some range of the chemical potential, each Fourier coefficient averages to zero. Thus this type of averaging would not lead to period halving. However, if we consider a ring with fixed number of electrons, then the Fourier coefficients in Eq. (2.5) as a function of  $N_{\rho}$  alternate in sign for odd l, but do not change sign for even l. This implies that if we average over an ensemble of isolated rings, where the number of electrons in each ring is fixed but varies randomly from one ring to the other, only term with even l survive. This result in a  $\phi_0/2$  periodicity of the persistent current. Note that the above argument does not involve elastic scattering along the ring (which is a common, though not necessary, scenario in the study of period halving in the resistance of two-terminal rings). We emphasize that various averaging procedures used in the magnetoresistance case do not result in period halving in our procedure.

For finite temperatures, the Fourier decomposition of the persistent current of a metal ring is given by Eq. (2.11), in which  $k_F \equiv \sqrt{2m\mu}/\hbar$ . Within the framework of the grand-canonical ensemble the average number of particles  $\overline{N}$  (which is a fluctuating quantity) is given in terms of  $\mu$  (which is a constant parameter). If we average over an ensemble of rings, each with a randomly selected  $\mu$ subject to the constraint that  $\overline{N}$  is an integer, we again obtain period halving. With increasing temperature, the large-*l* terms in Eq. (2.11) vanish exponentially faster than the small-*l* terms. Consequently, period halving as a consequence of finite temperature does not take place.

Next we consider the effect of similar averaging procedures in the presence of impurities. In the weakscattering limit there are small correction terms to the current in the free-electron limit. The odd-l terms still alternate in sign with  $N_e$ , hence the results of the above discussion remain qualitatively unchanged. In the strongscattering limit the l = 2 term is always smaller than l = 1term [cf. Eqs. (3.18) and (3.26), and Eq. (3.27) for a single impurity and many impurities, respectively]. Our results for  $\delta$ -function [Eq. (3.18)] and square potentials suggest that in the strong-scattering limit the l=1 term does vanish upon averaging over particle number (ensemble of isolated rings with a random number of electrons). The second harmonic (in the strong-scattering limit) does not contain a coefficient which alternates with  $N_{e}$ , and will not vanish upon particle averaging. We propose that for general disorder, averaging over the particle number will lead to a period halving, even in the strong-scattering limit. Evidently in that limit the current amplitude is very small. We shall also have to average over a larger ensemble of rings (compared to the weak-scattering limit) in order to see the hc/2e periodicity. When averaging over the chemical potential rather than  $N_e$ , all Fourier components will vanish, and no period halving will be observed. This is similar to what happens in the pure case at T=0. Different choices of  $\mu$  define periodic functions  $I(\phi)$  which differ from each other in phase (as well as in shape). Averaging over those functions gives a vanishing expectation value of I.

### V. SUMMARY

We have derived expressions for the persistent current in small one-dimensional normal-metal rings of circumference L threaded by an external magnetic flux  $\phi$  as functions of the ring size L, flux  $\phi$  temperature T, and degree of disorder W. In a separate paper<sup>20</sup> we will discuss the generalization of these results and the new features of persistent currents in multichannel rings. Experimental studies of such persistent currents would allow one to probe the nature of the discrete band structure of submicrometer metal and semiconductor devices.

The principal properties of persistent currents in onedimensional loops are as follows.

(i) For a time-independent flux  $\phi$  applied to the ring, there are circulating currents that are periodic in  $\phi$  with period  $\phi_0 = hc/e$  and have a magnitude that is given by the sum over the velocities in all occupied levels. At zero temperature, the current *I* is dominated by the last filled level and different *I*- $\phi$  characteristics result depending on the filling of these levels. These results are summarized in Eqs. (2.4) and (2.5), and Fig. 3. The maximum amplitude  $I_0 = ev_F/L$  decreases inversely proportional to the ring circumference *L*. The history of these results is discussed in the Introduction.

(ii) At finite temperatures the quantum levels are occupied according to some probability distribution function, e.g., Eq. (2.10). The T = 0 steps in the  $I - \phi$  characteristics become rounded and the amplitudes of the currents reduced, as exhibited in Figs. 4 and 5. For metal rings Eq. (2.5) is replaced by Eq. (2.11), which shows an amplitude reduction of the *l*th harmonics,  $\sin(2\pi l \phi / \phi_0)$ , by factors  $\exp(-lT/T^*)$  that come to bear for  $T > T^*$ . The value of the characteristic temperature is determined by the level spacing at the Fermi surface, <sup>22</sup> Eq. (2.12), and it decreases inversely proportional to the ring circumference. Similar expressions apply to semiconductor rings, Eqs. (2.13) and (2.14). The decrease with temperature of the current amplitude was seen by Büttiker.<sup>13</sup>

(iii) Disorder that leads to elastic scattering in the ring was treated within the transfer-matrix formalism. We obtained simple formulas for the persistent current in terms of the transmission coefficient of the system, Eq. (3.11). These equations were analyzed numerically and, in the limits of weak and strong disorder, also analytically. All forms of disorder were found to round the T=0steps in the *I*- $\phi$  characteristic and to reduce the amplitude of the persistent current, Figs. 7 and 8. Weak disorder leads to corrections of order  $W^2$  only. For strong disorder, the *I*- $\phi$  characteristic is well described by the first harmonic in the flux,  $\sin(2\pi\phi/\phi_0)$ , with an amplitude that decays as  $\exp(-L/\xi)$ , where  $\xi$  is the localization length.

(iv) Several averaging procedures that lead to period halving in the problem of conductance of a two-terminal ring, do not do so here. Averaging procedures that do lead to such a change in periodicity are those in which ensembles of rings containing different numbers of particles are considered. They are not related to the "backscattering mechanism" in the conductance problem. The two problems, that of the conductance and that of the persistent current, differ from each other qualitatively. This can be seen, for example, by considering the limit of strong elastic scattering. In this limit the conductance is proportional to  $|t|^2$  (t being the total transmission amplitude) whereas  $I \propto |t|$ ; cf. Eq. (3.11).

Before concluding, a few remarks are in order.

(a) As already pointed out by Büttiker et al.<sup>12</sup> and Büttiker,<sup>13</sup> the currents considered here are genuinely persistent and do not decay to zero with time, even in the presence of some weak phase-smearing effects. A finite phase-breaking time,  $\tau_{\phi}$ , results in a diminished amplitude of the dc current I. One could then argue naively that after times larger than  $\tau_{\phi}$  the electron no longer remains in its original phase and I decays to zero. However, if the particle does not lose its coherence before completing several turns around the ring (this means  $v_F \tau_{\phi} >> L$  in the weak-scattering limit), the inelastic broadening of the discrete levels will be smaller than the level spacing and the persistent current does not vanish. In other words, finite magnetic flux introduces an asymmetry between electrons with clockwise and anticlockwise momentum, respectively (and thus leads to a thermodynamic state with a persistent current), provided that the phase-breaking length  $L_{\phi}$  is not too short compared to L.

(b) We postpone the discussion of order-of-magnitude estimates for the persistent current to a separate paper<sup>20</sup> dealing with the experimentally more relevant multichannel systems. However, one may note that for a onedimensional metal loop whose perimeter is 1  $\mu$ m the maximal zero-temperature persistent current is of the order of a few tenths of  $\mu$ A in the weak-scattering regime.

(c) We have shown that upon averaging over isolated one-dimensional rings with random numbers of particles we may obtain period halving of  $I(\phi)$ . It remains an open question whether a multichannel ring acts effectively as an ensemble of one-dimensional rings, thus self-averages  $I(\phi)$  yielding period halving.

(d) When the electron does not travel in a magneticflux-free space, one may obtain additional effects due to the spin of the electron. The Hamiltonian then contains an additional term  $\tilde{E} = -\sigma_z \mu_B H$ , where  $\mu_B$  is the Bohr magneton and  $\sigma_z$  assumes the values  $\pm 1$ . In order to be able to observe the oscillating nature of the persistent current with  $\phi$ , we should require that the change in  $\tilde{E}$ , when the flux is varied by  $\phi_0$ , be smaller than the energy oscillations in the absence of  $\tilde{E}$ . The latter are of the order of the level spacing (in the weak-scattering limit). This condition is satisfied for a circular ring of circumference  $L \simeq 10^{-4}$  cm. A more detailed discussion is required for the multichannel case.

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## APPENDIX: TEMPERATURE EXPANSION FOR THE PERSISTENT CURRENT

Temperature expansions for the persistent current are derived within the free-electron model and a general band-structure model of metals.

Generalizing Eq. (2.10), we write the persistent current as

$$I = -\frac{e}{L} \sum_{n} \frac{v_n}{e^{\beta(E_n - \mu)} + 1} , \qquad (A1)$$

where  $v_n$  and  $E_n$  are functions of the wave vector  $k_n$ , see, e.g., Eq. (2.2) for the free-electron model. We replace  $\sum_n f(n)$  by  $\int \sum_n f(x)\delta(x-n)dx$ , and substitute

$$\delta(x-n) = \int \exp[iq(x-n)] \frac{dq}{2\pi}$$

We first perform the sum over *n*, which yields  $\sum_{n} \exp(-iqn) = \sum_{l} 2\pi\delta(q-2l\pi)$ , and then the integral over *q*. The result is the Poisson summation formula,

$$\sum_{n=-\infty}^{\infty} f(n) = \sum_{l=-\infty}^{\infty} \int_{-\infty}^{\infty} f(x) e^{i2l\pi x} dx \quad .$$
 (A2)

Next we make the substitution  $k = (2\pi/L)(x + \phi/\phi_0)$  to obtain

$$I = \sum_{l=-\infty}^{\infty} I_1(l) , \qquad (A3)$$

where

n

$$I_{1}(l) = -e^{-i2l\pi\phi/\phi_{0}} \int_{-\infty}^{\infty} \frac{ev(k)e^{ilkL}}{e^{\beta[E(k)-\mu]}+1} \frac{dk}{2\pi} .$$
 (A4)

This formula is now discussed for the free-electron model (2.1) and a general band-structure model.

For free electrons, Eq. (A4) becomes

$$I_{1}(l) = -\frac{ek_{B}T}{\pi\hbar}e^{-i2l\pi\phi/\phi_{0}}\int_{-\infty}^{\infty}\frac{ye^{ily(2T/\tilde{T})^{1/2}}}{e^{\alpha+y^{2}}+1}dy , \quad (A5)$$

with the reduced chemical potential  $\alpha = -\beta\mu$  and the characteristic temperature  $k_B \tilde{T} = \hbar^2 / mL^2$ .

(i) Insulators,  $\alpha \gg l$ . In this case, the Fermi distribution function can be expanded

$$[\exp(\alpha + y^{2}) + 1]^{-1} = \sum_{n=1}^{\infty} (-1)^{n+1} e^{-n(\alpha + y^{2})}, \qquad (A6)$$

where the first term is equivalent to taking the Boltzmann distribution. We now perform the resulting Gaussian integrals in (A5) to obtain

$$I = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} (-1)^n \frac{elk_B T}{n\hbar} \left[ \frac{2T}{n\pi \tilde{T}} \right]^{1/2} \exp\left[ -n\alpha - \frac{l^2 T}{2n\tilde{T}} \right] \times \sin\left[ \frac{2l\pi\phi}{\phi_0} \right].$$
(A7)

Equation (2.15) is the n = 1 term of this expression. The first term (n = 1, l = 1) is the leading term of the double sum when

$$2\sqrt{2} \exp\left[\alpha - \frac{T}{4\tilde{T}}\right] \gg 1 \gg 2 \exp\left[-\frac{3T}{2\tilde{T}}\right].$$
 (A8)

(ii) Semiconductors and metals. In this case, (A5) can be evaluated by contour integration in the complex y plane. For l = 0, the integral vanishes. For l > 0, the path can be closed in the upper y plane. The poles in the upper y plane are located at

$$y = \pm \frac{1}{\sqrt{2}} \{ -\alpha + [\alpha^2 + (2n-1)^2 \pi^2]^{1/2} \}^{1/2} + \frac{i}{\sqrt{2}} \{ \alpha + [\alpha^2 + (2n-1)^2 \pi^2]^{1/2} \}^{1/2} , \qquad (A9)$$

with n = 1, 2, 3, ... For l < 0, one observes  $I_1(-l) = [I_1(l)]^*$ , the resulting expression for the current (A3) is

$$I = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{4ek_B T}{\hbar} \cos\left[l \left[\frac{T}{\tilde{T}}\right]^{1/2} \{-\alpha + [\alpha^2 + (2n-1)^2 \pi^2]^{1/2}\}^{1/2}\right] \times \exp\left[-l \left[\frac{T}{\tilde{T}}\right]^{1/2} \{\alpha + [\alpha^2 + (2n-1)^2 \pi^2]^{1/2}\}^{1/2}\right] \sin\left[\frac{2l\pi\phi}{\phi_0}\right].$$
(A10)

The first term (n = 1, l = 1) is the leading term of the double sum when

$$\exp\left[-\left[\frac{T}{\tilde{T}}\right] [\alpha + (\alpha^2 + 9\pi^2)^{1/2}]^{1/2}\right] < \exp\left[-\left[\frac{T}{\tilde{T}}\right]^{1/2} [\alpha + (\alpha^2 + \pi^2)^{1/2}]^{1/2}\right] < 1.$$
(A11)

From formula (A10) one obtains the persistent current in two limits. (a) Small chemical potential. Setting  $\alpha = 0$  in (A10), we get

$$I = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{4ek_B T}{\hbar} \cos\left[ \left[ \frac{(2n-1)\pi l^2 T}{\tilde{T}} \right]^{1/2} \right] \exp\left[ - \left[ \frac{(2n-1)\pi l^2 T}{\tilde{T}} \right]^{1/2} \right] \sin\left[ \frac{2l\pi\phi}{\phi_0} \right].$$
(A12)

Equation (2.13) is the (n = 1) term of this expression. The (l = 1, n = 1) term is the leading term of the double sum when  $\sqrt{T} \gtrsim (\tilde{T}/\pi)^{1/2}$ .

(b) Metals. For metals,  $\alpha$  is large and negative. Expanding the arguments of the cosine and exponential in (A10) to leading order in  $(-\alpha^{-1})$ , we obtain

$$I = \sum_{l=1}^{\infty} \sum_{n=1}^{\infty} \frac{4ek_B T}{\hbar} \cos(lk_F L) \exp\left[-\frac{l(2n-1)T}{T^*}\right] \times \sin\left[\frac{2l\pi\phi}{\phi_0}\right], \qquad (A13)$$

with the characteristic temperature  $T^*$ ,

$$k_B T^* = \left[\frac{2\mu k_B \tilde{T}}{\pi^2}\right]^{1/2} = \frac{\Delta}{2\pi^2}$$
, (A14)

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- <sup>1</sup>Y. Imry, in *Directions in Condensed Matter Physics*, edited by G. Grinstein and G. Mazenko (World Scientific, Singapore, 1986), p. 101.
- <sup>2</sup>S. Washburn and R. A. Webb, Adv. Phys. **35**, 375 (1986).
- <sup>3</sup>B. L. Al'tschuler, A. G. Aronov, and B. Z. Spivak, Pis'ma Zh. Eksp. Teor. Fiz. **33**, 101 (1981) [JETP Lett. **33**, 94 (1981)].
- <sup>4</sup>D. Yu. Sharvin and Yu. V. Sharvin, Pis'ma Zh. Eksp. Teor. Fiz. 34, 285 (1981) [JETP Lett. 34, 272 (1981)]; B. L. Al'tschuler, A. G. Aronov, B. Z. Spivak, D. Yu. Sharvin, and Yu. V. Sharvin, *ibid.* 35, 476 (1982) [*ibid.* 35, 588 (1982)].
- <sup>5</sup>Y. Gefen, Y. Imry, and M. Azbel, Phys. Rev. Lett. **52**, 129 (1984); Surf. Sci. **142**, 203 (1984).
- <sup>6</sup>R. Webb, S. Washburn, C. Umbach, and R. Laibowitz, Phys. Rev. Lett. **54**, 2696 (1985); V. Chandrasekhar, M. Rooks, S. Wind, and D. Prober, *ibid.* **55**, 1610 (1985); S. Datta, M. Melloch, S. Bandyopadhyay, R. Noren, M. Vaziri, M. Miller, and R. Reifenberger, *ibid.* **55**, 2344 (1985).
- <sup>7</sup>M. Murat, Y. Gefen, and Y. Imry, Phys. Rev. B 34, 659 (1986); also Y. Gefen (unpublished).
- <sup>8</sup>A. D. Stone and Y. Imry, Phys. Rev. Lett. 56, 189 (1986).
- <sup>9</sup>D. A. Browne, J. P. Carini, and S. R. Nagel, Phys. Rev. Lett. 55, 136 (1985).
- <sup>10</sup>R. Landauer and M. Büttiker, Phys. Rev. Lett. 54, 2049 (1985).
- <sup>11</sup>M. Büttiker, in New Techniques and Ideas in Quantum Measurement Theory, edited by D. N. Greenberger [Ann. N.Y. Acad. Sci. 480, 194 (1986)].
- <sup>12</sup>M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. **96A**, 365 (1983).
- <sup>13</sup>M. Büttiker, Phys. Rev. B 32, 1846 (1985).
- <sup>14</sup>N. Byers and C. N. Yang, Phys. Rev. Lett. 7, 46 (1961).
- <sup>15</sup>F. Bloch, Phys. Rev. 137, A787 (1965); 166, 415 (1968).
- <sup>16</sup>M. Schick, Phys. Rev. 166, 401 (1968).
- <sup>17</sup>L. Gunther and Y. Imry, Solid State Commun. 7, 1391 (1969); also Y. Imry and L. Gunther (unpublished). We thank Y.

whose value is determined by the spacing of the energy levels at the Fermi surface  $\Delta = 2\pi \hbar v_F/L$ . Performing the sum over *n* yields Eq. (2.11).

The formulas (A13) and (2.11) for the persistent current in metal rings are valid for a general band for metals. Returning to Eq. (A4), assuming that the two energy branches near the Fermi surface can be approximated by the linearized dispersion law

$$E(k) = \mu \pm \hbar v_F(k \mp k_F) , \qquad (A15)$$

and performing a contour integration, similar to the one leading to Eq. (A10), for the poles at

$$k = \pm k_F + \frac{i(2n-1)\pi k_B T}{\hbar v_F}, \quad n = 1, 2, 3, \dots$$
 (A16)

one obtains again the current (A13) with  $T^*$  defined by  $k_B T^* = \Delta/2\pi^2$  of (A14).

Imry for showing the latter work to us.

- <sup>18</sup>F. Bloch, Phys. Rev. B 2, 109 (1970).
- <sup>19</sup>For a preliminary report of this work, see H. F. Cheung, Y. Gefen, E. K. Riedel, and W.H. Shih, Bull. Am. Phys. Soc. 32, 920 (1987).
- <sup>20</sup>H. F. Cheung, Y. Gefen, and E. K. Riedel (unpublished); IBM J. Res. Dev. (to be published).
- <sup>21</sup>Y. Aharonov and D. Bohm, Phys. Rev. 115, 485 (1959).
- <sup>22</sup>Estimates of  $T^*$  indicate that for experiments on one-channel systems the condition  $T < T^*$  would be less restrictive than the temperature required to ensure  $L \ll L_{\phi}$ .
- <sup>23</sup>P. Erdös and R. C. Hernson, Adv. Phys. **31**, 65 (1982).
- <sup>24</sup>P. D. Kirkman and J. B. Pendry, J. Phys. C 17, 4327 (1984).
- <sup>25</sup>P. W. Anderson and P. A. Lee, Supp. Prog. Theor. Phys. 69, 212 (1980).
- <sup>26</sup>Equation (3.2) was chosen for reasons of convenience. For other choices, see Ref. 23. If the energy range of (3.2) is not sufficient to cover the whole spectrum, one shifts the potential by a constant amount for all j such that one can sweep through another energy range.
- <sup>27</sup>For a review, see M. L. Mehta, *Random Matrices* (Academic, New York, 1967).
- <sup>28</sup>U. Sivan and Y. Imry, Phys. Rev. B 35, 6074 (1987); B. L. Al'tschuler and B. I. Shklolskii, Zh. Eksp. Teor. Fiz. 91, 220 (1986) [Sov. Phys.—JETP 64, 127 (1986)]; and references therein.
- <sup>29</sup>D. J. Thouless, in Critical Phenomena, Random Systems, Gauge Theories, Les Houches, Session XLIII, 1984 edited by K. Osterwalder and R. Stora (Elsevier, Amsterdam, 1986), p. 681.
- <sup>30</sup>P. A. Lee and T. V. Ramakrishnan, Rev. Mod. Phys. **57**, 287 (1985).
- <sup>31</sup>R. Landauer, Philos. Mag. 21, 863 (1970).
- <sup>32</sup>P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B 22, 3519 (1980).
- <sup>33</sup>M. Kappus and F. J. Wegner, Z. Phys. B 45, 15 (1981).
- <sup>34</sup>E. Abrahams and M. J. Stephen, J. Phys. C 13, L377 (1980);
   M. Y. Azbel, *ibid*. 13, L797 (1980); 14, L225 (1981).