Relation between persistent current and band structure of finite-width mesoscopic rings

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The energy bands of a finite-width mesoscopic multichannel ring are calculated using the transfer-matrix method. Two approaches are developed, the diagonal approximation and the multichannel model. We apply these results to the calculation of the persistent current in mesoscopic rings enclosing the magnetic flux Φ in the ballistic regime. It is shown that the interchannel coupling in a finite-width mesoscopic ring produces a halving of the fundamental period h/e of the persistent current $I_A^{(\tilde{n})}(\Phi)$.

I. INTRODUCTION

During the past decade the intense research on mesoscopic systems has led to the discovery of interesting physical phenomena. Among them there are Aharonov-Bohm (AB) oscillations of the conductivity as well as various mesoscopic fluctuation effects. There is increasing interest in the question of persistent currents induced in a mesoscopic ring by an AB flux. The intriguing question of the persistent current was discussed first in connection with the flux quantization in superconducting rings.[1,2] The work of Büttiker *et al.*[3] on persistent currents in strictly one-dimensional normal-metal rings initiated a renewal of interest in the persistent-current topic.[4–13] The origin of the persistent current is the relation between the static magnetic flux Φ threading the ring and the boundary conditions for the single-particle wave function. The potential acting on an electron moving along the strictly one-dimensional ring has a period equal to the circumference L. The energy spectrum of such a ring has the band sructure characteristics of a one-dimensional periodic lattice $E_n(k)$, where different values of the applied flux correspond to different values of $k = -k_0\Phi/\Phi_0$ ($k_0 = 2\pi/L$, the flux quantum $\Phi_0 = h/e$). Hence, the electron eigenenergies $E_n(\Phi)$ of a strictly one-dimensional ring are periodic functions of Φ with period Φ_0: $E_n(\Phi) = E_n(\Phi+\Phi_0)$. An electron in the state $E_n(\Phi)$ carries a current $I_n = -dE_n(\Phi)/d\Phi$. The total current in the system, given by the sum over all occupied states up to the Fermi energy weighted by the appropriate occupation probability, is finite.

As is known,[14] there are two possible methods of experimental investigation of the persistent currents in mesoscopic rings: the study (i) of a single ring or (ii) of a large number of independent rings. Such persistent currents have been detected by Lévy *et al.*[15] by using 10^7 mesoscopic copper rings in an experiment of the latter type. They observed an oscillatory response; however, the fundamental period was not h/e, but half of a flux quantum $h/(2e)$. This result is believed to be due to the large number of loops in the sample according to the ensemble averaging.[14,16–20] It is shown that, for a finite persistent current in the disconnected mesoscopic rings studied in Ref. 15, the number of electrons is conserved (canonical ensemble) while the chemical potential exhibits mesoscopic fluctuations.[21] Further, the periodicity of the persistent current is $\Phi_0/2$ instead of Φ_0. But averaging on the disorder at fixed chemical potential (grand canonical ensemble) yields a vanishingly small persistent current periodic in Φ_0. The inclusion of the electron-electron interaction gives also a finite ensemble average of the persistent current with periodicity $\Phi_0/2$. Up to now it is still controversial whether the experiment can be quantitatively explained within a model of noninteracting electrons in a random potential (disorder), or whether the electron-electron interaction is important.

Recently, Chandrasekhar *et al.*[22] have reported the observation of the persistent current in a single gold loop and Mailly *et al.*[23] in a single GaAs-$Ga_{1-x}Al_xAs$ loop. As distinct from the above-mentioned papers, our study is stimulated by an experiment in one mesoscopic semiconductor ring in the ballistic regime, which has recently been accomplished.[23] Because of a small number of impurities in the ring, there is no necessity for any ensemble averaging. Nevertheless, it will be shown that the halving of the fundamental period of the persistent current in a single ring of a finite width may occur due to the interchannel coupling.

II. THE MODEL

We consider a finite-width mesoscopic ring in the x-y plane of inner radius R_1 and outer radius R_2 threaded axially by an AB flux of radius $R_{AB} < R_1$ through the hole of the ring. It is assumed that the electrons are confined in a zero-thickness x-y plane along the z direction. The single-particle Hamiltonian of the electron in the x-y

plane outside the AB flux reads

$$H = \frac{1}{2m_e}\left\{-\hbar^2\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}\right)+\left[\frac{i\hbar}{r}\frac{\partial}{\partial\varphi}+eA_\varphi(r)\right]^2\right\} + V_C(r,\varphi)+V_S(r,\varphi), \quad (1)$$

where m_e is the effective conduction-band-edge mass and $A_\varphi(r) = BR_{\rm AB}^2/(2r)$ is the φ component of the vector potential outside the AB flux $\Phi = B\pi R_{\rm AB}^2$. The confining potential $V_C(r,\varphi)$ in the x-y plane is taken as zero in the region $R_1 < r < R_2$ and infinite otherwise, and the impurity potential $V_S(r,\varphi)$ is responsible for elastic scattering. Because the Hamiltonian does not depend on the spin operator, we can restrict the wave function to being a scalar function describing the orbital motion. In the AB case it is suitable to work in a gauge for the vector potential in which the magnetic field does not appear in the Hamiltonian, but enters the wave function via the flux-modified periodicity condition $\Psi(r,\varphi+2\pi) = \exp(i2\pi\Phi/\Phi_0)\Psi(r,\varphi)$. Hence, the eigenstates and energies of the finite-width ring are periodic in Φ with period Φ_0. The wave function is represented by the expansion $\Psi(r,\varphi) = \sum_K Q_K(\varphi)\chi_K(r)$, where $\{\chi_K(r)\}$ is the set of radial wave functions that are the eigenfunctions of Bessel's differential equation. The radial boundary conditions of vanishing $\chi_K(r)$ at the radii R_1 and R_2 result in the relation

$$J_\nu(\kappa R_1)N_\nu(\kappa R_2) - J_\nu(\kappa R_2)N_\nu(\kappa R_1) = 0, \quad (2)$$

where $J_\nu(x)$ is the Bessel function of the first kind and $N_\nu(x)$ is the Neumann function. On the one hand, this equation determines for each given ν ($\nu^2 \geq 0$) the discrete infinite set of roots $\{\kappa_K(\nu)\}_{K=1}^{\infty}$, where $K = 1,2,\ldots$. On the other hand, for each given $\kappa \geq \kappa_K(0)$ Eq. (2) determines a set of $K_{\rm open}$ real values $\{\nu_K(\kappa)\}_{K=1}^{K_{\rm open}}$, which describe open channels, and an infinite set of complex values $\{\nu_K(\kappa)\}_{K=K_{\rm open}+1}^{\infty}$, corresponding to the virtual channels. In the following, K is the radial quantum number denoting both open and virtual channels. The virtual channels assure a continuous reconstruction of the energy bands [and hence the continuity of the persistent current of Eq. (7) below] immediately under the thresholds of the open channels: $\kappa < \kappa_K(0)$, $\kappa_K(0)-\kappa \ll \kappa_K(0)-\kappa_{K-1}(0)$. The analytical result $\kappa_K(0) \approx K\pi/(R_2-R_1)$ follows from Eq. (2) under the condition $\kappa R_1, \kappa R_2 \gg 1$ for $\nu = 0$. From this relation the number of open channels at a given energy E is $K_{\rm open}(E) \leq (R_2-R_1)\sqrt{2m_eE}/(\pi\hbar)$. For a narrow-width ring, where the condition $(R_2-R_1) \ll (R_2+R_1)/2$ is fulfilled, the analytic dependence $\nu_K(\kappa) \approx \sqrt{\kappa^2-\kappa_K^2(0)}(R_2+R_1)/2$ is valid. With the use of the orthonormalization of the radial wave functions (see the Appendix) $\int_{R_1}^{R_2}(dr/r)\chi_K(r)\chi_{K'}(r) = \delta_{KK'}$, the azimuthal wave function is the eigenfunction of

$$\left[\frac{d^2}{d\varphi^2}+\nu_K^2(\kappa)\right]Q_K(\varphi) = \frac{2m_e}{\hbar^2}\sum_{K'=1}^{\infty}Q_{K'}(\varphi)\int_{R_1}^{R_2}dr\,r\chi_K(r)V_S(r,\varphi)\chi_{K'}(r). \quad (3)$$

This set of equations ($K = 1,2,\ldots$) determines the eigenfunctions $Q_{K\tilde{n}}(\varphi) \equiv Q_{K\tilde{n}}(\kappa_{\tilde{n}}(\Phi),\varphi)$ corresponding to the eigenvalues $\kappa_{\tilde{n}}(\Phi)$, $\tilde{n} = 1,2,\ldots$, from which we obtain the energy bands $E_{\tilde{n}}(\Phi)$.

III. PERSISTENT CURRENT

The current density is defined as a variational derivative

$$\mathbf{j}(\mathbf{x}) \equiv -\frac{\delta\langle H\rangle}{\delta\mathbf{A}(\mathbf{x})}, \quad (4)$$

where $\langle H\rangle \equiv \langle\Psi|H|\Psi\rangle$ denotes the mean value of H. If the mesoscopic ring is threaded by the AB flux Φ, the corresponding vector potential has only a φ component which is azimuthally symmetric: $\mathbf{A}(\mathbf{x}) = A_\varphi(r)\mathbf{e}_\varphi$, $A_\varphi(r) = \Phi/(2\pi r)$. In this case we obtain from Eq. (4)

$$j_\varphi(\mathbf{x}) = -2\pi r\Psi^*(\mathbf{x})\frac{\partial H(\mathbf{x},\Phi)}{\partial\Phi}\Psi(\mathbf{x}). \quad (5)$$

Starting with the current density given in Eq. (5), the azimuthal current may be defined as

$$I_A \equiv \frac{1}{2\pi}\int_0^{2\pi}d\varphi\int_{R_1}^{R_2}dr\,j_\varphi(\mathbf{x}). \quad (6)$$

Let us consider now as $\Psi(\mathbf{x})$ an eigenstate of H, $H\Psi_{\tilde{n}}(\mathbf{x}) = E_{\tilde{n}}\Psi_{\tilde{n}}(\mathbf{x})$, where H is, for instance, in the present problem given by Eq. (1). Using Eq. (5) in Eq. (6), we find the azimuthal current in the final form,

$$I_A^{(\tilde{n})}(\Phi) = -\frac{\partial E_{\tilde{n}}(\Phi)}{\partial\Phi}. \quad (7)$$

It is important to note that this equation relates the energy bands $E_{\tilde{n}}(\Phi)$ of a general ring (finite width and height) to the azimuthal current (single-band current), defined in Eq. (6). Hence, Eq. (7) generalizes the well-known relation between the one-dimensional persistent current I_n and the bands $E_n(\Phi)$ of a strictly one-dimensional ring[3] to any mesoscopic ring of finite width and height.

For the numerical calculation we specify our model by using the impurity potential $V_S(r,\varphi) = \sum_{s=1}^{N_S}V_s/r_s\delta(r-r_s)\delta(\varphi-\varphi_s)$ and bring Eq. (3) to the form

$$\left[\frac{d^2}{d^2\varphi}+\nu_K^2(\kappa)\right]Q_K(\varphi) = \sum_{K'=1}^{\infty}\sum_{s=1}^{N_S}\Gamma_{KK'}^{(s)}(r_s)\delta(\varphi-\varphi_s)Q_{K'}(\varphi), \quad (8)$$

with $\Gamma_{KK'}^{(s)}(r_s) = (2m_eV_s/\hbar^2)\chi_K(r_s)\chi_{K'}(r_s)$. The azimuthal wave function fulfills the boundary conditions $Q_K(\varphi_s+0) = Q_K(\varphi_s-0)$ and $dQ_K(\varphi)/d\varphi|_{\varphi=\varphi_s+0} - dQ_K(\varphi)/d\varphi|_{\varphi=\varphi_s-0} = \sum_{K'}\Gamma_{KK'}^{(s)}(r_s)Q_{K'}(\varphi_s)$.

Let us start with the impurity-free narrow-width ring. In this case, if $(R_2 - R_1) \ll (R_2 + R_1)/2$ is valid in the absence of impurities, the radial and azimuthal motions are independent and the simple analytical result follows

$$E_{K,m}(\Phi) = \frac{\hbar^2}{2m_e}\left\{\frac{\pi^2 K^2}{(R_2 - R_1)^2} + \frac{[m + (\Phi/\Phi_0)]^2}{(R_1 + R_2)^2/4}\right\}. \quad (9)$$

Here the general band index $\tilde{n}$ turns into a pair (K, m), where $K = 1, 2, \ldots$ indicates the level of the size-quantized radial motion, while $m = 0, \pm 1, \pm 2, \ldots$ numbers the bands corresponding to the azimuthal motion. This is the generalization of the well-known result $E_m(\Phi) = (\hbar^2/2m_e)\{[m + (\Phi/\Phi_0)]/R\}^2$ for the impurity-free strictly one-dimensional ring.[7] The persistent current corresponding to the above-described energy,

$$I_A^{(K,m)}(\Phi) \approx -\frac{\hbar^2}{m_e \Phi_0}\frac{m + (\Phi/\Phi_0)}{(R_1 + R_2)^2/4}, \quad (10)$$

is linear in Φ and independent of the size-quantization index K: the radial motion, as long as it is independent of the azimuthal motion, does not contribute to the formation of the persistent currents.

There are in principle two different possibilities for solving Eq. (8) in the presence of impurities, briefly developed below.

IV. DIAGONAL APPROXIMATION

Accounting for the mutual influence of the radial and azimuthal motions in the presence of impurities in the finite-width ring, one may use the diagonal approximation $\Gamma^{(s)}_{KK'} \propto \delta_{KK'}$, i.e., neglect the coupling between different channels. This can be done at least for the weak-scattering case and will be validated below from the point of view of more exact approaches.

According to Eq. (8), there are N_S impurities in the ring. Then the azimuthal wave function has in the region $\varphi_{s-1} < \varphi < \varphi_s$ the form $Q_K(\varphi) = A_K^{(s)} \exp(i\nu_K \varphi) + B_K^{(s)} \exp(-i\nu_K \varphi)$. Using the boundary conditions for $Q_K(\varphi)$, we obtain on the basis of the transfer-matrix method

$$\begin{pmatrix} A_K^{(N_S+1)} \\ B_K^{(N_S+1)} \end{pmatrix} = \mathrm{T}_K(\varphi_1, \ldots, \varphi_{N_S}) \begin{pmatrix} A_K^{(1)} \\ B_K^{(1)} \end{pmatrix}, \quad (11)$$

with $\mathrm{T}_K(\varphi_1, \ldots, \varphi_{N_S}) = \mathrm{T}_K^{(N_S)}(\varphi_{N_S}) \cdots \mathrm{T}_K^{(2)}(\varphi_2)\mathrm{T}_K^{(1)}(\varphi_1)$. Here the 2×2 transfer matrix is given by

$$\mathrm{T}_K^{(s)}(\varphi_s) = \begin{pmatrix} 1 - i\Gamma^{(s)}_{KK}(r_s)/(2\nu_K) & -i\Gamma^{(s)}_{KK}(r_s)/(2\nu_K)\exp(-2i\nu_K\varphi_s) \\ i\Gamma^{(s)}_{KK}(r_s)/(2\nu_K)\exp(2i\nu_K\varphi_s) & 1 + i\Gamma^{(s)}_{KK}(r_s)/(2\nu_K) \end{pmatrix}. \quad (12)$$

On the other hand, the boundary condition at $\varphi = 0$ gives

$$\begin{pmatrix} A_K^{(N_S+1)} \\ B_K^{(N_S+1)} \end{pmatrix} = \mathrm{e}^{i2\pi(\Phi/\Phi_0)}\mathrm{T}_K(2\pi) \begin{pmatrix} A_K^{(1)} \\ B_K^{(1)} \end{pmatrix}, \quad (13)$$

with

$$\mathrm{T}_K(2\pi) \equiv \begin{pmatrix} \exp(-i2\pi\nu_K) & 0 \\ 0 & \exp(i2\pi\nu_K) \end{pmatrix}. \quad (14)$$

The two equations (11) and (13) result in the dispersion relation

$$\det\left[\mathrm{e}^{i2\pi(\Phi/\Phi_0)}\mathrm{T}_K(2\pi) - \mathrm{T}_K(\varphi_1, \ldots, \varphi_{N_S})\right] = 0. \quad (15)$$

This equation, where in the transfer matrices $\nu_K = \nu_K(\kappa)$ is a solution of Eq. (2), determines the energy bands $E_{K,n_K}(\Phi), n_K = 1, 2, \ldots$ for each channel $K = 1, 2, \ldots$. So the general band index $\tilde{n}$ turns in this approximation into the pair (K, n_K), where K is the number of the channel and n_K numbers the bands originating from this channel.

Assuming two impurities $(s = 1, 2)$ in the finite-width mesoscopic ring, we obtain the dispersion relations in the form

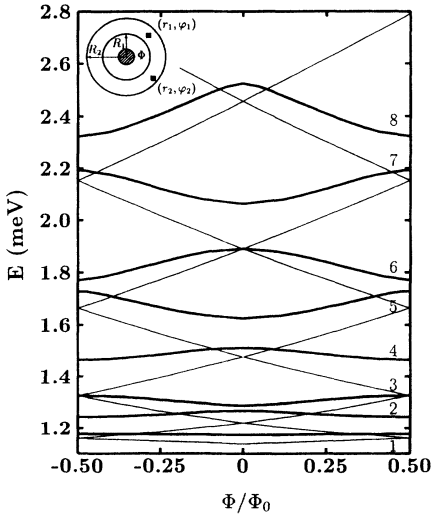

FIG. 1. Energy spectrum $E_{1,n_1}(\Phi)$ of a finite-width mesoscopic ring (R_1=50 nm, R_2=120 nm) without impurities (thin solid lines) and with two impurities (heavy solid lines): $V_1 = V_2 = 10^{-18}$ eV m^2, $r_1 = r_2 = 85$ nm, $\varphi_2 - \varphi_1 = 4\pi/3$, originating from the channel $K = 1$ in the diagonal approximation calculated from Eq. (16).

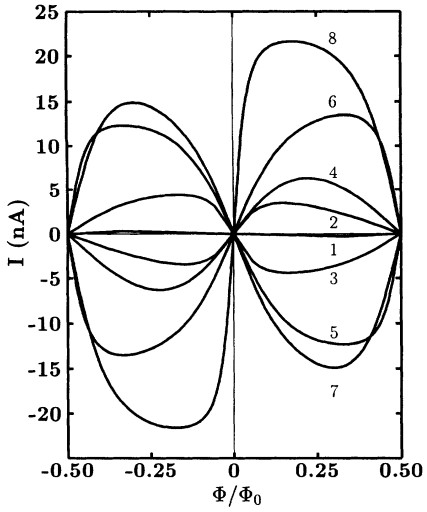

FIG. 2. Persistent currents $I_A^{(1,n_1)}$ carried by the energy bands $E_{1,n_1}(\Phi)$ of Fig. 1 over one period of the magnetic flux, calculated from Eq. (7). Parameters are the same as in Fig. 1.

$$\cos(2\pi\nu_K)+\frac{\Gamma_{KK}^{(1)}+\Gamma_{KK}^{(2)}}{2\nu_K}\sin(2\pi\nu_K) -\frac{\Gamma_{KK}^{(1)}\Gamma_{KK}^{(2)}}{4\nu_K^2}\{\cos(2\pi\nu_K) -\cos[2\nu_K(\varphi_2-\varphi_1-\pi)]\}-\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)=0, \quad (16)$$

independent of each other for all $K=1,2,\ldots$, where $\nu_K=\nu_K(\kappa)$ is a solution of Eq. (2).

We have chosen for numerical work material parameters typical for mesoscopic semiconductor rings (GaAs, $m_e=0.06624m_0$). Figure 1 shows the energy spectrum of a finite-width ring with two impurities originating from the channel $K=1$. For the sake of comparison, the energies are also exhibited for the finite-width ring without impurities. It is seen that the presence of the impurities opens gaps at the points $\Phi/\Phi_0=0$ and ±0.5 of the intersection of the corresponding energy bands of the impurity-free ring. We note that in the considered case the energy bands resulting from the higher channels $K=2,3,\ldots$ lie high above the energies plotted here, e.g., $\min\{E_{2,1}(\Phi)\}=4.611$ meV. The persistent currents $I_A^{(1,n_1)}$ carried by the levels $E_{1,n_1}(\Phi)$ of Fig. 1 are plotted in Fig. 2. Due to the scattering of the electrons, the persistent currents $I_A^{(K,n_K)}$ as a function of the magnetic flux vanish at the points $\Phi/\Phi_0=0$ and ±0.5.

V. MULTICHANNEL MODEL

The diagonal approximation is good only if the separation between the energy bands of the same channel is much smaller than that between the bands belonging to different channels. In the opposite case *interchannel coupling* (ICC) occurs between the different channels. In this case a possibility to solve Eq. (8) is to restrict oneself to a finite number M of channels $K\le M$, i.e., to use (respectively for $M=2,3,\ldots$) the two-, three-, ..., channel model. Using the boundary condition for $Q_K(\varphi)$, we obtain for the M-channel model on the basis of the transfer-matrix method

$$\begin{pmatrix} A_1^{(N_S+1)}\\ B_1^{(N_S+1)}\\ \cdots\\ A_M^{(N_S+1)}\\ B_M^{(N_S+1)}\end{pmatrix}=\mathcal{T}_M(\varphi_1,\ldots,\varphi_{N_S})\begin{pmatrix} A_1^{(1)}\\ B_1^{(1)}\\ \cdots\\ A_M^{(1)}\\ B_M^{(1)}\end{pmatrix}, \quad (17)$$

with $\mathcal{T}_M(\varphi_1,\ldots,\varphi_{N_S})=\mathcal{T}_M^{(N_S)}(\varphi_{N_S})\cdots\mathcal{T}_M^{(2)}(\varphi_2)\mathcal{T}_M^{(1)}(\varphi_1)$, where $\mathcal{T}_M^{(s)}(\varphi_s)$ is the $2M\times2M$ transfer matrix. The boundary condition at $\varphi=0$ gives

$$\begin{pmatrix} A_1^{(N_S+1)}\\ B_1^{(N_S+1)}\\ \cdots\\ A_M^{(N_S+1)}\\ B_M^{(N_S+1)}\end{pmatrix}=e^{i2\pi(\Phi/\Phi_0)}\mathcal{T}_M(2\pi)\begin{pmatrix} A_1^{(1)}\\ B_1^{(1)}\\ \cdots\\ A_M^{(1)}\\ B_M^{(1)}\end{pmatrix}, \quad (18)$$

with

$$\mathcal{T}_M(2\pi)\equiv\begin{pmatrix} \mathrm{T}_1(2\pi) & & & 0\\ & \mathrm{T}_2(2\pi) & & \\ & & \ddots & \\ 0 & & & \mathrm{T}_M(2\pi)\end{pmatrix}.$$

The two equations (17) and (18) result in the dispersion relation

$$\det\left[e^{i2\pi(\Phi/\Phi_0)}\mathcal{T}_M(2\pi)-\mathcal{T}_M(\varphi_1,\ldots,\varphi_{N_S})\right]=0, \quad (19)$$

which implicitly binds the energy [via the functions $\nu_K(\kappa)$ entering the matrices in Eqs. (17) and (18)] with the magnetic flux Φ. Note that in the energy interval where $K_{\mathrm{open}}(E)\ge M$ this scheme operates only with the open channels, while for $K_{\mathrm{open}}(E)<M$ it takes into consideration also $M-K_{\mathrm{open}}(E)$ virtual channels.

Assuming, for example, the two-channel model and two impurities ($s=1,2$) in the finite-width mesoscopic ring, we obtain the dispersion relation in the form

$$\cos\left(2\pi\frac{\Phi}{\Phi_0}\right)=\tfrac{1}{2}\left(\mathcal{A}_1+\mathcal{A}_2\pm\sqrt{(\mathcal{A}_1-\mathcal{A}_2)^2+\mathcal{B}}\right), \quad (20)$$

with

$$\mathcal{A}_K=\cos(2\pi\nu_K)+\frac{\Gamma_{KK}^{(1)}+\Gamma_{KK}^{(2)}}{2\nu_K}\sin(2\pi\nu_K) +\frac{D_{KK}}{2\nu_K}\sin[(2\pi-\varphi_2+\varphi_1)\nu_K], \quad (21)$$

$$D_{KK'}=\sum_{K''=1}^{2}\frac{1}{\nu_{K''}}\Gamma_{KK''}^{(2)}\Gamma_{K''K'}^{(1)}\sin[\nu_{K''}(\varphi_2-\varphi_1)], \quad (22)$$

and

$$\mathcal{B} = \frac{1}{\nu_1\nu_2}\Big([\Gamma_{12}^{(1)2} + \Gamma_{12}^{(2)2}]\sin(2\pi\nu_1)\sin(2\pi\nu_2)$$
$$+2\Gamma_{12}^{(1)}\Gamma_{12}^{(2)}\Big\{\cos[(\nu_1-\nu_2)(\varphi_2-\varphi_1)]\sin^2[\pi(\nu_1+\nu_2)] - \cos[(\nu_1+\nu_2)(\varphi_2-\varphi_1)]\sin^2[\pi(\nu_1-\nu_2)]\Big\}$$
$$+D_{21}\Big\{\Gamma_{12}^{(1)}\sin(2\pi\nu_1)\sin[(2\pi-\varphi_2+\varphi_1)\nu_2] + \Gamma_{12}^{(2)}\sin(2\pi\nu_2)\sin[(2\pi-\varphi_2+\varphi_1)\nu_1]\Big\}$$
$$+D_{12}\Big\{\Gamma_{12}^{(1)}\sin(2\pi\nu_2)\sin[(2\pi-\varphi_2+\varphi_1)\nu_1] + \Gamma_{12}^{(2)}\sin(2\pi\nu_1)\sin[(2\pi-\varphi_2+\varphi_1)\nu_2]\Big\}$$
$$+D_{12}D_{21}\sin[(2\pi-\varphi_2+\varphi_1)\nu_1]\sin[(2\pi-\varphi_2+\varphi_1)\nu_2]\Big). \tag{23}$$

This equation describes two branches corresponding to the $\pm$ signs in Eq. (20) if the condition $(\mathcal{A}_1-\mathcal{A}_2)^2 + \mathcal{B} \geq 0$ is satisfied. In its turn, for a given value of the flux Φ, each of these branches defines allowed ($|\cos(2\pi\Phi/\Phi_0)| \leq 1$) electron states $E_{\tilde{n}}(\Phi)$ if $|(\mathcal{A}_1 + \mathcal{A}_2 \pm \sqrt{(\mathcal{A}_1-\mathcal{A}_2)^2+\mathcal{B}})/2| \leq 1$; otherwise one obtains forbidden electron states. Being considered as a function of the flux Φ, these forbidden states form gaps in the energy spectrum.

The energy bands $E_{\tilde{n}}(\Phi)$ obtained within the framework of the two-channel model for two different values of the impurity potential are displayed in Fig. 3. The ICC due to the presence of the impurities leads to a hybride-type spectrum of the energy bands which have extrema not only at $\Phi/\Phi_0 = 0, \pm 0.5$, but at some values $0 < |\Phi/\Phi_0| < 0.5$ with gaps between neighbor extrema. With increasing energy band number $\tilde{n}$, these gaps grow, while the functions $E_{\tilde{n}}(\Phi)$ become smoother.

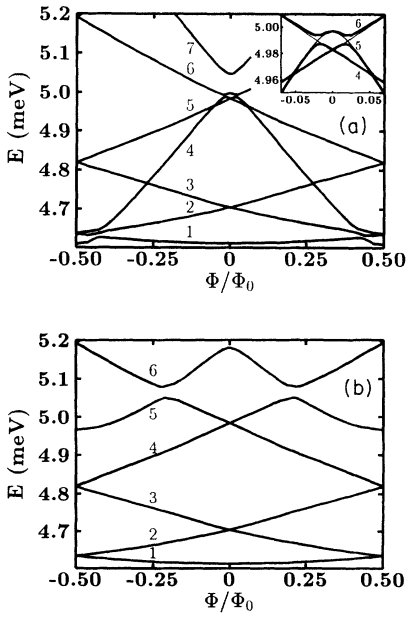

FIG. 3. The energy spectrum $E_{\tilde{n}}(\Phi)$ of a finite-width mesoscopic ring (R_1=50 nm, R_2=120 nm) with two impurities: $r_1 = r_2 = 85$ nm, $\varphi_2 - \varphi_1 = 4\pi/3$, $V_1 = V_2 = 10^{-18}$ eV m^2 (a), $V_1 = V_2 = 4\times10^{-18}$ eV m^2 (b), obtained by using the two-channel model from Eq. (20). Thin lines correspond to the diagonal approximation.

We emphasize that there are no crossings between the bands $\tilde{n}=2$ and $\tilde{n}=3$, $\tilde{n}=3$ and $\tilde{n}=4$, $\tilde{n}=4$ and $\tilde{n}=5$ in Figs. 3(a) and 3(b). There are narrow gaps between the energy bands which are the manifestation of the repulsion of levels of quantum chaotic systems.[24] It should be possible to conclude that the level statistics have to be different in the center and at the boundary of the Brillouin zone ($\Phi/\Phi_0 = 0; \frac{1}{2}$) and inside the Brillouin zone ($0 < \Phi/\Phi_0 < \frac{1}{2}$). The reason is that a nonvanishing magnetic flux breaks the time-reversal symmetry. Systems with no time-reversal symmetry are described by the Gaussian unitary ensemble, while systems with this symmetry are described by the Gaussian orthogonal ensemble. Because of the periodicity of the electronic spectrum of the ring, time-reversal symmetry is present at $\Phi/\Phi_0 = 0$ and $\frac{1}{2}$. For a metallic ring with the diffusive regime of the electron motion, such properties have been demonstrated recently.[25,26] This rearrangement of the band structure, specific for the finite-width rings, produces substantial changes in the persistent currents as a

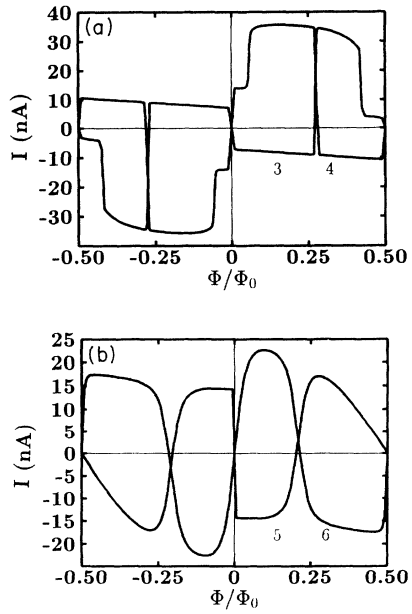

FIG. 4. Persistent currents $I_A^{(\tilde{n})}$ carried by the energy bands $E_{\tilde{n}}(\Phi)$ of Fig. 3 over one period of the magnetic flux, calculated from Eq. (7). Parameters are the same as in Fig. 3.

function of the magnetic flux shown in Fig. 4. Due to the ICC in the finite-width rings, the Fourier expansion of the persistent currents acquires a rich structure of harmonics, where the second harmonic ($\Phi_0/2$) is the most pronounced. Thus, the halving of the fundamental period Φ_0 in the spectrum of persistent currents in finite-width mesoscopic rings may be attributed to the coupling of the radial and azimuthal electron motions caused by the impurity scattering within a purely quantum-mechanical approach. The recent observation of the second harmonic along with the fundamental frequency in the spectrum of the persistent current in a single mesoscopic ring in the ballistic regime[23] confirms the results given in this paper.

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APPENDIX: ORTHONORMALITY OF THE RADIAL WAVE FUNCTIONS

A general solution of Bessel's differential equation

$$\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}+\kappa^2-\frac{\nu^2}{r^2}\right)\chi(r)=0, \tag{A1}$$

is $\chi(r)=aJ_\nu(\kappa r)+bN_\nu(\kappa r)\equiv\chi_{\nu,\kappa}(r)$. Imposing the boundary conditions relevant to a closed-ring problem, we arrive at a set of algebraic equations for a and b. This set has nontrivial solutions under the condition Eq. (2) which relates ν and κ to each other at the given values of R_1 and R_2. Taking Eq. (A1) for two different fixed pairs (ν_1,κ_1) and (ν_2,κ_2), we obtain straightforwardly the relation

$$(\nu_2^2-\nu_1^2)\int_{R_1}^{R_2}\frac{dr}{r}\chi_{\nu_2,\kappa_2}(r)\chi_{\nu_1,\kappa_1}(r)$$

$$=(\kappa_2^2-\kappa_1^2)\int_{R_1}^{R_2}dr\,r\chi_{\nu_2,\kappa_2}(r)\chi_{\nu_1,\kappa_1}(r). \tag{A2}$$

Let the parameter κ be fixed: $\kappa_1=\kappa_2=\kappa$. Then the boundary problem [see Eq. (2)] gives a finite set of roots $\nu_K(\kappa), K=1,2,\ldots,K_{\rm open}(E)$. Choosing two of them as $\nu_1=\nu_K(\kappa)$ and $\nu_2=\nu_{K'}(\kappa)$, one obtains from Eq. (A2)

$$[\nu_{K'}(\kappa)^2-\nu_K(\kappa)^2]\int_{R_1}^{R_2}\frac{dr}{r}\chi_{\nu_{K'}(\kappa),\kappa}(r)$$

$$\times\chi_{\nu_K(\kappa),\kappa}(r)=0. \tag{A3}$$

For nondegenerate bands when $\nu_K(\kappa)\neq\nu_{K'}(\kappa)$ it means the orthogonality of the functions $\chi_{\nu_K(\kappa),\kappa}(r)$ and $\chi_{\nu_{K'}(\kappa),\kappa}(r)$ with the weight $1/r$:

$$\int_{R_1}^{R_2}\frac{dr}{r}\chi_{\nu_{K'}(\kappa),\kappa}(r)\chi_{\nu_K(\kappa),\kappa}(r)=0. \tag{A4}$$

Now the function $\chi_{\nu_K(\kappa),\kappa}(r)$ may be normalized with the same weight:

$$\int_{R_1}^{R_2}\frac{dr}{r}\chi^2_{\nu_K(\kappa),\kappa}(r)=1. \tag{A5}$$

Thus, the orthonormality of the set of functions $\{\chi_{\nu_K(\kappa),\kappa}(r)\}$ exists on the ring $R_1<r<R_2$ with the weight $1/r$.

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