Eur. Phys. J. B **25**, 497–503 (2002)
DOI: 10.1140/epjb/e20020055

THE EUROPEAN PHYSICAL JOURNAL B
EDP Sciences

Persistent currents in one-dimensional aperiodic mesoscopic rings

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Received 22 January 2001 and Received in final form 25 October 2001

Abstract. In the tight-binding approximation, we have investigated the behaviour of persistent currents in a one-dimensional Thue-Morse mesoscopic ring threaded by a magnetic flux. By applying a transfer-matrix technique, the energy spectra and the persistent currents in the system have been numerically calculated. It is shown that the flux-dependent eigenenergies form “band” structures and the energy gaps will enlarge if the site energy increases. Actually, the site energy and the filling-up number of electrons are two important factors which have much influence upon the persistent current. Increment of the site energy in the system will lead to a dramatic suppression of the currents. When the highest-occupied energy level is on the top of the band, the total current is limited; otherwise, the persistent current increases by several orders of magnitude. Generally, this kind of large scale change in the magnitude of the current can easily be observed in the vicinity of band gaps. The parity effect in the Thue-Morse ring is also discussed.

PACS. 73.23.Ra Persistent currents – 61.44.Br Quasicrystals

1 Introduction

With the development of technology for the fabrication of submicrometer devices, mesoscopic systems have attracted much attention in the past 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 distinguishing features of quantum interference. Although this phenomenon was predicted by Büttiker *et al.* [1] a long time ago, and there has been a lot of theoretical and experimental work [2–5] performed, the problem is still not well understood. For example, the currents measured by experiments are much larger than the theoretical expectations [2,3].

The disorder of the system and the electron-electron interaction are supposed to be the two important factors affecting the persistent current [6,7]. It has been shown that the short-range Coulomb repulsion enhances the amplitude of PC in the system of spinless fermions [8,9]. In order to clarify the large PC discrepancy between the theory and the experiment, more realistic systems, such as the spinful system and also two- and three-dimensional models, have been taken into account [11–14]. In addition, the importance of many-channel-effect and geometrical influence are recently reported [15,16]. However, previous studies concentrate most on either periodic or disordered systems. Only a few studies [17] are based on the structure between periodic and disordered ones.

It is well known that the Thue-Morse (TM) structure is a typical example in a one-dimensional (1D) aperiodic system [18]. Theoretical studies show that a TM lattice has a singular continuous Fourier spectrum [19,20], Cantor-like energy spectrum [19] and phonon behaviour [21]. The property of TM lattice may be in between that of a periodic and a quasiperiodic lattice [22,23]. Experimentally, since the first realization of Fibonacci superlattices by Merlin *et al.* [24], much attention has been paid to the exotic wave phenomena in Fibonacci systems. A TM superlattice, at the same time, has also been fabricated and investigated by Raman scattering [25] and by X-ray diffraction [26]. In principle a mesoscopic ring with TM structure can be achieved experimentally. In this paper, we investigate the behaviour of persistent current in a 1D TM mesoscopic ring. Our calculations provide detailed information about the structural influence on currents.

2 Theoretical model

The Thue-Morse sequence can be obtained by the substitution rule $A \rightarrow AB$ and $B \rightarrow BA$ with the initial generation $S_1 = \{AB\}$. For example, $S_4 = \{ABBABAABBAABABBA\}$. In general, the jth generation of TM lattice consists of 2^{j-1} A and B units, respectively. Here the TM mesoscopic ring is constructed

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by a finite TM sequence with N sites, where the site energy is $v_{\rm A}$ or $v_{\rm B}$, respectively. Obviously $N = F_j$ holds, where $F_j = 2^j$ is the TM number. Considering the tight-binding approximation with on-site model, the Schrödinger equation for an electron in a 1D aperiodic mesoscopic ring can be written as [17]

$$t\psi_{l+1} + t\psi_{l-1} + v_l\psi_l = E\psi_l, \tag{1}$$

where l is the site index, the site energy $v_l = v_{\rm A}$ (or $v_{\rm B}$) if the lth atom is A (or B), and t is the hopping integral. In this on-site model, we can choose $v_{\rm A} = -v_{\rm B} = v$ and $t = -1$ without loss of generality. Equation (1) can 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

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

A magnetic flux Φ threaded through the ring will lead to the twisted boundary conditions for the wave functions of the electrons [1], hence the equation for the global transfer matrix takes the form

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = M_j \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = {\rm e}^{{\rm i}2\pi\Phi/\Phi_0} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{3}$$

where $\Phi_0 = hc/e$ is the flux quantum and $M_j = \prod_{l=1}^{N} T_{l+1,l}$.

By denoting $\chi_j = \frac{1}{2}{\rm tr}M_j$, the flux-dependent energy spectra of an electron in the mesoscopic ring can be obtained from

$$\chi_j = \cos(2\pi\Phi/\Phi_0). \tag{4}$$

The trace map of TM lattice [27] follows

$$\chi_{j+1} = 4\chi_{j-1}^2(\chi_j - 1) + 1, \tag{5}$$

and the initial conditions have the form

$$\chi_1 = \left(E - v^2\right)/2 - 1,\ \chi_2 = \left(E - v^2\right)^2/2 - 2E^2 + 1.$$

Here we do not distinguish $v_{\rm A}$ and $v_{\rm B}$ since $v_{\rm A}^2 = v_{\rm B}^2$ under the condition $v_{\rm A} = -v_{\rm B} = v$.

The persistent current in the ring can be achieved by

$$I = -c\frac{\partial}{\partial\Phi}E(\Phi). \tag{6}$$

For an individual energy level, the contribution to the persistent current is

$$\begin{aligned} I_n(\Phi) &= -c\frac{\partial E_n(\Phi)}{\partial\Phi} = -c\frac{\partial E_n}{\partial\chi_j}\frac{\partial\chi_j}{\partial\Phi} \\ &= \frac{2\pi c}{\Phi_0}\frac{\sin(2\pi\Phi/\Phi_0)}{\partial\chi_j/\partial E_n}. \end{aligned} \tag{7}$$

From the trace map of TM lattice, $\partial\chi_j/\partial E_n$ can be obtained recursively as

$$\frac{\partial\chi_{j+1}}{\partial E} = 4\chi_{j-1}^2\frac{\partial\chi_j}{\partial E} + 8\chi_{j-1}\frac{\partial\chi_{j-1}}{\partial E}(\chi_j - 1) \tag{8}$$

with the initial conditions

$$\frac{\partial\chi_1}{\partial E} = E, \qquad \frac{\partial\chi_2}{\partial E} = 2E(E^2 - v^2) - 4E.$$

At zero temperature, the number of electrons in the spinless fermion system $N_{\rm e}$ equals the highest-occupied level labeled by the index m. So the energy of the system follows

$$E(\Phi) = \sum_{n=1}^{m} E_n(\Phi), \tag{9}$$

and the total persistent current in the system satisfies

$$I = \sum_{n=1}^{m} I_n(\Phi) = \frac{2\pi c}{\Phi_0}\sum_{n=1}^{m}\frac{\sin(2\pi\Phi/\Phi_0)}{\partial\chi_j/\partial E_n}. \tag{10}$$

3 Results and discussion

It is easy to understand that the properties of the persistent currents are ultimately determined by the flux-dependent energy of the system. Therefore we first consider the energy spectra of the TM mesoscopic rings threaded by a magnetic flux Φ. Based on equations (4, 5) and (9), we carry out numerical calculations on the energy spectra. Figures 1a and b give the flux-dependent energy spectra for $v = 0.1$ and $v = 0.5$ respectively in the TM ring with $j = 7$ ($N = 128$). The electron eigenenergies form a "band" structure. When the on-site energy v increases, the energy gap enlarges accordingly, as it happens in other system [19]. This feature becomes much clearer in Figures 1c and d, where the details of the energy spectra are shown. The parameter v represents the on-site energy of the electrons. In our case in order to simplify the calculation, we choose v_A and v_B for the two building units A and B, respectively, which have the same absolute value and are opposite in sign, *i.e.* $v_A = v$ and $v_B = -v$. Therefore, in some sense, the quantity v represents the strength of non-periodicity. Here we discuss a spinless fermion system with tight-binding approximation, which means that each electron occupies only a single energy level. When the aperiodic strength of the structure v increases, the dependence of the energy levels on the flux is deformed and smoothed as shown in Figures 1c and d, which is similar to the influence of disorder on the energy levels reported by Kusmartsev [28]. This explains why the energy levels split into groups and the energy gaps enlarge when v increases (also see Figs. 1e and f). Certainly this feature will eventually affect the behaviour of the persistent currents. Figures 1e and f show the energy eigenvalues of the corresponding systems when the magnetic flux is kept at $\Phi/\Phi_0 = 0.3$, and $v = 0.1$ and $v = 0.5$, respectively. The difference of the neighbouring energy levels

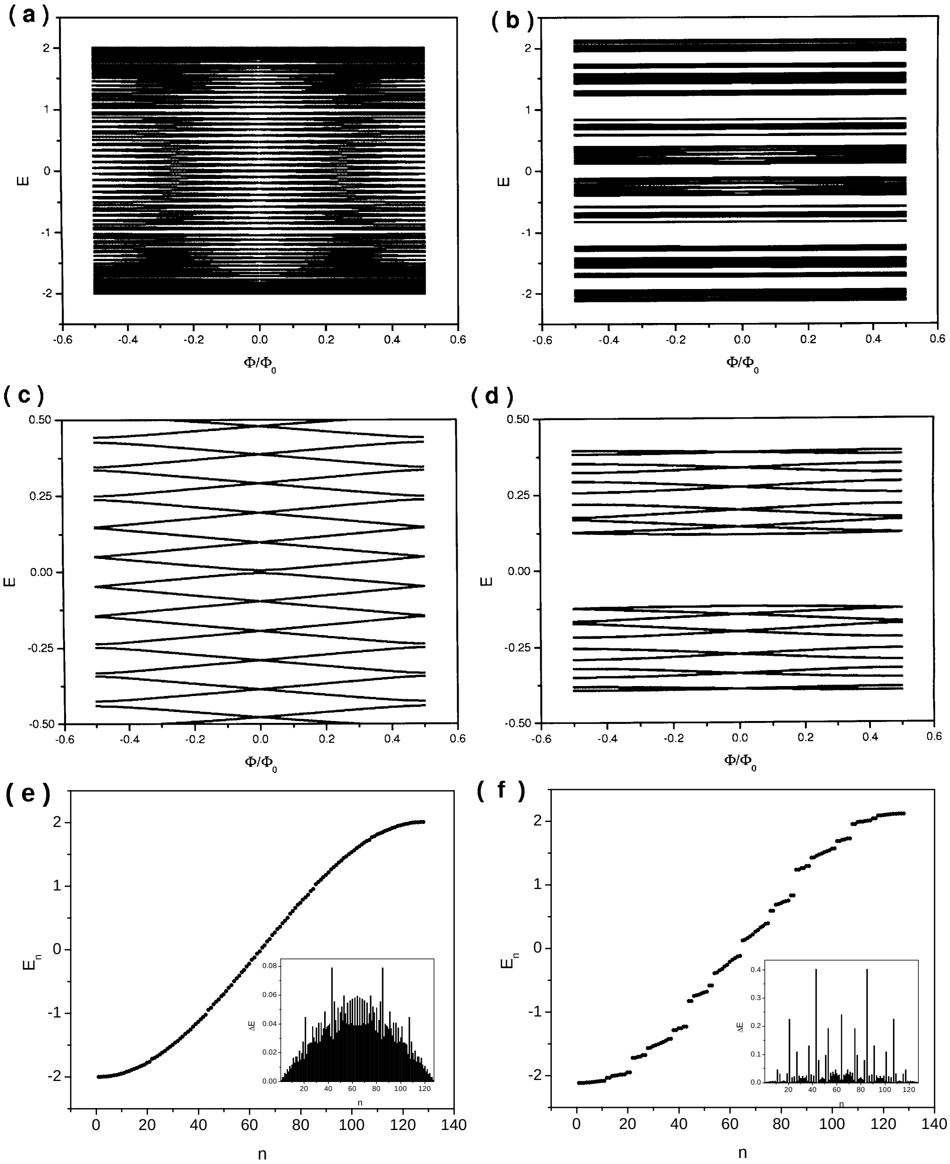

Fig. 1. The flux-dependent energy spectra in a mesoscopic Thue-Morse ring: (a) and (b) show the spectra for $-1/2 < \Phi/\Phi_0 < 1/2$ with different on-site energy v: (a) $v = 0.1$, (b) $v = 0.5$. (c) and (d) show the details of the spectra (a) and (b), which demonstrates the deforming and smoothing of energy-flux dependence caused by non-periodicity of the structure. While (e) and (f) show the energy eigenvalues for $\Phi/\Phi_0 = -0.3$ with different v: (e) $v = 0.1$, (f) $v = 0.5$. The inserts give the difference between the neighbouring energy levels.

in the case of $v = 0.5$ is one order of magnitude larger than that in the case of $v = 0.1$. Unlike the Fibonacci structure, here the flux-dependent energy spectra do not exhibit apparent self-similarity; actually it is symmetric. The origin of the symmetric nature can be traced back to the property of the transfer matrix of the TM structure. If we transform energy from E to $-E$, the transfer matrix will be changed accordingly following $T_{AB} \to -T_{BA}$ and $T_{BA} \to -T_{AB}$. Then it can be proven that the trace map of $M_j = \prod_l T_{l+1,l}$ is unchanged. Therefore the energy spectra should be symmetric.

The persistent current in a Thue-Morse mesoscopic ring can be obtained from equations (7, 8) and (10). The calculations indicate that the persistent current is dominated by two important factors. One is the filling the number of electrons in the system, and the other is the site energy. Figures 2a and b demonstrate the behaviour of persistent currents for different filling-up numbers and for different site energies ($v = 0.1$ and 0.5, respectively). We are particularly interested in the properties near the edge of large energy gaps. The insets of Figures 1e and f illustrate that there is a big gap between the 84th and the 85th levels. Figure 2a plots the persistent current I against the magnetic flux Φ/Φ_0 when the number of electrons varies from $n = 84$ to $n = 86$ at $v = 0.1$. The magnitude of the current is dramatically suppressed when

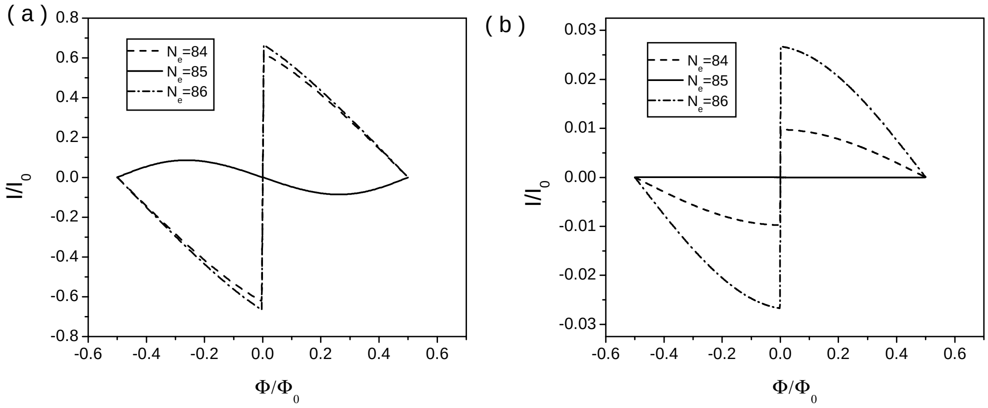

Fig. 2. The persistent current I *vs.* flux Φ for various filling-up number of electrons $N_{\rm e}$: (a) $v = 0.1$, (b) $v = 0.5$.

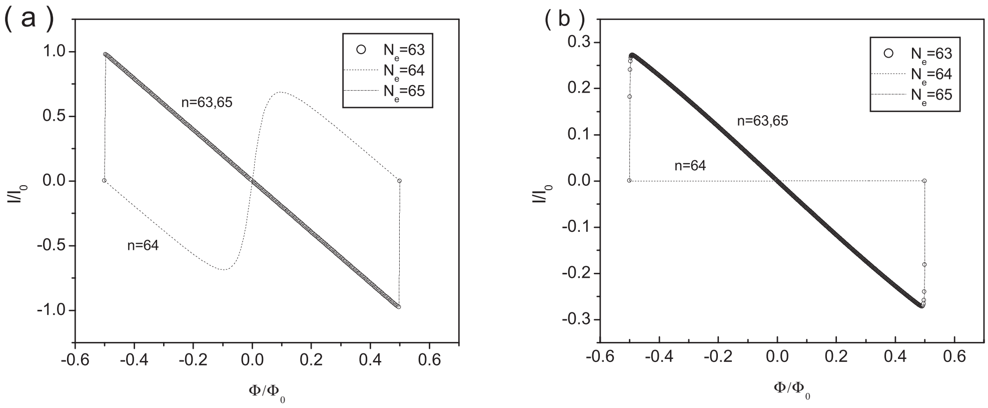

Fig. 3. The persistent current I *vs.* flux Φ for various filling-up numbers of electrons at half-filling case: (a) $v = 0.1$, (b) $v = 0.5$.

the filling number of electrons is $n = 85$. When v becomes larger, for example, $v = 0.5$ (Fig. 2b), the suppression of the currents becomes more evident. Actually the current decreases by four orders of magnitude when comparing the cases of $n = 84$ or 86. Generally, when the electrons in the system are filled just up to the "top" of a band, the current is strongly limited, otherwise the current in the system becomes fairly large. However, an exception happens in the case of half-filling, as shown in Figures 3a and b. Meanwhile as v becomes larger, the current drops dramatically when the number of electrons equals 64 ($n = 64$). The physical origin of this feature remains unclear.

The persistent current in the aperiodic ring is also determined by the site energy in the system. Figure 4 gives the persistent currents for different values of v. It is evident that for a system with fixed electron number, the increment of v always suppresses the magnitude of the current. The similar characteristics on the conductance have been discussed by Avishai and Berend [29]. It can be understood from the following two aspects. On one hand, when the potential strength in the ring increases, the scattering rate is enhanced, hence the current must decrease. On the other hand, increasing v means that the non-periodicity of the structure becomes stronger, then the dependence of energy level on the flux becomes smoother as was mentioned above. Therefore the current contribution coming from these energy levels will decrease according to equation (7). Consequently the total currents will decrease. If the number of electrons changes in the system, the behaviour of the currents will be much complicated. It is interesting to note that when the electrons are filled up to the edge of a large energy gap, a slight increment of the site energy will decrease the persistent current dramatically. In some case the change of currents $\Delta I(v)$ can be as high as one order of magnitude (as shown in Fig. 4a). On the other hand, due to the fact that the contributions to the current from the nearby two energy levels are opposite in sign, the change of currents $\Delta I(v)$ in the system with an even number of electrons is much less than that with an odd number of electrons. This feature can easily be seen by comparing Figure 4a ($N_{\rm e} = 43$)) and Figure 4b ($N_{\rm e} = 44$), as well as Figure 4c ($N_{\rm e} = 7$) and Figure 4d ($N_{\rm e} = 6$). However, an exception exists in the case of half-filling (as shown in Figs. 5a and b). Unlike the other cases, the systems with $N_{\rm e} = 64$ (even electrons) and with $N_{\rm e} = 63$ (odd electrons) have dramatically decreased current.

It can be inferred from Figure 4 that the parity effect is an important feature of persistent current in a mesoscopic ring. Kusmartsev *et al.* [30] have discussed the parity effect in the interacting fermion systems and in the spinful

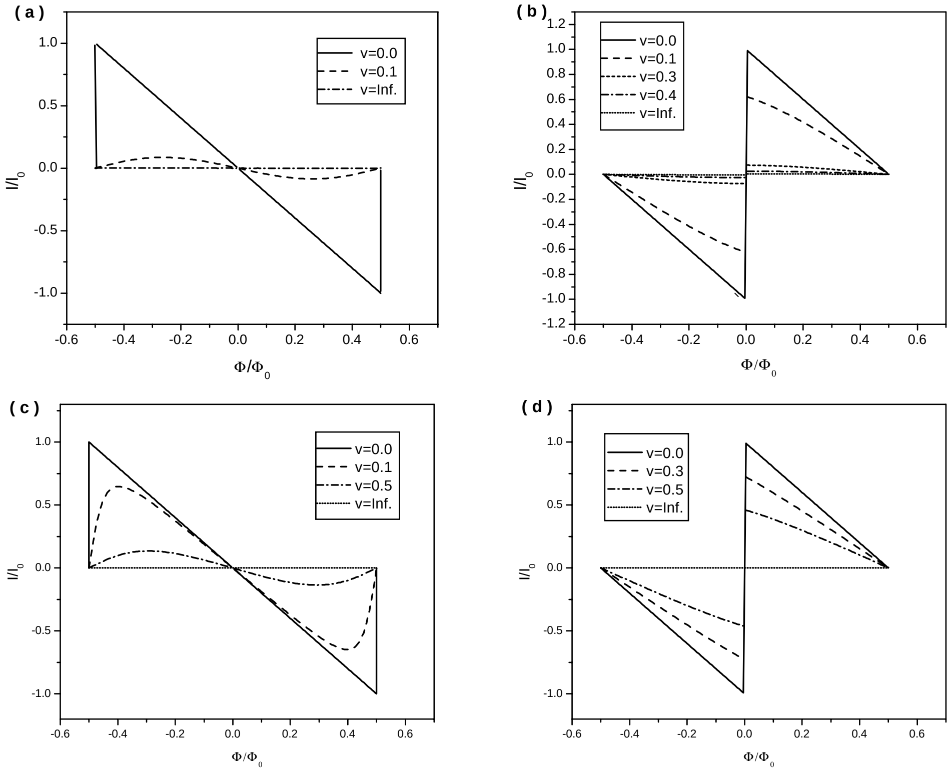

Fig. 4. The persistent current I *vs.* flux Φ for various on-site energies v: (a) $N_{\mathrm{e}} = 43$, (b) $N_{\mathrm{e}} = 44$, (c) $N_{\mathrm{e}} = 7$, (d) $N_{\mathrm{e}} = 6$.

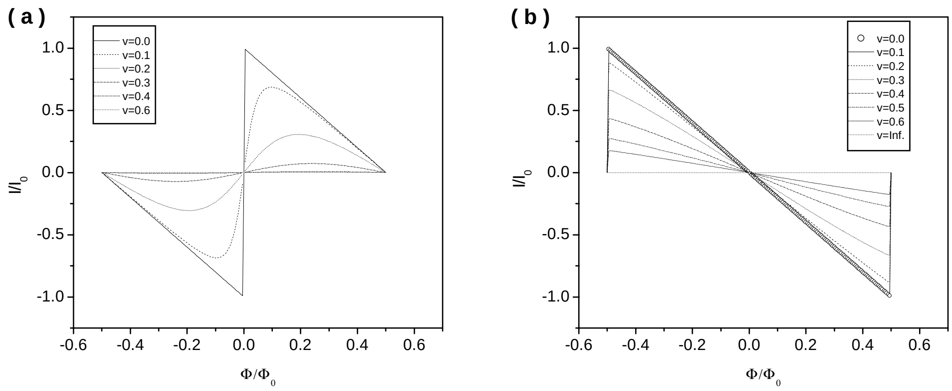

Fig. 5. The persistent current I *vs.* flux Φ for various on-site energies at half-filling case: (a) $N_{\mathrm{e}} = 64$, (b) $N_{\mathrm{e}} = 63$.

systems. For a TM mesoscopic ring, there are three interesting features related to the parity effect. First, in a system with odd electrons, the flux-dependent persistent current (shown in Figs. 4a or 4c) behaves like a diamagnet, whereas in the system with even electrons, the dependence of currents on magnetic flux (shown in Figs. 4b or 4d) is like a paramagnet. This type of parity effect in the TM ring is similar to the results in the disordered ring [30] and in the Fibonacci structure [17]. But in our case, there exits a difference, *i.e.*, the persistent currents depend linearly on the magnetic flux in the even-electron systems. Only in the half-filled case, the plot of the current *vs.* the flux is linear in an odd-electron system ($N_{\mathrm{e}} = 63$, to see Fig. 5b) and is a sine-function in an even-electron system ($N_{\mathrm{e}} = 64$, to see Fig. 5a) (in this case, the current shifts half a flux quantum compared with the non-half-filled cases). Second, if the electrons are filled just to the bottom of a big energy gap, a small increment of the site energy will lead to the significant suppression of the PC. Meanwhile if an electron is added or removed, the PC suppression will be kept but the current-flux dependence will shift a half flux quantum. If the electrons are not filled up to the bottom of big gaps, the PC will not change significantly by adding or removing an electron in the system. In other words, in this case the parity effect of electrons is not obvious. Third, the current is less sensitive to the

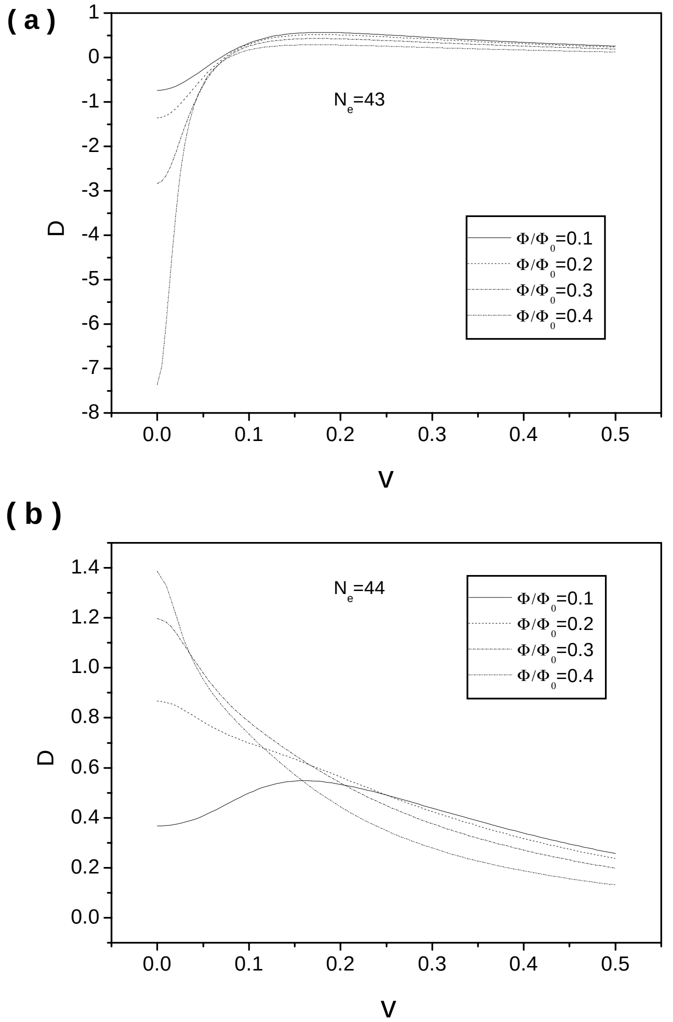

Fig. 6. The variation of the charge stiffness D with the on-site energy v when $\Phi/\Phi_0 = 0.1$, 0.2, 0.3, and 0.4, respectively.

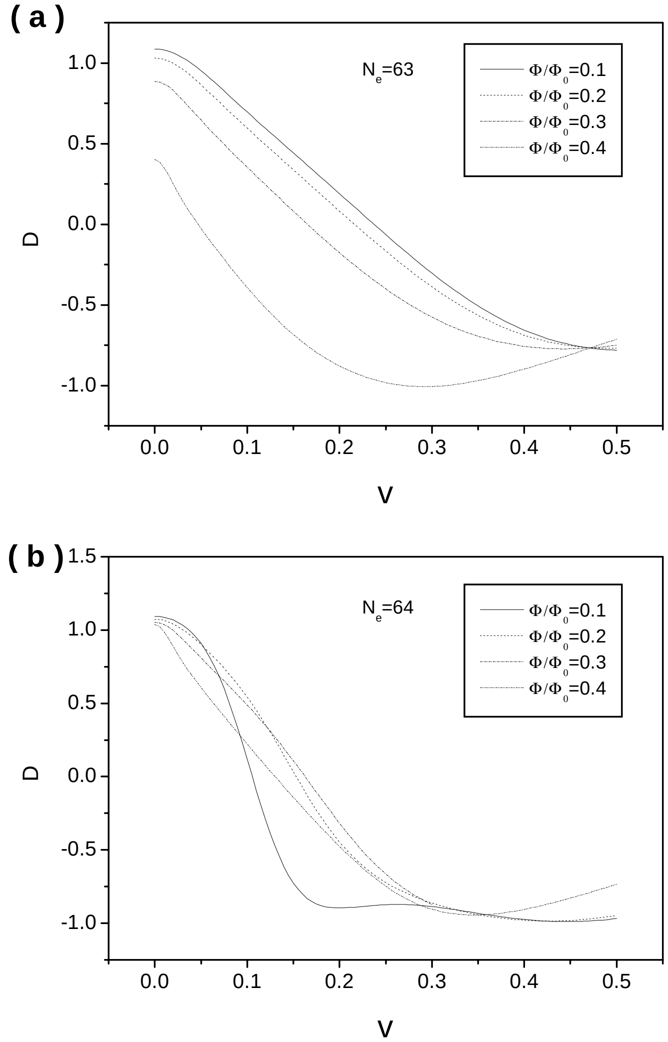

Fig. 7. The variation of the charge stiffness D with the on-site energy v at half-filling case when $\Phi/\Phi_0 = 0.1$, 0.2, 0.3, and 0.4, respectively.

change of the site energy when the number of electrons in the ring is even compared with the case of odd electrons, as demonstrated in Figures 4a and 4b.

In order to address the response of the persistent currents to the magnetic flux, the charge stiffness is also calculated. The charge stiffness is defined as

$$D = \frac{F_j}{4\pi^2} \frac{\partial^2 E(\Phi)}{\partial(\Phi/\Phi_0)^2} \cdot \tag{11}$$

To carry on the calculation, we use the second-order derivatives of the trace map

$$\frac{\partial^2 \chi_{j+1}}{\partial E^2} = 4\chi_{j-1}\left(4\chi_{j-1}\frac{\partial \chi_{j-1}}{\partial E}\frac{\partial \chi_j}{\partial E} + \chi_{j-1}\frac{\partial^2 \chi_j}{\partial E^2}\right) + 8(\chi_j - 1)\left(\frac{\partial \chi_{j-1}}{\partial E}\frac{\partial \chi_{j-1}}{\partial E} + \chi_{j-1}\frac{\partial^2 \chi_{j-1}}{\partial E^2}\right) \tag{12}$$

with

$$\frac{\partial^2 \chi_1}{\partial E^2} = 1, \quad \frac{\partial^2 \chi_2}{\partial E^2} = 2(E^2 - v^2) + 4E^2 - 4.$$

Figures 6a and b give the charge stiffness with different site energy, magnetic flux and number of electrons. Obviously, the charge stiffness is sensitive to the parity of electrons in the system. It is noteworthy that if the number of electrons is odd, there is a maximum in the curve. When v is larger than the "critical point", the persistent current becomes insensitive to the flux. If the number of electrons is even, the charge stiffness always goes down as the on-site energy v increases. The near-half-filling case (shown in Figs. 7a, b) is different from the situations presented above and seems rather complicated. An inflection point can be found when the external flux becomes sufficiently strong.

4 Summary

Based on a tight-binding model, we have studied the energy spectra and the persistent currents in one-dimensional Thue-Morse mesoscopic rings threaded by a magnetic flux Φ. It is shown that the electron eigenenergies $E(\Phi)$ form a "band" structure and the energy gaps will enhance if the site energy increases. Meanwhile, the persistent currents in the rings exhibit a rich structure, which depends on the number of electrons and the site energy. When the highest-filling band is just at the top of an energy band, the current is very limited. Otherwise the large current can be observed in the TM ring. The increment of site energies always diminishes the magnitude of the current in the system. The parity effect of electrons has been discussed in an aperiodic mesoscopic ring. Generally, the ring behaves as a diamagnet in the odd-electron system and as a paramagnet in the even-electron system. An exception can always be found in the half-filling case. The reason for this behaviour remains unclear.

This work was supported by grants from the National Nature Science Foundation of China and the State Key Program for Basic Research from the Ministry of Science and Technology of China. One of the authors (YL) thanks Dr. Xiangsong Chen for the help in the numerical calculation.

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