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Multiple Delocalization of Electrons and Persistent Currents in Random *n*-mer Mesoscopic Rings

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We demonstrate that the electronic property of a mesoscopic ring can be alternatively tuned between metallic and insulative states by changing the Fermi level. The one-dimensional mesoscopic ring is constructed based on random *n*-mer model and threaded by magnetic flux. Multiple localization–delocalization transitions of electrons have been found. When the Fermi level approaches the resonant energy, persistent current approaches the behavior of free electrons regardless of the disorder, corresponding to the metallic feature. Away from the resonant state, the current is dramatically diminished, indicating an insulative feature. We suggest our results have potential application in designing quantum switch devices.

Keywords: Persistent Currents, Mesoscopic Rings, The Random *n*-mer Model.

1. INTRODUCTION

With the development of technology for the fabrication of submicrometer devices, much attention has been paid to the mesoscopic system in the past few decades. It is well known that in mesoscopic systems the semiclassical transport theory is invalid and quantum effects have to be taken into account. The persistent current (PC) is one of the distinguished features of quantum interference. In 1983, Büttiker et al.[1] first predicted the persistent current (PC) in one-dimensional (1D) mesoscopic rings threaded by a magnetic flux. Since then, considerable interests have been paid to the PC in 1D metal or semiconductor mesoscopic rings.[2–9] The experimental studies on the PC have been carried out since last decade. In the early experiment made by Lévy et al.,[2] PC measured on 10^7 copper rings is in agreement with the theoretical prediction. However, 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 noninteracting theory. Some models have been presented to explain this puzzle.[7] Recently more experiments bring new challenges to the theory, such as the sign of PC near zero field,[8] the correlation of PC with phase coherence time etc.[9] Generally speaking, disorder of the system and electron–electron interaction are the two important factors affecting the magnitude of the PC. Here we are interested in persistent currents in the correlated disordered system.

A famous example in the correlated disordered systems is the random-dimer model (RDM) introduced by Dunlap, Wu, and Phillips in 1990.[10] In RDM, one of two site energies is randomly assigned to pairs in the lattice. It has been demonstrated that $\sqrt{N}$ extended electronic states exist in RDM with length N; otherwise, localization occurs. This localization–delocalization transition has also been found in random trimer and random dimer-trimer, and even random *n*-mer systems.[11] Naturally one may ask whether similar phenomenon of electrons may occur in a mesoscopic ring. In this work, we investigate the electronic delocalization and its influence on PC in a 1D random *n*-mer (RN) mesoscopic ring threaded by a magnetic flux. Multiple localization–delocalization transitions of electrons have been observed in the RN ring. Due to the electronic delocalization in the RN system, PC presents a rich feature depending on its energy spectrum and Fermi level. The PC can approach the behavior of free electrons regardless of the disorder if the Fermi level is around the resonant energy, while the PC can be depressed dramatically if the Fermi level is far away from the resonant energy. As a result, the electronic property of a mesoscopic ring can be alternatingly tuned between metallic and insulative states by changing the Fermi level.

2. THE THEORETICAL MODEL

Consider the electron behavior in a 1D random *n*-mer (RN) mesoscopic ring threaded by the magnetic flux.

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There are two kinds of sites A and B in the ring which contains M sites. Site "A" and the impurity cluster of sites "$B\cdots B$" (the number of atom B is n) are randomly assigned in the ring as

$$\cdots\underbrace{A\cdots A}_{X_1}\underbrace{B\cdots B}_{Y_1}\underbrace{A\cdots A}_{X_2}\underbrace{B\cdots B}_{Y_2}\cdots\underbrace{A\cdots A}_{X_j}\underbrace{B\cdots B}_{Y_j}\cdots$$

where X_j is the number of site A in the jth cluster of A, which is random. $Y_j = nZ_j$ is the number of site B in the jth cluster of B. Obviously, $Y_j = 2Z_j$ in the random-dimer model. In other words, the number of site B in the jth cluster of B is even because site B exists in pairs in the random-dimer model. $Y_j = 3Z_j$ in the random-trimer model, and in general $Y_j = nZ_j$ in the random n-mer model, respectively. Here, Z_j is an integer. The RN model shown here is an extension of the RD model and other correlated models.[5,11] With tight-binding approximation, Schrödinger equation for a spinless electron in a RN ring can be written in a transfer matrix form as

$$\begin{pmatrix}\psi_{l+1}\\ \psi_l\end{pmatrix} = T_l\begin{pmatrix}\psi_l\\ \psi_{l-1}\end{pmatrix} \tag{1}$$

where T_l is the transfer matrix that correlates the adjacent site amplitudes ψ_l and $\psi_{l\pm 1}$. In the on-site model, T_l is set as $T_l = \begin{pmatrix}(E-\varepsilon_l)/t & -1\\ 1 & 0\end{pmatrix}$, and the site energy ε_l is taken as $\varepsilon_l = \varepsilon_a$ (or ε_b) if atom A (or B) occupies the site. For generality, the nearest hopping integral t is set as a constant (here $t = -1$) in the following calculation.

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

$$\begin{pmatrix}\psi_{M+1}\\ \psi_M\end{pmatrix} = \overline{T}\begin{pmatrix}\psi_1\\ \psi_0\end{pmatrix} = e^{i2\pi\Phi/\Phi_0}\begin{pmatrix}\psi_1\\ \psi_0\end{pmatrix} \tag{2}$$

where $\overline{T} = \Pi_{l=1}^{M} T_l$ is the global transfer matrix, and $\Phi_0 = hc/e$ is the flux quantum. We can calculate the flux-dependent energy spectra from equation $Tr(\bar{T}) = 2\cos(2\pi\Phi/\Phi_0)$. At zero temperature, if the number of electrons equals N_e, total PC in the ring satisfies

$$I(\Phi) = \sum_{h=1}^{N_e} I_h(\Phi) = -c\sum_{h=1}^{N_e}\frac{\partial E_h(\Phi)}{\partial\Phi} \tag{3}$$

For the RN ring, the global transfer matrix can be written as

$$\overline{T} = \cdots (T_b)^{Y_j}(T_a)^{X_j}\cdots(T_b)^{Y_2}(T_a)^{X_2}(T_b)^{Y_1}(T_a)^{X_1} \tag{4}$$

where T_a (or T_b) is the matrix T_l when ε_l equals to ε_a (or ε_b), and $(T_b)^{Y_j} = [(T_b)^n]^{Z_j}$. From the theory of matrices,[12] the nth power of the 2×2 unimodular matrix T_b can be written as

$$(T_b)^n = u_{n-1}(\chi)T_b - u_{n-2}(\chi)I \tag{5}$$

where $\chi = \frac{1}{2}tr(T_b)$, I is an unit matrix, $u_n(\chi)$ is the nth Chebyshev polynomial of the second order. If $|\chi| \le 1$, $u_n(\chi)$ has the form of

$$u_n(\chi) = \sin(n+1)\theta/\sin\theta(\theta = \arccos\chi) \tag{6}$$

For $n \ge 2$, if

$$\chi = \chi_g = \cos(g\pi/n), \quad g = 1, 2, \ldots, n-1 \tag{7}$$

we obtain $u_{n-1}(\chi_g) = 0$ and $u_{n-2}(\chi_g) = (-1)^{g+1}$. In this case, Eq. (5) turns to $(T_b)^n = (-1)^g I$, and the total matrix of Eq. (4) is only composed of matrices T_a and $(-1)^g I$. Thus, the RN structure appears as a monoatomic (i.e., atom A only) system. Based on the above matrix theory, resonant energies satisfy

$$E_g = \varepsilon_b - 2\cos(g\pi/n), \quad g = 1, 2, \ldots, n-1 \tag{8}$$

According to Eq. (8), there are $n-1$ resonant energies exist in the RN ring. Physically, at the resonant energies, impurity cluster of $B\cdots B$ does not influence the electronic wave function, thereafter, the behavior of electron in the RN ring is similar to that in a homogeneous ring of atom A. From this point of view, localization–delocalization transition of electrons indeed takes place at the resonant energy given by Eq. (8). Finally, at the resonant energy, PC in RN ring will approach that in the ordered (periodic) mesoscopic ring.

3. THE NUMERICAL CALCULATIONS

The above analysis can be demonstrated by numerical calculation of the energy spectrum and the persistent current in 1D RN mesoscopic ring threaded by a magnetic flux Φ. Let us take the random trimer ring as an example, which corresponds to the RN system with $n = 3$. In a random trimer ring, the total number of atoms is $N_{tot} = 600$, and the number of atom A is same as that of atom B. Besides, the site energy is set as $\varepsilon_a = 0.4$ and $\varepsilon_b = 0.0$, respectively. According to Eq. (8), the resonant energies are $E_g = 1$ and $E_g = -1$ for $n = 3$. The flux-dependent energy spectra around the resonant energies $E_g = -1$ and 1 are shown in Figures 1(a) and (b), respectively. Obviously, around E_g, the energy levels have no gap at $\Phi/\Phi_0 = 0$ and ± 0.5. This feature is quite similar to that in an ordered ring. However, if the energy is deviated from E_g, distinct energy gaps appear and the energy levels become much more flat (as shown in Figs. 1(c and d)).

The PC is ultimately determined by the flux-dependent energy spectrum. Figures 2(a) and (b) present the flux-dependent PC when the Fermi levels are close to the resonant energies $E_g = -1$ (corresponding to the electron-filling number $N_e = 176$) and $E_g = 1$ (corresponding to $N_e = 380$), respectively. Obviously, the unsuppressed current is observed at E_g in the random trimer ring. On the

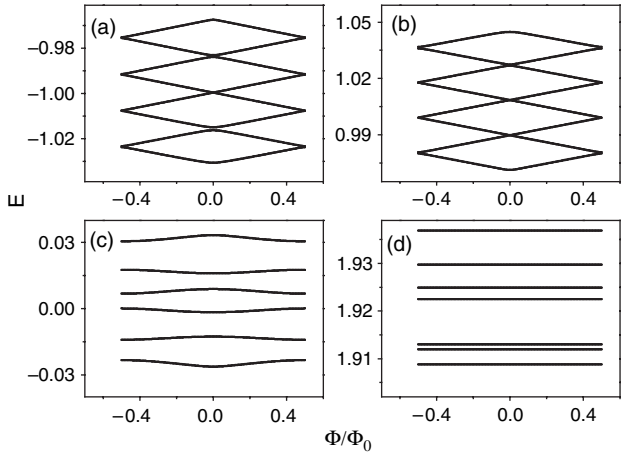

Fig. 1. The flux-dependent energy spectra of the random trimer ring, where the total number of atoms $N_{\text{tot}} = 600$, $\varepsilon_a = 0.4$, $\varepsilon_b = 0.0$, and $t = -1$. (a) The spectrum around the resonant energy $E_g = -1$; (b) The spectrum around the resonant energy $E_g = 1$; (c) and (d) The spectra when the energy is away from the resonant energy.

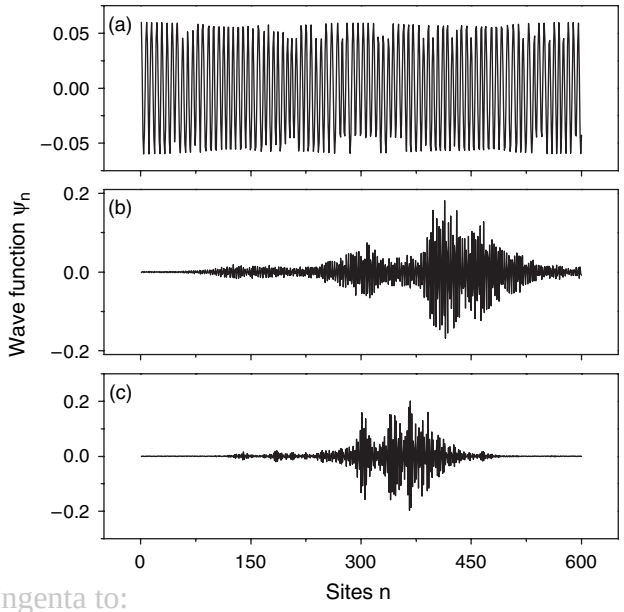

Fig. 3. The wave-function amplitudes on each site of the random timer ring when the Fermi level corresponds to the different cases in Figure 2, where $\Phi/\Phi_0 = -0.252$. The electronic state is (a) extended when $N_e = 176$ and $E = -1.0036724213594$, (b) intermediated when $N_e = 442$ and $E = 1.5337400345322$, and (c) localized when $N_e = 500$ and $E = 1.9119807396496$.

other hand, if the Fermi level deviates from the resonant energy E_g, PC will be significantly reduced (shown in Figs. 2(c and d)). In Figures 2(c and d), we also show the results for odd N_e with dashed curves. It is found that the parity effect of electronic filling with odd and even number is similar to that of the periodic system.

In order to understand the behavior of PC in a random trimer ring clearly, electronic wave function has been studied. Figure 3 shows wave functions of electron in the ring with different Fermi levels, where $\Phi/\Phi_0 = -0.252$. It is shown that the wave function is extended (shown in Fig. 3(a)) when the Fermi level is close to the resonant energy $E_g = -1$. In this case, the electron propagates through the whole ring without decay. Figures 3(b) and (c) show the intermediated and the localized wave functions, respectively, when Fermi level deviates from the resonant energy. Therefore, in a random trimer ring, PC is almost not suppressed when there is an extended electronic state at the Fermi level. The behavior of PC resembles the case of a free electron, although disorder exists in the ring. The electronic delocalization indeed occurs at the resonant energy in this correlated disordered ring. However, if the electronic state is intermediated or localized at the Fermi level, PC is significantly suppressed.

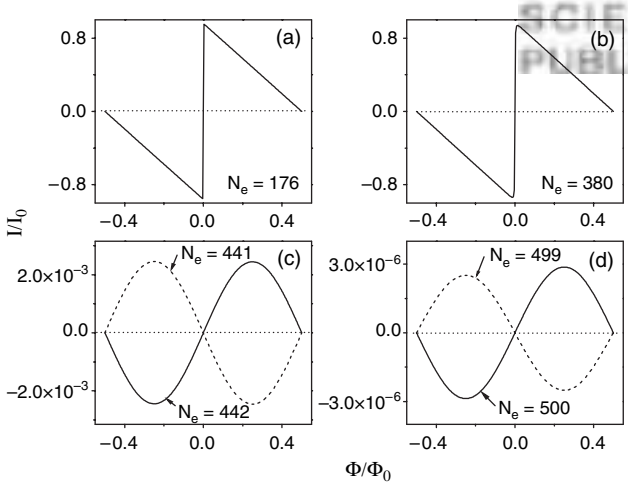

Fig. 2. The persistent current (PC) versus the magnetic flux Φ in the random trimer ring, where $I_0 = (4\pi c/N\Phi_0)\sin(N_e\pi/N)$ and the parameters are the same as those in Figure 1. The electron-filling number is: (a) $N_e = 176$; (b) $N_e = 380$; (c) $N_e = 442$ for the solid curve and $N_e = 441$ for the dashed curve; and (d) $N_e = 500$ for the solid curve and $N_e = 499$ for the dashed curve.

We can generalize the random trimer system to a random n-mer (RN) ring. In the calculation the parameters are taken as $\varepsilon_a = 0.25$, $\varepsilon_b = 0.0$, and the total number of atoms $N_{\text{tot}} = 1200$ for each ring. According to Eq. (8), there is one resonant energy in the random-dimer ring, i.e., $E_g = 0$. There are two resonant energies in the RT ring, i.e., $E_g = -1$ and $E_g = 1$. There are three resonant energies in the random-tetramer ring, i.e., $E_g = -\sqrt{2}$, $E_g = 0$, and $E_g = \sqrt{2}$. For random 5-mer ring, four resonant energies exist, which are $E_g = -(1+\sqrt{5})/2$, $E_g = -(-1+\sqrt{5})/2$, $E_g = (-1+\sqrt{5})/2$, and $E_g = (1+\sqrt{5})/2$, respectively. At these resonant energies, the electron can propagate through the whole RN ring, and large PC can be observed. Figure 4 shows the absolute value of the PC in several RN rings versus the number of filling electrons N_e when $\Phi/\Phi_0 = -0.252$. Due to the delocalization of electron at resonant energies, $n-1$ peaks appear in the PC curve (shown in Figs. 4(a–d)). For instance, there is one

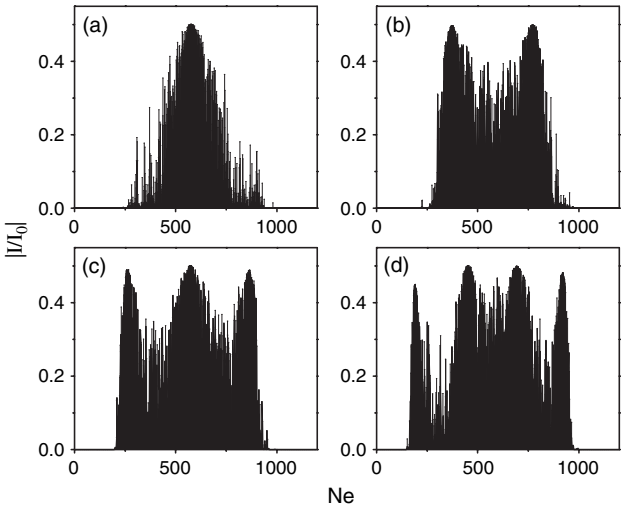

Fig. 4. The absolute value of the persistent current versus the number of filling electrons N_e in several random n-mer (RN) rings. At each ring, the number of atom A is the same as that of atom B, and the total number of atoms $N_{tot} = 1200$. The other parameters are set as $\varepsilon_a = 0.25$, $\varepsilon_b = 0.0$, $t = -1$, and $\Phi/\Phi_0 = -0.252$. (a) The random dimer ring, i.e., $n = 2$; (b) The random trimer ring, i.e., $n = 3$; (c) The random 4-mer ring, i.e., $n = 4$; (d) The random 5-mer ring, i.e., $n = 5$.

peak for the random-dimer ring, two peaks for the random-trimer ring, three peaks for the random 4-mer ring, and four peaks for the random 5-mer ring, respectively. The PC can be close to the periodic case when the Fermi level comes to these resonant energies. In details, the absolute value of I/I_0 can be more than 0.4 if the Fermi energy takes some peculiar values. I_0 is the maximum of PCs in a periodic structure. We can expect that once RN ring is sufficiently large, the peak will gradually become a single mode, which is very similar to δ-function. Therefore, in a sufficiently large RN ring, when the Fermi level approaches the resonant energies (Eq. (8)), large PC can be observed and the ring is metal-like. While the Fermi level deviates from the resonant energy, the dramatically-suppressed PC can be observed and the ring becomes insulator-like. By changing the Fermi level, RN ring may demonstrate metallic and insulative properties alternately. This feature may have potential applications in designing quantum-switch devices.

4. SUMMARY

With tight-binding approximation, flux-dependent energy spectra, electronic wavefunctions, and persistent currents have been investigated in 1D random n-mer (RN) mesoscopic ring. Multiple localization–delocalization transitions of electrons have been found in the RN ring. The persistent current in the mesoscopic ring is determined by the energy spectrum and the Fermi level. When the Fermi level approaches the resonant energy, persistent current approaches the behavior of free electrons regardless of the disorder, corresponding to the metallic feature. Away from the resonant state, the current is dramatically diminished, indicating an insulative feature. We demonstrate that the electronic property of a mesoscopic ring can be alternatingly tuned between metallic and insulative states by changing the Fermi level. Our results may have potential application in designing quantum switch devices.

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