Electronic delocalization and persistent currents in nonsymmetric-dimer mesoscopic rings threaded by magnetic flux

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(Presented on 9 January 2004)

We investigate electronic delocalization and magnetic-flux-induced persistent current in the mesoscopic ring, which is constructed according to the nonsymmetric-dimer (NSD) model. The flux-dependent energy spectra, electronic wavefunctions, and persistent currents are theoretically obtained. It is demonstrated that due to the localization-delocalization transition of electrons, the electronic state in the NSD ring can be localized, extended, and the intermediate case between extended states and localized ones. The persistent current (PC) approaches the behavior of free electrons if the Fermi level is around the near-resonant energy. Otherwise, the PC is depressed dramatically. This conclusion could be generalized to other correlated-disordered systems. © *2004 American Institute of Physics.* [DOI: 10.1063/1.1651801]

Since Anderson presented the electronic localization theorem based on a model with a site-diagonal disorder in 1958,[1] much attention has been paid to the problem of electronic localization in one-dimensional (1D) disordered systems.[2] Recently, some fascinating issues have added fresh insight into the localization problem. It is shown that extended states can still exist in the system with correlated disorder. One typical case is the random-dimer model (RDM) introduced by Dunlap, Wu, and Phillips in 1990.[3] In the RDM, one of two site energies ϵ_a and ϵ_b is randomly assigned to pairs in the lattice, and an invariable nearest-hopping integral V connects the sites. Provided that $|\epsilon_a - \epsilon_b| \leqslant 2V$, there are $\sqrt{N}$ extended electronic states in the RDM with length N; otherwise, localization occurs. This kind of localization-delocalization transition has also been found in the random trimer, random dimer-trimer, and even the random n-mer model.[4] The widely accepted understanding of the electronic delocalization in RDM-like systems is that the impurity possesses internal symmetry, and this short-range correlated disorder can make the localization length comparable to the length of the system at resonant energies.[3,5] However, near-resonant scattering was found in nonsymmetric-dimers chains in 1994.[6] Very recently, resonant scattering phenomenon has been observed in n-mer chains with inversely symmetric impurities.[7] It is shown that the internal mirror symmetry is not a necessary condition for the presence of electronic delocalization: Instead, the short-range spatial correlation plays an important role in such systems with correlated disorder. Considering the analogy between electronic transport in a 1D chain and that in a mesoscopic ring,[8] we may ask whether a similar resonant phenomenon may occur in a mesoscopic ring.

In this paper, we investigate electronic delocalization and its effect on the persistent current in a 1D disordered mesoscopic ring threaded by a magnetic flux. The mesoscopic ring is constructed according to the nonsymmetric-dimer (NSD) model, where the defect clusters are randomly embedded into a monoatomic host system, but each cluster contains two kinds of defects, i.e., the cluster is nonsymmetric, and thus it is different from the RDM. It is well known that Büttiker, Imry, and Landauer first theoretically predicted the persistent current (PC) in the flux-threaded mesoscopic ring in 1983.[8] The experimental work on persistent currents has been carried out since the last decade. In an early experiment by Lévy *et al.*,[9] the PC measured on 10^7 copper rings is in agreement with the theoretical prediction under the diffusive case. However, the experimental observation by Chandrasekhar *et al.*[10] indicated that the current in a single Au ring is one or two orders of magnitude larger than the value predicted by the noninteracting theory. Some models have been presented to explain this puzzle.[11] In our case, due to the electronic localization-delocalization transition in the NSD system, the PC in the NSD mesoscopic rings presents a rich feature. The PC can approach the behavior of free electrons regardless of the disorder if the Fermi level is around the energy of near-resonant scattering, while the PC can be depressed dramatically if the Fermi level is far away from the energy of near-resonant scattering. Our investigations provide another reasonable model to explain the anomalously large PC observed in the experiments.

Consider a 1D aperiodic mesoscopic ring threaded by the magnetic flux. There are N sites in the ring, and the lth site is occupied by the atom a_l ($l=1,2,\ldots,N$). In the tight-binding approximation, without an electron-electron interaction, the Schrödinger equation for a spinless electron in a 1D aperiodic mesoscopic ring threaded by a magnetic flux Φ can be written as

$$(E-\epsilon_l)C_l = V_{l,l+1}C_{l+1} + V_{l,l-1}C_{l-1}, \tag{1}$$

where C_l is the amplitude of wavefunction on the lth site, $V_{l,l\pm 1}$ is the nearest hopping integral, and the site-energy ϵ_l

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is taken as $\epsilon_l = \epsilon_a$ (or ϵ_b, ϵ_c) if atom a (or b, c) occupies the site. Equation (1) can also be expressed in the matrix form

$$\begin{pmatrix} C_{l+1} \\ C_l \end{pmatrix} = M_{l+1,l} \begin{pmatrix} C_l \\ C_{l-1} \end{pmatrix}, \tag{2}$$

where the transfer matrix

$$M_{l+1,l} = \begin{pmatrix} \dfrac{E-\epsilon_l}{V_{l,l+1}} & -\dfrac{V_{l,l-1}}{V_{l,l+1}} \\ 1 & 0 \end{pmatrix}. \tag{3}$$

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

$$\begin{pmatrix} C_{N+1} \\ C_N \end{pmatrix} = \overline{M} \begin{pmatrix} C_1 \\ C_0 \end{pmatrix} = e^{i2\pi\Phi/\Phi_0} \begin{pmatrix} C_1 \\ C_0 \end{pmatrix}, \tag{4}$$

where $\overline{M} = \Pi_{l=1}^{N} M_{l+1,l}$ and $\Phi_0 = hc/e$ is the flux quantum. By denoting the trace of $\overline{M}$ as $\chi = \frac{1}{2}\mathrm{Tr}\,\overline{M}$, the flux-dependent energy $E_n(\Phi)$ 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 follows:

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

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

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

In our case, the mesoscopic ring is constructed according to the NSD model. The NSD model contains three kinds of atoms: a, b, and c. The host atom a and the paired impurity atoms bc are distributed randomly on the sites, and there is a total of N sites in the NSD model. Without loss of generality, we let the nearest hopping interval of atoms $a-a$, $a-b$, and $a-c$ be the same as $V_{a,a} = V_{a,b} = V_{a,c} = V$, but the nearest hopping interval of atoms $b-c$ is $V_{b,c} = \overline{V}$. As we know, near-resonant scattering can happen if the reflection coefficient[6]

$$|r|^2 = 1 - \frac{4V^2\overline{V}^2 \sin^2 k}{[\overline{V}^2 - V^2 - W_b W_c - V(W_b + W_c)\cos k]^2 + V^2[(W_b - W_c)^2 + 4\overline{V}^2]\sin^2 k} \tag{8}$$

is close to zero in the nonsymmetric-dimer chain, where $W_b = \epsilon_a - \epsilon_b$, $W_c = \epsilon_a - \epsilon_c$, and k is the wavevector. [According to Eq. (8), we have $|r|^2 = 0$ only in the case of $W_b = W_c$ and $\overline{V} = V$, i.e., a symmetric dimer. Therefore, there is only near-resonant scattering in a nonsymmetric-dimer structure.] Once in the case of near-resonant scattering, the energy satisfies

$$E \cong E_g = \epsilon_a + 2V\cos k. \tag{9}$$

Thus, the impurity cluster seems to not have affected the amplitude of the electronic wave function, and the NSD structure looks like the monoatomic (i.e., the atom "a") system. The behavior of electrons in the NSD ring is exactly like that in the NSD chain: the wave vector k is determined by the magnetic flux Φ in the ring, i.e., $kL = 2\pi\Phi/\Phi_0$ ($\Phi_0 = hc/e$ is the flux quantum and L is the length of the ring). Near-resonant scattering will happen in the NSD mesoscopic ring if the Fermi level is close to the near-resonant energy given by Eqs. (8) and (9) when $|r|^2$ approaches zero. Thereafter, the PC in this ring with correlated disorder will approach that in the ordered (periodic) mesoscopic rings.

The above analysis can be demonstrated by the numerical calculation on the energy spectrum and the persistent current in the 1D NSD mesoscopic ring. In the following calculation, the parameters are taken as $N = 595$, $\epsilon_a = 0.4$, $\epsilon_b = 1.0$, $\epsilon_c = 1.22$, $V = -1.48$, $\overline{V} = 1.183$, and the numbers of atoms a, b, and c in the ring are almost the same, which correspond to the most disordered case. The flux-dependent energy spectrum can be obtained according to Eqs. (3)–(5). Figure 1(a) shows the energy levels around the near-resonant energy $E_g = 2.05$. Obviously in the vicinity of the near-resonant energy, the energy level has narrow gaps at $\Phi/\Phi_0 = 0$ and $\Phi/\Phi_0 = \pm 0.5$ [shown in Fig. 1(a)], which is quite similar to that in the ordered ring. Figure 1(b) presents the flux-dependent eigenenergy which is away from the near-resonant energy. The energy level shows large gaps and is much smoother in the case here the energy deviates from the resonant energy [shown in Fig. 1(b)].

Based on Eqs. (6) and (7), the persistent current can be calculated. Figure 2(a) presents the total persistent current

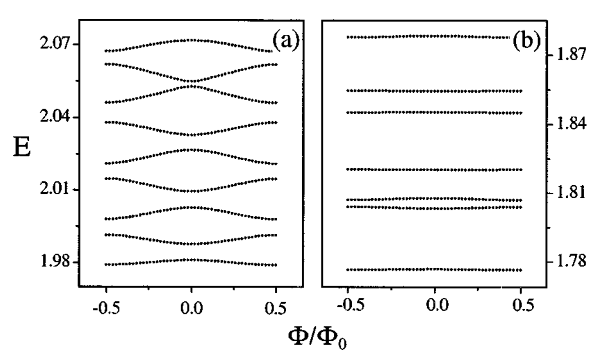

FIG. 1. The flux-dependent energy level of the 1D NSD mesoscopic ring, where $N = 595$, $\epsilon_a = 0.4$, $\epsilon_b = 1.0$, $\epsilon_c = 1.22$, $V = -1.48$, and $\overline{V} = 1.183$. (a) Around the near-resonant energy $E \cong E_g = 2.05$. (b) Away from the near-resonant energy.

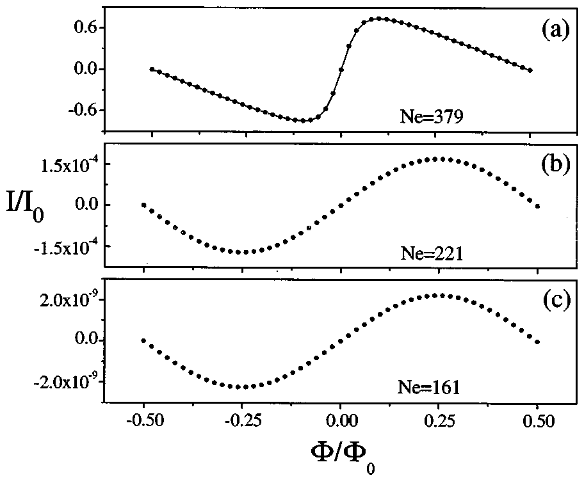

FIG. 2. The persistent current in the NSD mesoscopic ring with the same parameters as in Fig. 1, where $I_0=(4\pi c/N\Phi_0)\sin(N_e\pi/N)$. (a) Large persistent current when $N_e=379$ ($E=2.0353937\sim2.0587578$). (b) Suppressed persistent current when $N_e=221$ ($E=-0.2204804\sim-0.2028655$). (c) Infinitesimal persistent current when $N_e=161$ ($E=-0.9383504\sim-0.9210108$).

when the Fermi level is closest to the near-resonant energy $E_g=2.05$. This Fermi level corresponds to the electron- filling number $N_e=379$. It is shown that the current is quite large ($I/I_{0\ \max}\simeq0.75$, with slight suppression), although the correlated disorder exists in the NSD system. The behavior of the PC in this case approaches that of a free electron. On the other hand, if the Fermi level occupies the off-resonant energy, the persistent current will be significantly reduced. Figures 2(b) and 2(c) illustrate the significantly depressed PC with different magnitudes.

In order to understand the behavior of the PC in the NSD ring, the electronic wave function has been studied. Applying Eqs. (2) and (3) in the initial conditions of $C_0=0$ and $C_1=1$, we have obtained the amplitude of the electronic wavefunction on each site of the ring. Figures 3(a)–3(c) are the wave function on the Fermi level corresponding to the different highest-occupied electrons in Figs. 2(a)–2(c), where $\Phi/\Phi_0=0.25$. It is obvious that the wave function is almost extended [shown in Fig. 3(a)] if the Fermi energy is closest to the near-resonant energy $E_g=2.05$. It propagates through the whole ring with very little decay. Figures 3(b) and 3(c) show intermediated and localized wave functions, respectively, when the Fermi level deviates from the near-resonant energy. Therefore, in the NSD mesoscopic ring, the persistent current is almost not suppressed if there is an extended electronic state at the Fermi level. The behavior of the PC resembles the case of a free electron, although there is the disorder in the NSD ring. The electronic delocalization indeed occurs in the NSD ring. However, if the electronic state is intermediated or localized at the Fermi level, the persistent current is significantly decreased.

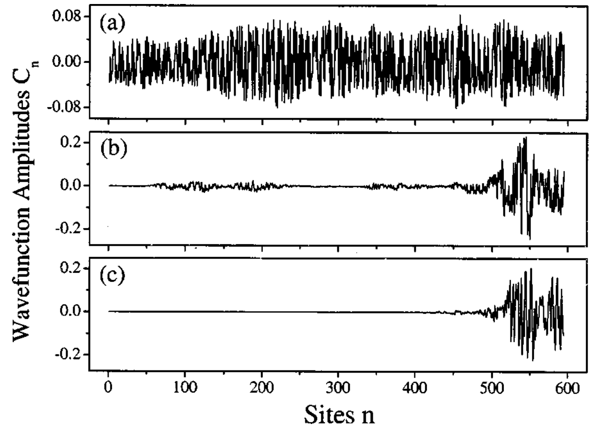

FIG. 3. The wave-function amplitudes on each site of the NSD ring when the Fermi level corresponds to the cases in Figs. 2(a)–2(c), respectively, where $\Phi/\Phi_0=0.25$. The highest-occupied electronic state is (a) almost extented when $N_e=379$ and $E=2.0487790107727$, (b) intermediated when $N_e=221$ and $E=-0.204\,360\,395\,669\,9$, and (c) localized when $N_e=161$ and $E=-0.938\,350\,439\,071\,6$.

This work was supported by the grants from National Nature Science Foundation of China (90201039, 10274029, 10374042, 10021001), the State Key Program for Basic Research from the Ministry of Science and Technology of China (C01CB610602, G1998061410), Provincial Nature Science Foundation of Jiangsu (BK2002408), and partially by the Fok Ying Tung Education Foundation.

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