Magnetic-flux-induced persistent currents in symmetric-polymer mesoscopic rings

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(Presented on 1 November 2005; published online 27 April 2006)

We investigate magnetic-flux-induced persistent currents in one-dimensional symmetric-polymer (SP) mesoscopic ring, where a defect cluster is embedded into two periodic clusters and the whole cluster possesses mirror symmetry. Under tight-binding approximation, the flux-dependent energy spectra, electronic wave functions, and persistent currents are obtained. It is shown that the energy spectra form band structure and the defect modes appear in the band gap. The persistent current (PC) depends on the magnetic flux, the site energy, and the Fermi level. Particularly, by changing the Fermi level, the SP ring presents metallic and insulative features alternately. Our investigations provide a possible model to explain the anomalously large PC observed in some experiments and contribute to the potential application in quantum-switch devices. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2172562]

In mesoscopic systems, one of the quantum effects is the persistent current (PC) in mesoscopic rings threaded by a magnetic flux. This phenomenon was predicted by Büttiker *et al.*[1] in 1983, and there has been a lot of theoretical and experimental work[2–6] performed. However, the problem is still not well understood. For example, the experimental observation of Chandrasekhar *et al.*[3] indicated that the current in single Au ring is one or two orders of magnitude larger than the value predicted by the noninteracting theory. Recently more experimental work brought challenges to the theoretical work, such as the sign of the PC near zero field,[7] the correlation of the PC with the phase coherence time, etc.[8]

Generally speaking, the disorder in the system and the electron-electron interaction are two important factors influencing the PC. In this work, we investigate magnetic-flux-induced persistent currents in a one-dimensional (1D) mesoscopic ring, which is constructed according to the symmetric-polymer (SP) model. In a SP model, the defect cluster is embedded into two periodic clusters and the whole cluster possesses mirror symmetry. It is shown that the energy spectra form band structure and the defect modes appear in the band gap. The number of defect modes depends on the number of atoms in the defect cluster. The PC is determined by the magnetic flux, the site energy, and the Fermi level. Particularly, by changing the Fermi level, the SP ring presents metallic and insulative properties alternately. Our investigations provide a possible model to explain the anomalously large PC observed in some experiments and may contribute to the potential application in quantum-switch devices.

We consider the electronic behavior in the 1D SP ring threaded by a magnetic flux. The SP ring contains N sites. Atom A or B occupies the sites according to the sequence $R(m,n)=(BA)^m B^n (AB)^m$, where m and n are the repeating numbers of the units. Obviously, the defect cluster B^n is embedded into two periodic clusters and the whole cluster possesses mirror symmetry in the SP ring. Under the tight-binding approximation, without the electron-electron interaction, the Schrödinger equation for a spinless electron in a 1D SP mesoscopic ring can be written as

$$(E-\varepsilon_l)\psi_l = t_{l,l+1}\psi_{l+1} + t_{l,l-1}\psi_{l-1}, \tag{1}$$

where ψ_l is the amplitude of wave function on the lth site index, $t_{l,l\pm1}$ is the nearest hopping integral, and the site energy ε_l is taken as $\varepsilon_l=\varepsilon_A$ (or ε_B) if atom A (or B) occupies the site. Without loss of generality, we choose the on-site model, for example, $\varepsilon_A=-\varepsilon_B=\varepsilon$, and $t_{l,l\pm1}$ is set as a constant as $t_{l,l\pm1}=-1$. Equation (1) can also be expressed in the matrix form,

$$\begin{pmatrix} \psi_{l+1} \\ \psi_l \end{pmatrix} = T_{l+1,l}\begin{pmatrix} \psi_l \\ \psi_{l-1} \end{pmatrix}, \tag{2}$$

where the transfer matrix is

$$T_{l+1,l} = \begin{pmatrix} -(E-\varepsilon_l) & -1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

Because a magnetic flux Φ threaded through the ring will lead to the twisted boundary conditions for the wave functions of the electrons, the equation for the global transfer matrix has the form as

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = \bar{T}\begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = e^{i2\pi\Phi/\Phi_0}\begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{4}$$

where $\bar{T}=\Pi_{l=1}^{N} T_{l+1,l}$ and $\Phi_0=hc/e$ is the flux quantum. By denoting the trace of matrix $\bar{T}$ as $\chi=\frac{1}{2}\mathrm{tr}\,\bar{T}$, the flux-dependent energy spectra of an electron in the mesoscopic ring can be obtained from

$$\chi = \cos(2\pi\Phi/\Phi_0), \tag{5}$$

and the persistent current in the ring contributed by the nth energy level is as follows:

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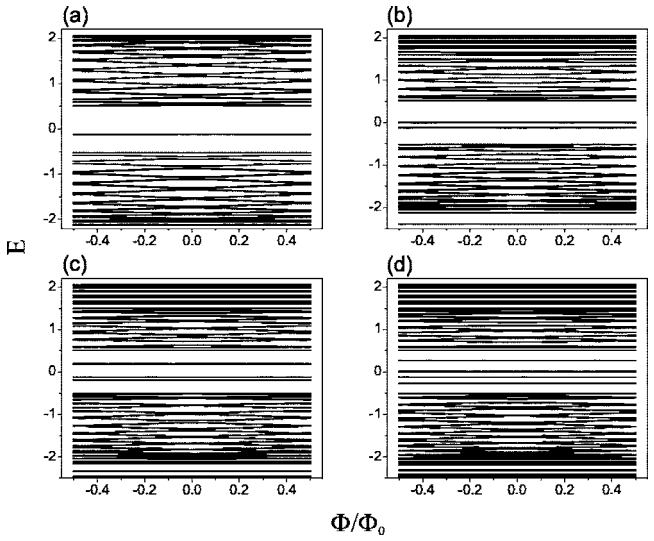

FIG. 1. The flux-dependent energy spectra of the SP rings $R(10,n)$, where $\varepsilon_A=-\varepsilon_B=0.5$ and $t_{l,l\pm1}=-1$. (a) $n=1$, (b) $n=7$, (c) $n=13$, and (d) $n=19$.

$$I_n(\Phi) = -c\frac{\partial E_n(\Phi)}{\partial \Phi}, \tag{6}$$

where c is the velocity of light. At zero temperature, if the number of electrons equals N_e in the spinless fermion system, the total persistent current in the mesoscopic ring satisfies

$$I(\Phi) = \sum_{n=1}^{N_e} I_n(\Phi). \tag{7}$$

Due to the fact that the properties of the persistent current (PC) are ultimately determined by the flux-dependent energy of the system, we first consider the energy spectra of the SP mesoscopic rings by a magnetic flux Φ. Based on Eqs. (3)–(7), we carry out the numerical calculation on the energy spectra. Figure 1 shows the flux-dependent energy spectra of several SP rings $R(10,n)$ in the case of $\varepsilon=0.5$. The electron eigenenergies form a "band" structure and the defect modes appear in the band gap [shown in Figs. 1(a)–1(d)]. The number of defect modes increases with increasing the number of atoms in the defect cluster. For example, there are one defect mode in SP ring $R(10,1)$ [shown in Fig. 1(a)], two defect modes in SP ring $R(10,7)$ [shown in Fig. 1(b)], three defect modes in $R(10,13)$ [shown in Fig. 1(c)], and four defect modes in $R(10,19)$ [shown in Fig. 1(d)], respectively. Thus, with increasing n, more and more defect modes appear in the band gap. While if we increase the value of m in the SP ring $R(m,n)$, the number of defect modes will not change, but the energy band will become more dense. Therefore, in the SP ring, the energy spectrum forms a "band" structure and the defect mode in the band gap can be tuned by selecting the construction of a SP ring.

The PC in SP ring can be obtained from Eqs. (6) and (7). The calculations indicate that the PC is dominated by the magnetic flux, the site energy, and the filling number of electrons corresponding to the Fermi level. Figure 2 presents the flux-dependent PC in the SP ring $R(10,1)$ with different site energies and different filling numbers of electrons. First, the PC shows a sinusoidal-like relation with respect to the magnetic flux. Second, the PC is gradually suppressed if the site of energy ε increases [as shown in Figs. 2(a) and 2(b)]. Increasing ε means that the scattering rate is enhanced and then the dependence of the energy level on the flux becomes smoother. Thereafter the current contribution coming from these energy levels will decrease according to Eq. (6). Consequently, the total current will decrease. Third, at the zero-temperature limit, the sign of the PC is determined by the parity effect. In a ring with an odd number of electrons, the flux-dependent PC is like that in a diamagnet [as shown in Figs. 2(a) and 2(c)]. While in a ring with an even number of electrons, the flux-dependent PC behaves like that in a paramagnet [as shown in Figs. 2(b) and 2(d)]. Finally, the magnitude of PC is also influenced by the electron-filling number N_e or the Fermi level. If the Fermi level is in the energy band, the PC is unsuppressed, while if the Fermi level is around the defect mode in the band gap of energy, the PC is suppressed dramatically. Figures 2(c) and 2(d) show the PC in the ring $R(10,1)$. It is found that if the filling number of electron is 20 or 21, the Fermi level comes to the defect mode; eventually the PC is suppressed dramatically. In this case the ring behaves like an insulator. Once the Fermi level has a slight deviation to the defect mode, the PC becomes unsuppressed and the ring looks like a metal.

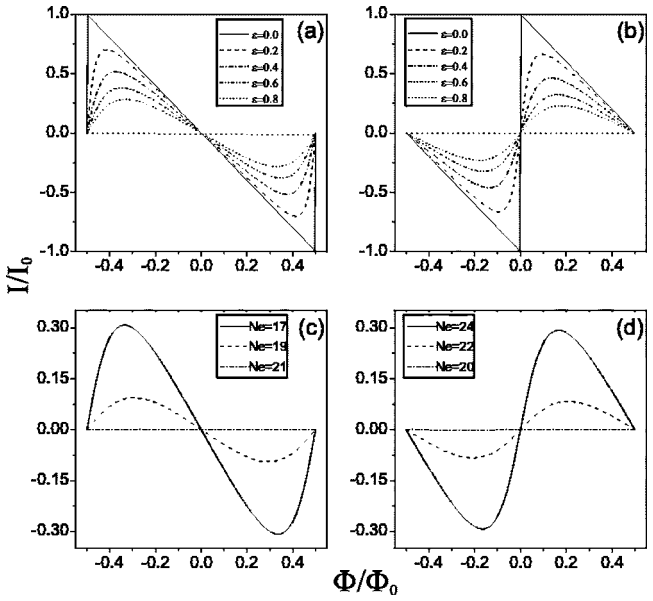

FIG. 2. The persistent current (PC) vs the magnetic flux Φ in the SP ring $R(10,1)$, where $I_0=(4\pi c/N\Phi_0)\sin(N_e\pi/N)$. (a) and (b) show the PC under different site energies ε: (a) $N_e=15$ and (b) $N_e=16$. (c) and (d) show the PC under different electron-filling numbers N_e, where $\varepsilon=0.5$.

It is worthwhile to show the overall behavior of the PC in the SP mesoscopic ring. Figure 3 plots the PC in several SP rings $R(10,n)$ versus the number of filling electrons N_e when $\Phi/\Phi_0=-0.252$ and $\varepsilon=0.5$. Now we are interested in how to observe the large PC in the SP ring. Obviously in each SP ring, the PC can be close to the periodic case when N_e comes to some special values. In details, the absolute value of I/I_0 can be more than 0.4 if the Fermi energy takes some peculiar values [as shown in Figs. 3(a)–3(d)]. Here I_0 is the maximum of PCs in a periodic structure. In these cases, the PC is absent of suppression, large PC can be observed in the SP ring, and the ring behaves like a metal. On the other

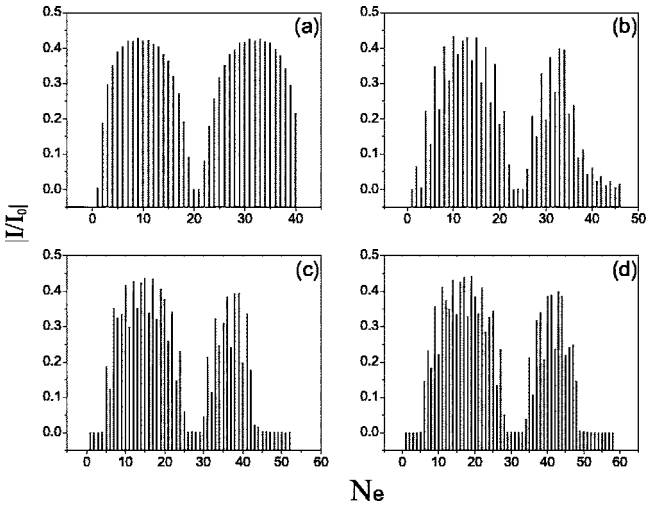

FIG. 3. The absolute value of persistent currents PC vs the number of filling electrons N_e in the SP rings $R(10,n)$, where $\varepsilon=0.5$ and $\Phi/\Phi_0=-0.252$. (a) $n=1$, (b) $n=7$, (c) $n=13$, and (d) $n=19$.

hand, it is also very interesting to observe the dramatically suppressed PC in the SP ring. As shown in Fig. 3, with increasing n in the SP ring $R(10,n)$, more and more Fermi energies correspond to the dramatically suppressed PCs. We define E_{fc} as the Fermi energy corresponding to the dramatically suppressed PC. Around the defect mode, there are two kinds of E_{fc} in the ring $R(10,1)$, three kinds of E_{fc} in the ring $R(10,7)$, four kinds of E_{fc} in the ring $R(10,13)$, and five kinds of E_{fc} in the ring $R(10,19)$, respectively. That is to say, at each E_{fc}, the PC is dramatically suppressed and the ring behaves like an insulator. Therefore, by changing the Fermi level, the SP ring presents the features of metallic and insulative properties alternately.

In order to understand the behavior of the PC in the SP ring clearly, the electronic wave function has been studied. Applying Eqs. (2) and (3) in the initial conditions of $\psi_0=0$ and $\psi_1=1$, we have obtained the amplitude of the electronic wave function on each site of the ring. Figure 4 shows the wave function at the Fermi level corresponding to the different highest-occupied electrons in the SP ring $R(10,19)$, where $\Phi/\Phi_0=-0.252$. It is shown that the wave function is almost extended [as shown in Fig. 4(a)] if the Fermi level is in the band of the energy spectra. In this case, the electron propagates through the whole ring, and the PC resembles the case of a free electron. Thus the SP ring looks like a metal. Figure 4(c) shows the localized wave functions if the Fermi level approaches the defect mode in the band gap of the energy spectra. Obviously, the electron cannot propagate through the whole ring. Thus the SP ring behaves like an insulator. The intermediate case of wave functions is given in Fig. 4(b), where the electron goes through the ring in part and the PC is significantly decreased. Therefore, if the Fermi level is gradually changed, the SP ring presents the features of metallic and insulative properties alternately. From this point of view, the SP ring provides a possible model to explain the anomalously large PC observed in some experiments. It is a structural model and different from other models.[6] Besides, the SP ring also gives a theoretical model

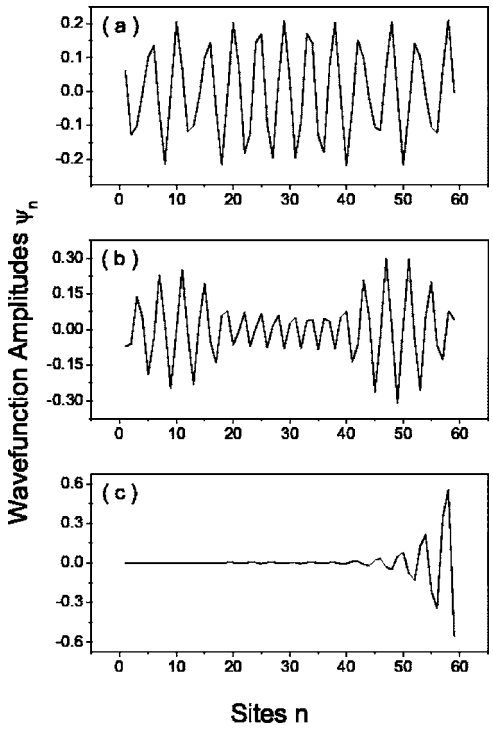

FIG. 4. The wave function amplitudes on each site of the SP ring $R(10,19)$, where $\Phi/\Phi_0=-0.252$. The electronic state is (a) almost extended when $N_e=25$ and $E=-0.801\,932\,784\,947\,375$, (b) intermediated when $N_e=35$ and $E=0.574\,291\,227\,825\,515$, and (c) localized when $N_e=31$ and $E=-0.118\,048\,341\,390\,78$.

to realize quantum switches. In the experiment, one may intentionally introduce suitable sites in the ring to realize the SP mesoscopic model. By changing the electron number in ring, we may obtain large PC and "zero" PC alternately and observe a similar metallic-insulative transition in the SP ring.

This work was supported by the grants from the National Natural Science Foundation of China (10374042, 90201039, 10274029, and 10021001), the State Key Program for Basic Research from the Ministry of Science and Technology of China (2004CB619005), NSF of Jiangsu (BK2004209), and partly by the Ministry of Education of China and Fok Ying Tung Education Foundation.

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