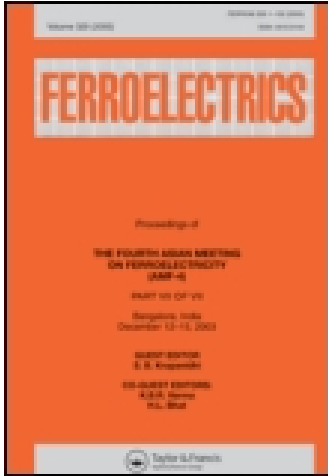


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Quantum Behavior in One-Dimensional Mesoscopic Thue-Morse Rings

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Using a tight-binding model, we have investigated the energy spectra and persistent currents in one-dimensional mesoscopic rings threaded with a magnetic flux ϕ . The mesoscopic ring is constructed by a Thue-Morse chain with N sites. By applying a transfer-matrix method, the flux-dependent energy spectra have been obtained. It is shown that the electron eigenenergies $E(\phi)$ gradually form "bands" as the disorder increases in the quantum system. Meanwhile, the persistent currents in the rings exhibit a rich structure, which depends on the number of electrons and the disorder of system. On the other hand, as increasing the disorder of system, the "bandwidths" are getting narrower in the energy spectra; thereafter the maximum persistent current decreases obviously in the rings. A metal-insulator transition can be easily found in the half-filled electron system.

Keywords: Thue-Morse; mesoscopic system; persistent currents

INTRODUCTION

Recently, the studies on domains have been extensively developed in many fields. In the mesoscopic systems, much attention has been paid to quantum interference phenomena related to domain walls and size

effects. One of the most attracting topics is the persistent current in one-dimensional metal or semiconductor mesoscopic rings threaded by magnetic flux^[1-6]. This phenomenon was predicted by Büttiker *et al.*^[1] in the 1980's. Later the experiments performed on both an ensemble of 10^7 Cu loops^[2] and single Au ring^[3] have confirmed their prediction, which have stimulated the extensive studies^[4-6]. But the question on the unexpectedly large magnitude of the measured currents is still open. It is shown that disorder and interaction play a very important role in the current amplitude^[5, 6]. For example, recently in the frame of Hubbard model, the strong electron-electron correlation is considered to explain the large magnitude of the observed persistent current^[7]. As to the disorder effect, most of the previous reports examined the behavior of periodic or disorder rings. However, as we know, only few studies^[8] are based on the structure between periodic and disorder case.

In this paper, we calculate the persistent currents in one-dimensional (1D) Thue-Morse (TM) ring. It is well known that the TM structure is aperiodic, in some sense, TM structure is an intermediate case between periodic and quasiperiodic structures^[9]. In the tight-binding approximation, we firstly give the basic formulas for the energy spectra and persistent currents in the TM ring threaded by a magnetic flux, the numerical results and discussions are then followed.

THE THEORETICAL MODEL

With two building units A and B, a TM chain can be formed according to the substitution rule $A \rightarrow AB$, $B \rightarrow BA$ and $S_1 = \{AB\}$. For example, the fourth generation of the TM lattice is expressed as $S_4 = \{ABBABAAB BAABABBA\}$. The k th-order TM lattice consists of 2^k atoms (A and B). Here a TM ring is constructed by finite TM chain with N site. A and B are considered as two kinds of site energies or hopping integrals. We suppose that $N = F_k$ where k is a generation number, and F_k is a TM number which obeying the relation $F_k = 2^k$. Considering an electron in a one-dimensional TM mesoscopic ring, we use the tight-binding approximation. The Schrödinger equation can be written as

$$t_{l+1}\psi_{l+1} + t_l\psi_{l-1} + v_l\psi_l = E\psi_l, \quad (1)$$

where l is the site index, t_l the hopping integral, and v_l the on-site energy. For simplicity, here the spin freedom is not taken into account. Without loss of generality, an on-site model is applied, i.e., t_l is taken to be constant as $t_l = -1$ and v_l is set to be v_A and v_B in the TM sequence. In the on-site model, Eq.(1) can be written as

$$t\Psi_{l+1} + t\Psi_{l-1} + v_l\Psi_l = E'\Psi_l, \tag{2}$$

where $v_A' = (v_A - v_B)/2 = -v_B'$ and $E' = E' - (v_A + v_B)/2$. The energy spectra of eq. (2) and eq. (1) are equal except for the origin of the coordinate. That means we can choose $v_A = -v_B = v$ without loss of generality. Then eq. (1) can be rewritten into a matrix form as

$$\begin{pmatrix} \Psi_{l+1} \\ \Psi_l \end{pmatrix} = \begin{pmatrix} -(E - v_l) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \Psi_l \\ \Psi_{l-1} \end{pmatrix}. \tag{3}$$

A magnetic flux ϕ threaded through the ring will lead to the twisted boundary conditions for the wave functions of the electrons in the ring. Then we have

$$\begin{pmatrix} \Psi_{N+1} \\ \Psi_N \end{pmatrix} = M_j \begin{pmatrix} \Psi_1 \\ \Psi_0 \end{pmatrix} = e^{i2\pi\phi/\phi_0} \begin{pmatrix} \Psi_1 \\ \Psi_0 \end{pmatrix}, \tag{4}$$

where $\phi_0 = hc/e$ is the flux quantum and $M_j = \prod_{l=1}^N T_{l+1,l}$.

Denoting $\chi_j = 1/2\text{tr}M_j$, so we have

$$\chi_j = \cos(2\pi\phi/\phi_0). \tag{5}$$

The trace map of TM lattice^[10] is

$$\chi_{j+1} = 4\chi_{j-1}(\chi_j - 1) + 1, \tag{6}$$

with the initial conditions

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

Here we do not separate v_A and v_B because $v_A^2=v_B^2$ under the condition of $v_A=-v_B$. The persistent current is defined as below:

$$I = -c \frac{\partial}{\partial \phi} E(\phi). \quad (7)$$

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

$$I_n = -c \frac{\partial}{\partial \phi} E_n(\phi) = -c \frac{\partial E_n}{\partial \chi_j} \frac{\partial \chi_j}{\partial \phi} = \frac{2\pi c}{\phi_0} \frac{\sin(2\pi\phi/\phi_0)}{\partial \chi_j / \partial E_n}. \quad (8)$$

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

$$\begin{aligned} \frac{\partial \chi_{j+1}}{\partial E} &= 4\chi_j^2 \frac{\partial \chi_j}{\partial E} + 8\chi_{j-1} \frac{\partial \chi_{j-1}}{\partial E} (\chi_j - 1), \\ \frac{\partial \chi_1}{\partial E} &= E, \\ \frac{\partial \chi_2}{\partial E} &= 2E(E^2 - v^2) - 4E. \end{aligned} \quad (9)$$

At zero temperature, the number of the electrons of the system N_e equals to the highest occupied-level index m , then the overall persistent current of the system is

$$I = \sum_{n=1}^m I_n(\phi) = -c \sum_{n=1}^m \frac{\partial E_n(\phi)}{\partial \phi} = \frac{2\pi c}{\phi_0} \sum_n \frac{\sin(2\pi\phi/\phi_0)}{\partial \chi_j / \partial E_n}. \quad (11)$$

RESULTS AND DISCUSSION

Based on eq.(5) and (6), the flux-dependent energy spectra of the system can be obtained. Figure 1(a) addresses the numerical result of the energy spectra for $j=7$ and $v=0.4$. At a fixed flux, there are $F_7=128$ eigenenergies. It is evidence that the spectrum doesn't possess obvious

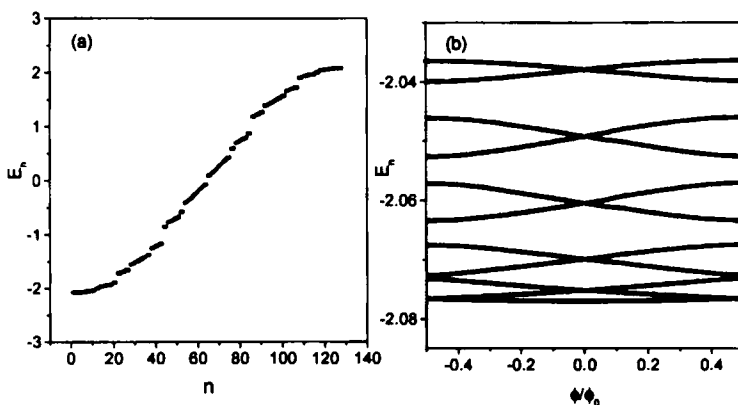


FIGURE 1. The energy eigenvalues of a mesoscopic Thue-Morse ring for the on-site model, where $j=7$ ($N=128$). (a) $v=0.4$ and $\phi/\phi_0=0.7$. (b) The lowest 11 bands for $v=0.4$, $1/2 < \phi/\phi_0 < 1/2$.

self-similarity but is symmetric about its center, which is decided by the structural characterization of the TM sequence. The several lowest energy bands are shown in Fig. 1(b). It is demonstrated that electron eigenenergies gradually form “bands” as on-site energy v increases. Since the degree of disorder is decided by the site energies, we can conclude that disorder affects the energy spectra of the system.

The persistent current in the mesoscopic ring is completely determined by the energy spectra of the system. According to eq.(11), the persistent currents in the TM rings depend on the number of electron N_e and the on-site energy v . We choose two different cases: near half-filled and far away from half-filled. And in each case, the parity of the electron number is also concerned. Figure 2(a) presents the persistent current $I(\phi)$ when the energy bands are half-filled and the number of electrons is even. It is easy to see that the plot of the persistent current I vs. the magnetic flux ϕ is taken to be sine-function at half-filling and that the persistent currents are suppressed dramatically with the increase of v . As v is the index of disorder, we can make the conclusion that a metal-insulator transition occurs at half-filling due to the increase of disorder. Our results confirm the previous claim that the persistent

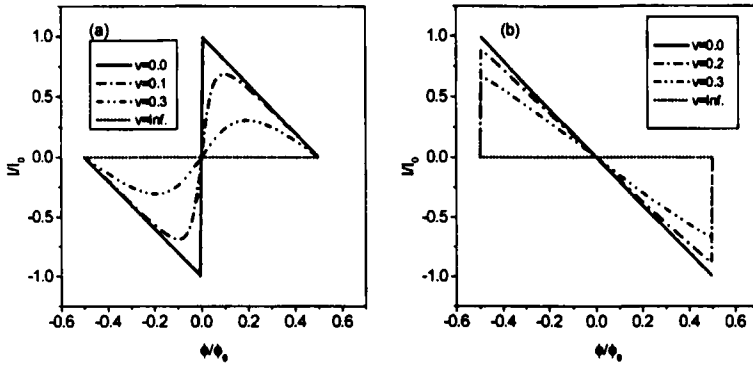


FIGURE 2. The persistent current I vs. magnetic flux ϕ for different on site energies, where $j=7$ ($N=128$), (a) $N_e=64$. (b) $N_e=63$

current will drop as a function of disorder. It is also in agreement with the conclusion we made above that disorder leads to the formation of the energy bands. Meanwhile, if the number of electrons deviates a little from half-filling and is odd, as plotted in Fig.2(b), the relationship between I and ϕ become linear and the suppression of persistent currents are much slower, and there is no obvious transition from the metal to insulator.

On the other hand, we have studied the behavior of persistent current when the energy bands are far away from half-filled. In the electron system where there has small gap near the highest-lying band, even if disorder is large, the situation is quite different from the half-filling case (shown in Fig. 3(a) and (b)). The curves in Fig. 3 are always quasi-linear while the suppression of persistent currents is not obvious, too. If there is a large gap near the highest-lying band, the behavior of the persistent current will change a lot. As Landauer and Büttiker have pointed out before^[1], persistent current strongly depends on the highest-

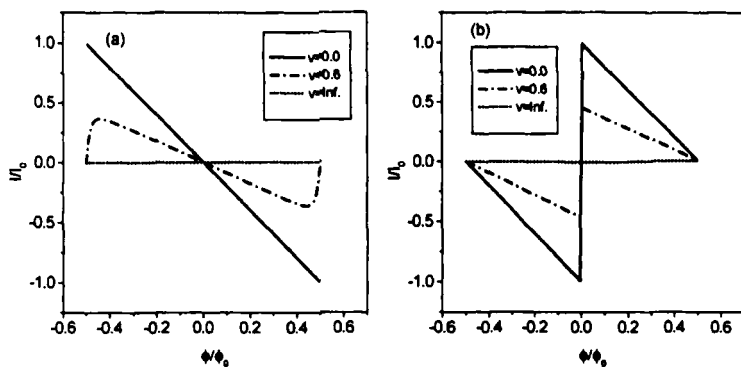


FIGURE 3. The persistent current I vs. magnetic flux ϕ when far away from half-filling, where $j=7(N=128)$ (a) $N_e=97$. (b) $N_e=96$.

-lying band. Therefore the number of electron near Fermi level is essential to the overall current.

CONCLUSION

In the frame of a tight-binding model, we have studied the energy spectra and persistent currents in one-dimensional mesoscopic rings threaded with a magnetic flux ϕ . It is shown that the electron eigenenergies $E(\phi)$ gradually form "bands" as the disorder increases in the quantum system. Meanwhile, the persistent currents in the rings exhibit a rich structure, which depend on the number of electrons and the disorder of system. In the case that the energy bands are near half-filled, the plot of the persistent current I vs. the magnetic flux ϕ is taken to be sine-function if the number of electron is even; but if the electron number is odd, the relationship between I and ϕ is changed to be linear. While in the case that the energy bands are far away from half-filled, $I(\phi)$ strongly depends on the gap near the highest-lying band and is rather complicated. On the other hand, as increasing the disorder of system, the "bandwidths" are getting narrower in the energy spectra, thereafter

the maximum persistent current decreases obviously in the rings. Interestingly, a metal-insulator transition has been found in the half-filled electron system.

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