

Absence of Suppression in the Persistent Current by Delocalization in Random-dimer Mesoscopic Rings

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We study the persistent current (PC) in one-dimensional (1D) magnetic-flux threaded mesoscopic rings, which is constructed according to the random-dimer (RD) model. It is found that the PC varies significantly when the Fermi energy is changed in the system. The PC can approach the behaviour of free electrons regardless of the disorder if there is the extended electronic state at the Fermi level; while the PC can be depressed dramatically if the highest-occupied electronic state is localized or in the intermediate case between the extended state and localized one. This property provides a possible explanation to the anomalously large PC observed in some experiments. Furthermore, it is demonstrated that the electronic delocalization leads to unsuppressed persistent currents and \sqrt{N} unscattered states exist around the resonant energy in the RD model from the viewpoint of the PC. The possibility to use 1D random-dimer mesoscopic rings as quantum-switch devices is also discussed.

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Based on the model with site-diagonal disorder distributed randomly, Anderson pointed out in 1958 that all electronic states are exponentially localized even for infinitesimal disorder in one-dimensional (1D) systems.¹⁾ Later, more theoretical and experimental studies have provided deeper insights into the problem of the electronic localization.^{2–17)} It is found that extended states can still exist in the 1D disordered system. One of the well-known examples is the random-dimer (RD) model, in which Dunlap *et al.*^{2–5)} presented the surprising absence of the electronic localization. Since then, much work has been carried out on the Lyapunov coefficient, transmission coefficient, and wavefunction behavior in the RD model, which have further confirmed the existence of the delocalization.^{6–10)} Actually, the delocalization originates from the fact that the defects in the RD model possess internal symmetry. This short-range correlated disorder can make the localization length comparable to the length of the system at some specific energies. The short-range spatial correlation among disorders has been applied to explain the hierarchy of electronic extended states in some 1D quasiperiodic structures,^{11,12)} and physical properties of correlated structures have also been studied.^{13–16)} Very recently, the experimental observation of the delocalization was reported in the random-dimer semiconductor superlattice.¹⁷⁾

In this paper, we investigate the effect of disorder on the persistent current (PC) in the 1D mesoscopic ring where two site energies ϵ_a and ϵ_b are constructed according to the RD model. In this case, ϵ_a and paired ϵ_b (i.e., ϵ_b always occurs in pairs) are randomly distributed on the sites of the ring. It is well known that Büttiker *et al.* first predicted the persistent current in flux-threaded mesoscopic rings,^{18,19)} then this subject has attracted much attention. The experimental work on persistent currents has been carried out since last decade. In the early experiment made by Lévy *et al.*, the persistent current measured on 10^7 copper rings is in agreement with the theoretical prediction under the diffusive case.²⁰⁾ However, the experimental observation of Chandrasekhar *et al.* indicated that the current in single Au ring is one or two orders of magnitude larger than the value predicted by the

noninteracting theory.²¹⁾ Some models have been presented to explain this puzzle.^{22,23)} In recent years, more experimental work came out and brought new challenges to the theoretical work, such as the sign of the PC near zero field, the correlation of the PC with the phase coherence time τ_φ etc.^{24–27)} Generally speaking, the disorder in the system and the electron–electron interaction play an important role on the persistent current in mesoscopic rings.^{28–37)} The effect of electron–electron interaction on the persistent current is complicated. Some reports have indicated that both long-range and short-range electron–electron interactions decrease the persistent current.^{28,29)} While other authors have claimed that the amplitude of the PC is enhanced due to the Coulomb interaction.^{30–32)} As for the effect of disorder, the general theorem is that the disorder always suppresses the persistent current.^{33–35)} However, our investigations show that the effect of disorder to the persistent current in 1D random-dimer mesoscopic rings is not so simple, because the electronic states in the system present quite different characteristics (that is, extended, localized or intermediated). The persistent current can approach the behavior of free electrons regardless of the disorder if there is the extended electronic state at the Fermi level; while the persistent current can be depressed dramatically if the highest-occupied electronic state is localized or in the intermediate case between the extended state and localized one.

Firstly we consider the electronic behavior in the 1D random-dimer mesoscopic ring threaded by a magnetic flux. The RD ring contains two kinds of atoms a and b . On the sites of the ring, the atom a and the paired atoms bb are arranged randomly, and totally there are N sites in the RD ring. Under the tight-binding approximation, without electron–electron interaction, the Schrödinger equation for a spinless electron in a 1D aperiodic mesoscopic ring can be written as

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

where C_l is the amplitude of wavefunction on the l th site, $V_{l,l\pm 1}$ is the nearest hopping integral, and the site-energy ϵ_l is taken as $\epsilon_l = \epsilon_a$ (or ϵ_b) if atom a (or b) occupies the site. In

this paper, we restrict ourself in the on-site model, that is, $V_{l,l\pm 1}$ is set as a constant V and as the energy unit. Equation (1) can be expressed in the matrix form

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

where the transfer matrix

$$M_{l+1,l} = \begin{pmatrix} \frac{E - \epsilon_l}{V} & -1 \\ 1 & 0 \end{pmatrix}.$$

Because a magnetic flux Φ threaded through the ring will lead to the twisted boundary condition for the wavefunction of the electrons,³³⁾ the equation for the global transfer matrix has the form as

$$\begin{pmatrix} C_{N+1} \\ C_N \end{pmatrix} = \bar{M} \begin{pmatrix} C_1 \\ C_0 \end{pmatrix} = e^{i2\pi\Phi/\Phi_0} \begin{pmatrix} C_1 \\ C_0 \end{pmatrix}, \quad (3)$$

$$I(\Phi) = \begin{cases} -I_0 \frac{\sin(2\pi\Phi/N\Phi_0)}{\sin(\pi/N)} & \left(\text{odd } N_e, -0.5 \leq \frac{\Phi}{\Phi_0} < 0.5 \right) \\ -I_0 \frac{\sin[(\pi/N)(2\Phi/\Phi_0 - 1)]}{\sin(\pi/N)} & \left(\text{even } N_e, 0.0 \leq \frac{\Phi}{\Phi_0} < 1.0 \right), \end{cases} \quad (6)$$

where $I_0 = \frac{4\pi c}{N\Phi_0} \sin(N_e\pi/N)$ is the persistent current at Fermi level. For large N , the above expressions approach the free-electron case

$$I(\Phi) = \begin{cases} -I_0 \frac{2\Phi}{\Phi_0} & \left(\text{odd } N_e, -0.5 \leq \frac{\Phi}{\Phi_0} < 0.5 \right) \\ -I_0 \left(\frac{2\Phi}{\Phi_0} - 1 \right) & \left(\text{even } N_e, 0.0 \leq \frac{\Phi}{\Phi_0} < 1.0 \right). \end{cases} \quad (7)$$

In order to make comparison later, we firstly give Figs. 1(a) and 1(b) to illustrate the persistent current in 1D ordered mesoscopic rings for even N_e and odd N_e , respectively. It can be seen that the current in Fig. 1(a) is shifted by $\frac{\Phi_0}{2}$ due to the parity effect, compared with that in Fig. 1(b). The

where $\bar{M} = \prod_{l=1}^N M_{l+1,l}$ and $\Phi_0 = hc/e$ is the flux quantum. Once the flux-dependent energy $E_n(\Phi)$ is obtained from eq. (3), the persistent current in the ring contributed by the n th energy level is expressed as

$$I_n(\Phi) = -c \frac{\partial E_n(\Phi)}{\partial \Phi}, \quad (4)$$

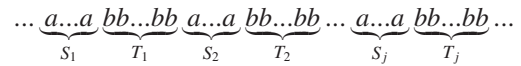
where c is the velocity of the light. At zero temperature, if the number of electrons in the spinless fermion system equals N_e , the total persistent current in the mesoscopic ring satisfies

$$I(\Phi) = \sum_{n=1}^{N_e} I_n(\Phi). \quad (5)$$

As well known, under the tight-binding approximation, the persistent current in periodic (or ordered) mesoscopic rings is³³⁾

persistent current has a sudden jump at $\frac{\Phi}{\Phi_0} = 0$ in the case of even N_e , while for odd N_e , the sudden jump exists at $\frac{\Phi}{\Phi_0} = \pm 0.5$.

Now we consider a 1D random-dimer mesoscopic ring with N sites which are arranged according to the random-dimer model as follows:



S_j is the number of atom a in the j th cluster composed of a , which is random. T_j is the number of atom b in the j th cluster composed of b , which must be even because b is inserted with pairs. Site energies ϵ_a and ϵ_b are assigned correspondingly.

The global transfer matrix is

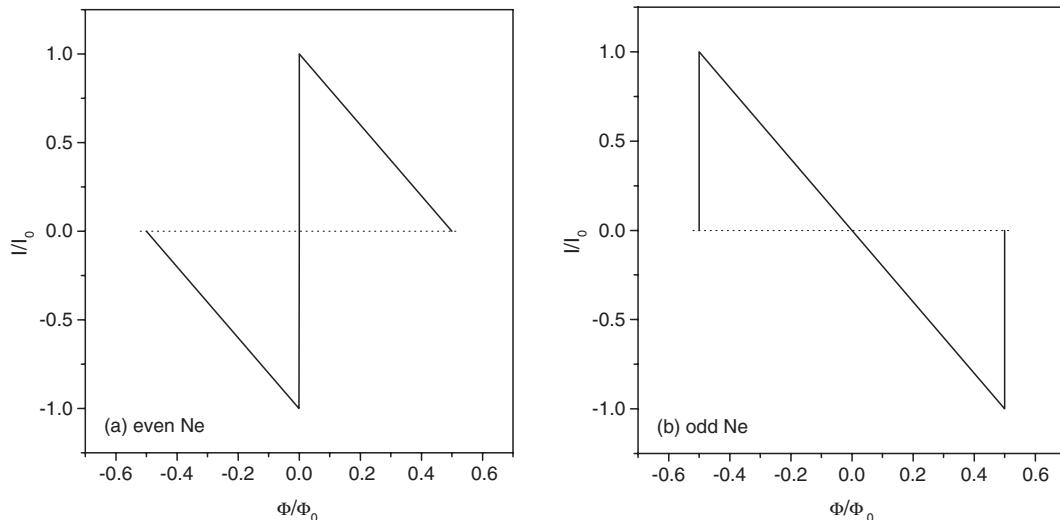


Fig. 1. The persistent current I versus the magnetic flux in 1D ordered mesoscopic rings. The electron-filling number N_e is (a) even and (b) odd, respectively. I_0 and Φ_0 are defined in the text.

$$\overline{M} = \dots (M_b)^{T_j} (M_a)^{S_j} \dots (M_b)^{T_2} (M_a)^{S_2} (M_b)^{T_1} (M_a)^{S_1}, \quad (8)$$

where M_a (or M_b) is the matrix $M_{l+1,l}$ when ϵ_l equals ϵ_a (or ϵ_b).

According to the matrices theory, the m th power of the 2×2 unimodular matrix M_b can be simplified in the form as¹¹⁾

$$(M_b)^m = u_{m-1}(\chi)M_b - u_{m-2}(\chi)I, \quad (9)$$

where $\chi = \frac{\text{Tr}(M_b)}{2}$ ($\text{Tr}(M_b)$ is the trace of M_b), and I is the unit matrix. u_m is the m th Chebyshev polynomial of the second order. If $|\chi| \leq 1$, u_m can be written as

$$u_m = \sin(m+1)\theta / \sin \theta \quad (\theta = \arccos \chi). \quad (10)$$

For $m \geq 2$, if

$$\chi = \chi_g = \cos\left(\frac{g\pi}{m}\right), g = 1, 2, \dots, m-1, \quad (11)$$

it can be readily obtained from eq. (10) that $u_{m-1}(\chi_g) = 0$ and $u_{m-2}(\chi_g) = (-1)^{g+1}$. Then eq. (9) turns to

$$(M_b)^m = (-1)^g I. \quad (12)$$

Based on the definition of χ , the energy corresponding to χ_g in eq. (11) is

$$E_g = \epsilon_b + 2V \cos(g\pi/m), g = 1, 2, \dots, m-1. \quad (13)$$

From eqs. (8)–(13), we can see that if the electronic energy satisfies $E = E_g$, the global transfer matrix \overline{M} is the product of matrices M_a and $(-1)^g I$. On these resonant energies $E = E_g$, the cluster composed of atom b does not affect the amplitude of the electronic wavefunction (sometimes it causes phase shift with π), and the RD ring looks like the system only made up of atom a (i.e., an ordered ring). Since T_j (the number of atom b in the j th cluster) is even in the RD mesoscopic ring, the resonant energy for the whole mesoscopic RD ring is $E_g = \epsilon_b$ according to eq. (13). It should be noted that the resonant energy is allowed only when $|\epsilon_a - \epsilon_b| \leq 2V$ is satisfied. The reason is that E is the energy of the remaining ordered chain composed of atom a , so it must meet the equation $E - \epsilon_a = 2V \cos k$, where k is the wave vector. Consequently the energy band should be in

the range of $[-2V + \epsilon_a, 2V + \epsilon_a]$. Thereafter, the allowed resonant energy must locate in the interval $[-2V + \epsilon_a, 2V + \epsilon_a]$, that is, $|\epsilon_a - E_g| \leq 2V$. Obviously, in the case of random-dimer model, the resonant energy is restricted by $|\epsilon_a - \epsilon_b| \leq 2V$, which is in agreement with the result of Dunlap *et al.*³⁾

Concerning the effect of the disorder on the persistent current in 1D flux-threaded mesoscopic rings, the commonly accepted standpoint is that the disorder always strongly suppresses the persistent current.^{33–35)} This property can be explained qualitatively based on the energy spectrum of electrons. For a free-electron model, the n th eigenenergy is $E_n = -\frac{\hbar^2}{2m} [\frac{2\pi}{N} (n + \frac{\Phi}{\Phi_0})]^2$ with $n = 0, \pm 1, \pm 2, \dots$. The energy curves versus flux $\frac{\Phi}{\Phi_0}$ form intersecting parabolas. Similar to the perturbation theory in the band-structure problem, the presence of disorder gives rise to the gap in the energy level at the intersection point (i.e., at $\frac{\Phi}{\Phi_0} = 0$ and ± 0.5) and the energy level repels each other. With the strength of disorder increasing, the ensuing level repulsion enhances and the flux-dependent energy level becomes much smoother. From eq. (4), the persistent current is proportional to the slope of the flux-dependent energy level. Therefore, the persistent current is intensively reduced by the disorder.

However, the above point can not be held at the resonant energies in the RD mesoscopic ring, despite the existence of site-diagonal disorders. At the resonant energy level, the global transfer matrix is the product of matrices M_a and $\pm I$, that is, the ring recovers the ordered ring that only consists of a . Naturally it is expected that the persistent current should be similar to the free-electron-like case. While at the off-resonant energy level, the persistent current decreases because the electron is scattered by the impurity b .

The above analysis can be verified by the numerical calculation on the persistent current in the 1D random-dimer mesoscopic ring. The following parameters are taken in our calculation: $N = 400$, $V = 1.0$, $\epsilon_a = -\epsilon_b = 0.4$, and the ratio of the total number of atom a and b in the ring is set to be $q = \sum S_j / \sum T_j = 1$, which corresponds to the most disordered case. Based on eq. (3), the flux-dependent eigenenergy can be obtained. Figure 2(a) plots the energy

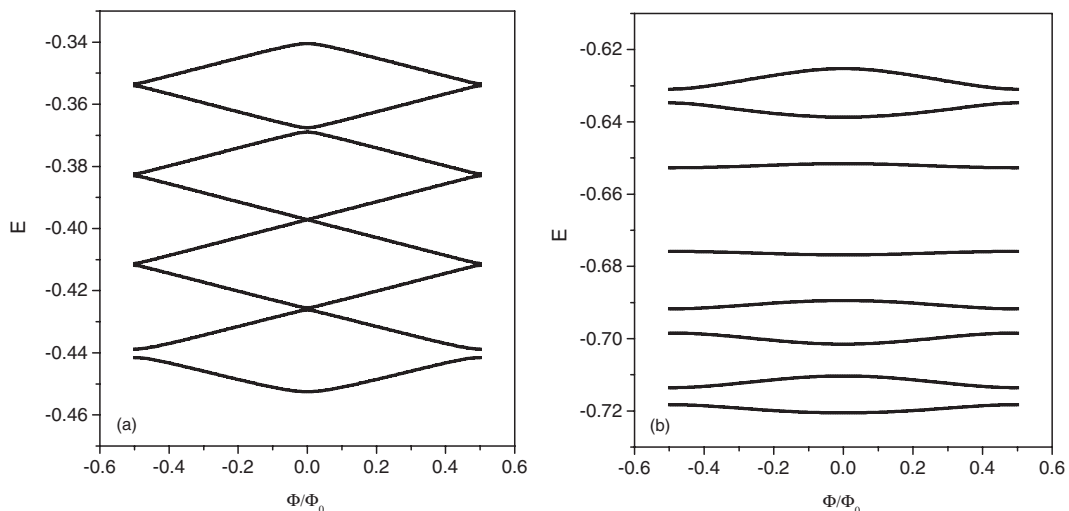


Fig. 2. The flux-dependent energy level of the 1D random-dimer mesoscopic ring, where $N = 400$, $V = 1.0$ and $\epsilon_a = -\epsilon_b = 0.4$. (a) Near the resonant energy $E = \epsilon_b = -0.4$; (b) Away from the resonant energy.

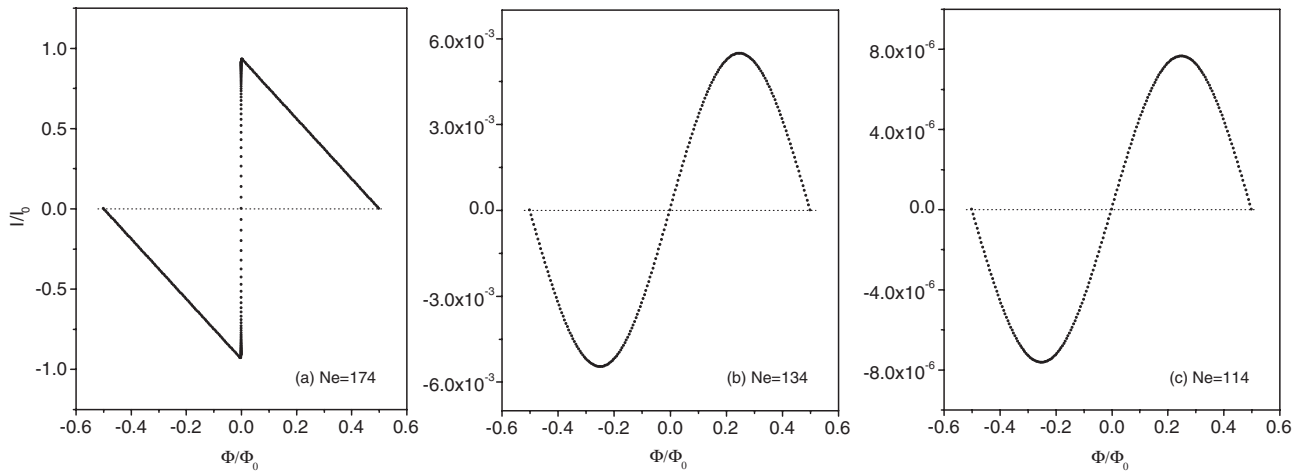


Fig. 3. The persistent current in the 1D random-dimer mesoscopic ring with the same parameters as Fig. 2. (a) Large persistent current when $N_e = 174$ ($E = -0.4112192 \rightarrow -0.3971527$), similar to that in ordered rings as demonstrated in Fig. 1(a); (b) Suppressed persistent current when $N_e = 134$ ($E = -0.9708473 \rightarrow -0.9705472$); (c) Infinitesimal persistent current when $N_e = 114$ ($E = -1.2035892 \rightarrow -1.2035889$).

levels which are near the resonant energy $E = \epsilon_b = -0.4$, and Fig. 2(b) shows the flux-dependent eigenenergy which is far away from the resonant energy. It is easy to find that in the vicinity of the resonant energy, the energy level has narrow gaps at $\frac{\Phi}{\Phi_0} = 0$ and $\frac{\Phi}{\Phi_0} = \pm 0.5$ [shown in Fig. 2(a)], which is quite similar to that in the ordered ring. However, the energy level shows large gaps and is much smoother if the energy deviates from the resonant energy [shown in Fig. 2(b)]. Then the persistent current is obtained by calculating the slope of the energy level according to eqs. (4) and (5). Figure 3(a) presents the total persistent current when the Fermi level is closest to the resonant energy $E = \epsilon_b = -0.4$. It is shown that the current is quite large ($I/I_{0max} \simeq 0.931$, almost without suppression), although the disorder exists in the system. Compared with Fig. 1(a), it is obvious that the persistent current in this case is very similar to that of the free electrons. Here, the electron-filling number $N_e = 174$. Actually, if the parameters of the RD ring, such as the length of the ring and site energy, are changed, the Fermi level may coincide with the resonant energy for odd N_e . Thus almost unreduced persistent current similar to Fig. 1(b) can also be found in the RD ring. On the contrary, if the Fermi level occupies the off-resonant energy, the persistent current will be significantly reduced and becomes a “sinusoidal” function of the flux. Only in this case, it follows the general theory that disorder always reduces the persistent current. Figures 3(b) and 3(c) illustrate the significantly depressed PC with different magnitudes.

Combining eq. (2) with the initial condition $C_0 = 0$ and $C_1 = 1$, it is straightforward to obtain the amplitude of the electronic wavefunction on each site of the ring. Figures 4(a)–4(c) are the wavefunction on the Fermi level corresponding to the different highest-occupied electrons in Figs. 3(a)–3(c), where $\Phi/\Phi_0 = 0.25$. In Fig. 4(a), the Fermi energy is closest to the resonant energy $E = \epsilon_b = -0.4$, and the wavefunction is extended. Though it is not Bloch-wave-like, it propagates through the whole ring without decay. Figures 4(b) and 4(c) show intermediated and localized wavefunctions, respectively, when Fermi level deviates from the resonant energy. Considering Figs. 3(a)–3(c) together

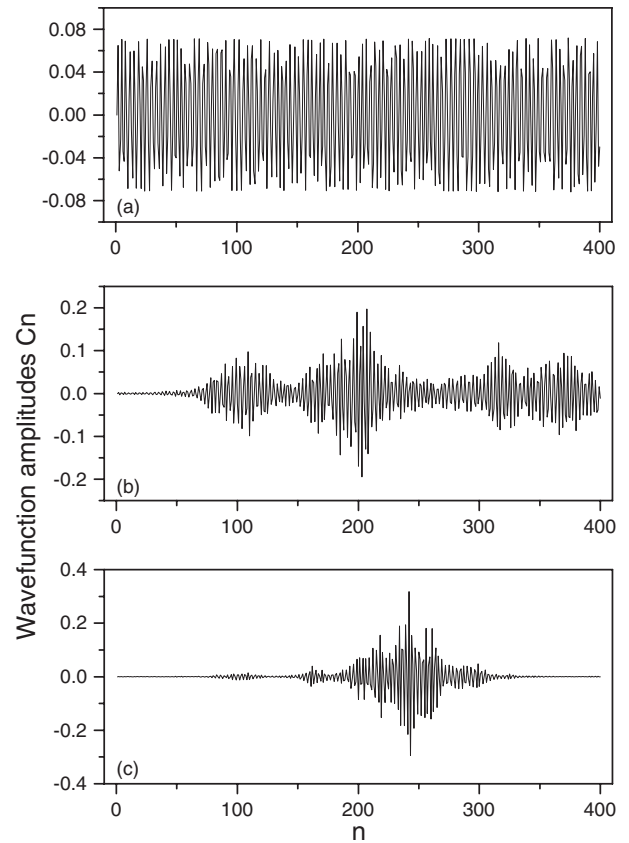


Fig. 4. The wavefunction amplitudes on the Fermi level corresponding to the cases in Figs. 3(a)–3(c), respectively, where $\Phi/\Phi_0 = 0.25$. The highest-occupied electronic state is (a) extended when $N_e = 174$ and $E = -0.4043449650423$, (b) intermediated when $N_e = 134$ and $E = -0.9706918941286$, and (c) localized when $N_e = 114$ and $E = -1.2035890660313$.

with Figs. 4(a)–4(c), it is reasonable to deduce that the highest-occupied electronic state determines the magnitude of the total persistent current $I(\Phi)$, though $I(\Phi)$ is contributed by all of the filled electrons [see eq. (5)]. Actually, we have compared the current contributed by the highest occupied level $I_{N_e}(\Phi)$ with the total current $I(\Phi)$ for

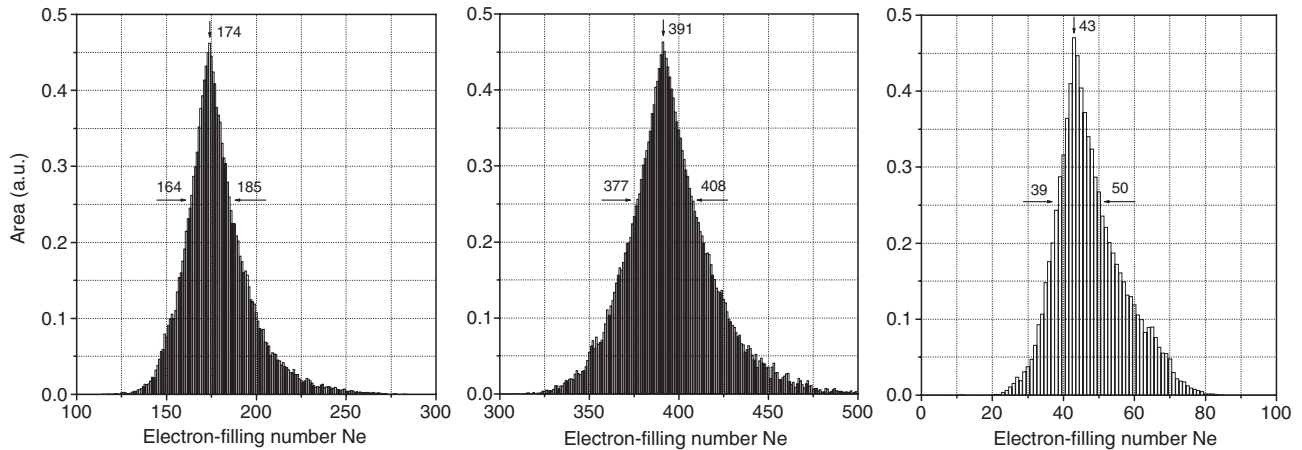


Fig. 5. The area enclosed by the curve of the total persistent current vs flux for various N_e in the RD rings, where $V = 1.0$, $\epsilon_a = -\epsilon_b = 0.4$. (a) $N = 400$, (b) $N = 900$, and (c) $N = 100$, respectively.

different electron-filling number N_e , and it is found that $I_{N_e}(\Phi)$ is the dominant factor determining the magnitude of $I(\Phi)$. The reason is that the current contribution from the levels of n and $n + 1$ ($n < N_e$ and $N_e \gg 1$) counteracts each other due to the opposite sign. Therefore, a general conclusion may be reached that in a 1D random-dimer mesoscopic ring, if there is the extended electronic state at the Fermi level, the persistent current is almost not suppressed and shows the free-electron-like behavior, in spite of the presence of disorder; while if the electronic state is intermediated or localized at the Fermi level, the current is significantly decreased. This conclusion could be generalized to any other systems possessing electronic delocalization.

It is worthwhile to show the overall behavior of the persistent current in the 1D random-dimer mesoscopic ring. In Fig. 5(a), we plot the area enclosed by the curve of the total persistent current vs flux as illustrated in Fig. 3 for different electron-filling number N_e . The result shown here is averaged over 100 samples with the same parameter as Fig. 3 in order to eliminate sample-dependent effect. In the case of ordered rings, the total area is 0.5 for arbitrary N_e . It is found that the area possesses maximum in the case of $N_e = 174$, that is, when the Fermi energy is closest to the resonant energy $E = \epsilon_b$. Then the area decays if the Fermi level deviates from the resonant energy. However, the area has relatively large magnitude in an interval around $E = \epsilon_b$. In fact, this property is related to the presence of extended states in the vicinity of the resonant energy in the random-dimer model. Dunlap *et al.* argued that around the resonant energy, there are \sqrt{N} unscattered states in the RD model with N sites.^{3,4} The authors of refs. 7–10 have confirmed the existence of delocalization in RD models and further claimed the number of extended states is $C\sqrt{N}$ (Dunlap *et al.* believed $C = 1$). However, Gangopadhyay and Sen found that the number of ballistic state is proportional to $N^{1/3}$ in large dimer chains.⁶ In our case, it has been shown that the highest-occupied electronic state determines the magnitude of the total persistent currents in 1D mesoscopic RD rings. It is naturally expected that the area enclosed by the curve of the total PC can be used as an index of the delocalization of the states in the system. Actually, if we set half-decay (i.e., when the area is 0.25) as the scale, the

number of cases where the area exceeds 0.25 is equal to 22, because the allowed N_e ranges from 164 to 185. This property is in agreement with the conclusion made by Dunlap *et al.* that there are \sqrt{N} , i.e., 20 (here $N = 400$) extended states in the RD model. In order to demonstrate that the \sqrt{N} rule is independent of the system sizes, we perform the similar calculation on the RD rings with $N = 900$ and $N = 100$ [as shown in Figs. 5(b) and 5(c), respectively]. According to the above scale, the number of extended states in the two cases is 32 and 12, respectively. The results obtained in the three RD rings with different length have matched well with the \sqrt{N} scale law. It can be expected that the \sqrt{N} rule will fit better in the system with larger size. Hence, \sqrt{N} unscattered states indeed exist around the resonant energy in the RD model from a completely new viewpoint of the persistent current.

A long-standing puzzle in mesoscopic physics is the large measured persistent current reported in ref. 21. The amplitude of the oscillatory component corresponds to the persistent current $I \simeq (0.3-2.0)ev_F/L$, which is one or two magnitude larger than the prediction of the noninteracting theory. It is well known that for a metallic ring with impurity, the magnitude of the persistent current $I \simeq I_0/l/L = (ev_F/L)l/L = e/\tau_D$, where l is the elastic mean free path, v_F is the electron Fermi velocity and $\tau_D = L^2/D$ is the time required for an electron to diffuse a ring whose perimeter is L ($D = v_F l$ is the diffusion constant). By estimating the mean free path l of Au, the theoretical value of the persistent current should be about $0.01ev_F/L$, which contradicts the measured current remarkably. Kirczenow²² and Ben-Jacob *et al.*²³ once respectively proposed the theoretical model considering grain boundaries, and all of them have obtained the same order of magnitude of persistent currents as observed experimentally. Anyway, it is interesting to discuss this problem from the viewpoint of the electronic delocalization. As we have seen in the above discussion on the 1D random-dimer mesoscopic ring, though the disorder exists in the system, the PC is indeed possible to be the order of I_0 ($I_0 = ev_F/L$) due to the electronic delocalization around the resonant energy. In fact, the mean free path l is very close to the localization length in 1D system. If the Fermi level locates in the vicinity of the resonant energy, the mean free path l is comparable with L ,

that is, $l \ll L$ for 1D disordered system is no longer valid under this case. Therefore we obtain the large PC with the same magnitude of I_0 . It might be possible that “the resonant transport” causes the persistent current $I \simeq (0.3-2.0)e v_F/L$ in the experiment of Chandrasekhar *et al.* The resonant transport may originate from the specific distribution of disorder in the ring and the chemical potential of the material. This assumption deserves the further confirmation in experiments.

In summary, we have investigated the persistent current in 1D random-dimer mesoscopic rings threaded by a magnetic flux. Contrary to the general viewpoint that disorder always reduces the persistent current, it is found that in the random-dimer ring, nearly unsuppressed currents can exist if the Fermi level is at the resonant energy, where the electronic state is extended; while the current is suppressed by the disorder as expected if Fermi level deviates from the resonant energy, where the electronic state is intermediated or localized. Around the resonant energy, large persistent currents preserve. Correspondingly, the area enclosed by the PC curve has large amplitude. We have also confirmed the \sqrt{N} law of the number of extended states in the 1D random-dimer system. The property that the persistent current is nearly unsuppressed due to the electronic delocalization in RD mesoscopic rings provides a possible explanation to the anomalously large measured current in the isolated Au ring.²¹⁾ The theoretical calculation of the persistent current in this paper, from a new point of view, presents further understanding of the electronic localization and delocalization in the random-dimer model. It is expected that, with the development of the fabrication technique, observing the persistent current in 1D flux-threaded mesoscopic rings could be one effective tool to explore the nature of electronic states since the persistent current is quite sensitive to the electronic state. Furthermore, because of the drastic transition of the persistent current when the Fermi energy is changed, it is possible to use the 1D random-dimer mesoscopic ring as quantum-switch devices.

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