Magnetic-flux-induced persistent currents in nonlinear mesoscopic rings

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(Presented 15 November 2010; received 27 September 2010; accepted 8 December 2010; published online 6 April 2011)

We investigate magnetic-flux-induced persistent currents (PCs) in a one-dimensional nonlinear mesoscopic ring based on the Frenkel–Kontorova (FK) model. By applying a transfer-matrix technique, the energy spectra, the PCs, and the Thouless exponent are theoretically obtained. It is shown that the energy spectrum splits into sub-bands when the on-site energy is gradually increased, and in the flux-dependent energy spectra, the energy levels show different behaviors over the *transition by breaking of analyticity*. Meanwhile, the PC is determined by the magnetic flux, the on-site energy, and the Fermi level. The increment of the on-site energy leads to a dramatic suppression of the PC. When the Fermi level is in the vicinity of "band" gaps, the PC is limited considerably; otherwise, the PC increases by several orders of magnitude. The suppressed PC is related to the electronic localization of the FK ring, which is described by the Thouless exponents. Our investigations provide detailed information about the influence of nonlinear structure on the PC and contribute to its potential application in quantum devices. © *2011 American Institute of Physics*. [doi:10.1063/1.3562257]

When a conducting ring is threaded by a magnetic flux, a persistent current (PC) will be induced due to the topologically determined quantum interference. Since the seminal proposal of PC by Büttiker *et al.*,[1] considerable attention has been paid to the PC in one-dimensional (1D) metal or semiconductor mesoscopic rings.[1–8] In an early experiment conducted by Chandrasekhar *et al.*,[4] the PC measured in a single Au ring is 1 or 2 orders of magnitude larger than the value predicted by noninteracting theory. Recently, an experimental observation of Bluhm *et al.*[5] indicated that the h/e PC in diffusive rings is in good agreement with theoretical predictions, though its sign and amplitude change between the rings. Generally, the PC depends on the particular realization of disorder and thus varies between nominally identical samples. It has been shown that disorder reduces the magnitude of the PC,[6] but in correlated disordered rings, the PC is not reduced at a particular Fermi level.[7] Meanwhile, periodic and quasiperiodic systems have also been investigated.[8] However, previous studies concentrate mostly on the linear systems, and few studies are based on the nonlinear systems such as the Frenkel–Kontorova model.

The Frenkel–Kontorova (FK) model describes a 1D chain of atoms with harmonic nearest-neighbor interaction placed in a periodic potential.[9] When the mean distance between consecutive atoms is in an irrational ratio to the period of the external potential, the corresponding state is incommensurate.[10] By changing the coupling constant, Aubry *et al.*[11] demonstrated that the transition from one configuration to another occurs, i.e., *the transition by breaking of analyticity*. The FK model has been used to model crystal dislocation,[12] charge density waves,[13] vortex transmission,[14] and epitaxial monolayers on the crystal surface.[15] In this work, we investigate magnetic-flux-induced PCs in 1D FK mesoscopic rings. "Band" structures of the electron eigenenergies have been formed. PC presents a rich feature depending on its energy spectrum and Fermi level. The increment of the amplitude of the on-site energy will lead to a dramatic suppression of the PC. When the Fermi level reaches a specific value, a large PC can be observed. The Thouless exponents have also been studied. Our investigations provide detailed information about the structural influence on PC and contribute to its potential application in quantum devices.

Consider the electron behavior in a 1D FK mesoscopic ring threaded by the magnetic flux. In the tight-binding approximation, the Schrödinger equation for a spinless electron in a FK ring can be written as

$$t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1} + \varepsilon_n\psi_n = E\psi_n, \tag{1}$$

where ψ_n is the amplitude of the wavefunction on the nth site index; $t_{n,n\pm1}$ is the nearest hopping integral, which is set to 1 in the following calculation; and the on-site energy ε_n is taken as $\varepsilon_n = V\cos(2\pi x_n^0)$. $\{x_n^0\}$ is the configuration of an incommensurate ground state of the FK model. In other words, $\{x_n^0\}$ minimizes the functional

$$H = \sum_n \left[\tfrac{1}{2}(x_{n+1} - x_n - a)^2 + K\cos(2\pi x_n)\right], \tag{2}$$

where K is a coupling constant and a is the equilibrium distance between consecutive atoms. It is well known that for each irrational a there exists a critical value K_c separating two configurations of ground state, i.e., *the transition by breaking of analyticity*. The largest $K_c = 0.02461...$ is achieved when a is equal to the golden mean. In the numerical calculations, we restrict ourselves to this particular value.

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Equation (1) can also be expressed in the matrix form

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = T_n \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}. \tag{3}$$

Here T_n is the transfer matrix that correlates the adjacent site amplitudes, and it reads

$$T_n = \begin{bmatrix} (E - \varepsilon_n) & -1 \\ 1 & 0 \end{bmatrix}. \tag{4}$$

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

$$\begin{pmatrix} \psi_{M+1} \\ \psi_M \end{pmatrix} = \bar{T} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = e^{i2\pi\Phi/\Phi_0} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{5}$$

where $\bar{T} = \prod_{n=1}^{M} T_n$ 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, the total PC in the ring satisfies

$$I(\Phi) = \sum_{h=1}^{n_e} I_h(\Phi) = -c \sum_{h=1}^{n_e} \frac{\partial E_h(\Phi)}{\partial \Phi}. \tag{6}$$

According to the above theoretical model, the PCs are ultimately determined by the flux-dependent energy spectra of the system. Figures 1(a) and 1(d) show the energy spectra against the amplitude of the on-site potential V in the FK rings with different values of the coupling constant K. Obviously, the band splits into sub-bands as V is increased from zero. When the amplitude of the on-site potential V becomes larger than a critical value, the energy levels tend to repel each other. In other words, the energy gap is enlarged by increasing V, as happens in other systems.[16] However the spectral properties display quite different behaviors for $K \leq K_c$ [Fig. 1(a)] and $K > K_c$ [Fig. 1(d)]. The eigenvalues are evenly spaced above the transition, densely filling the "bands," but the distribution of eigenvalues is more fragmented below the transition. This feature becomes much clearer in Figs. 1(b) and 1(e), which present the flux-dependent energy spectra when $V = 1.4$ and $K = 0.02$ and 0.04, respectively. Figures 1(c) and 1(f) are the enlargement of the energy regions around zero corresponding to Figs. 1(b) and 1(e), respectively. It is shown that when $K = 0.04$, the electronic gap appears around $E = 0$. However, there are several energy levels around $E = 0$ when $K = 0.02$. It is well known that the phase transition by the breaking of analyticity is manifested by the phonon gap for $K > K_c$ in other systems.[10,17] In fact, the electronic gap appears for $K > K_c$ in our system with a particular value of V.

Based on the energy spectra, the behavior of the PC in the FK ring can be obtained. Figures 2(a) and 2(b) plot the flux-dependent PCs in the FK ring with different amplitudes of the on-site potential V and different electron-filling numbers n_e. It is found that the PC is gradually suppressed if V

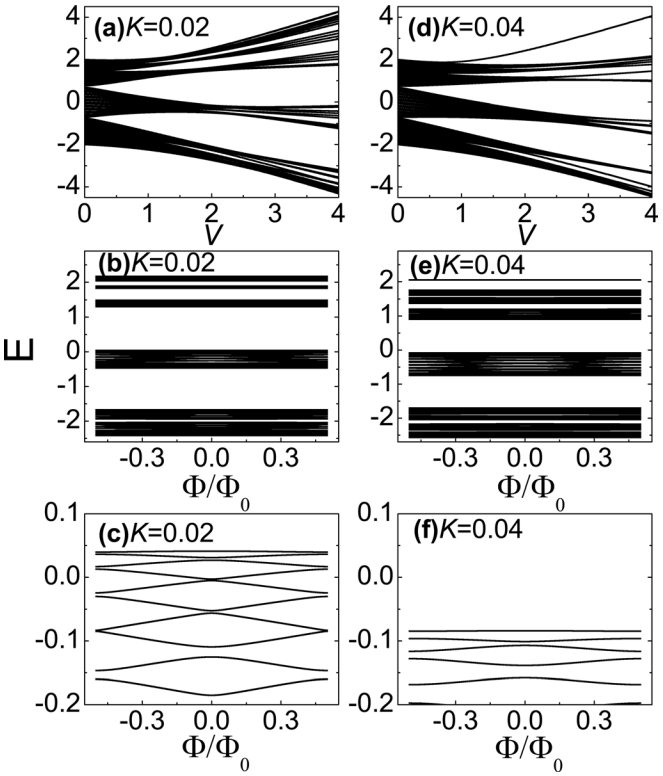

FIG. 1. The energy spectra of the FK ring, where the total number of atoms $N_{tot} = 89$. (a) and (d) show the spectra vs V with $\Phi/\Phi_0 = 0.3$ when $K = 0.02$ and $K = 0.04$, respectively. (b) and (e) present the flux-dependent energy spectra with $V = 1.4$ when $K = 0.02$ and $K = 0.04$, respectively. (c) and (f) illustrate the enlargement of the region around $E = 0$ corresponding to (b) and (e), respectively.

increases [as shown in Figs. 2(a) and 2(b)]. Increasing V means that the scattering rate is enhanced, and the dependence of the energy level on the flux becomes smoother [as shown in Figs. 1(c) and 1(f)]. Thereafter, the current will decrease according to Eq. (6). On the other hand, the flux-

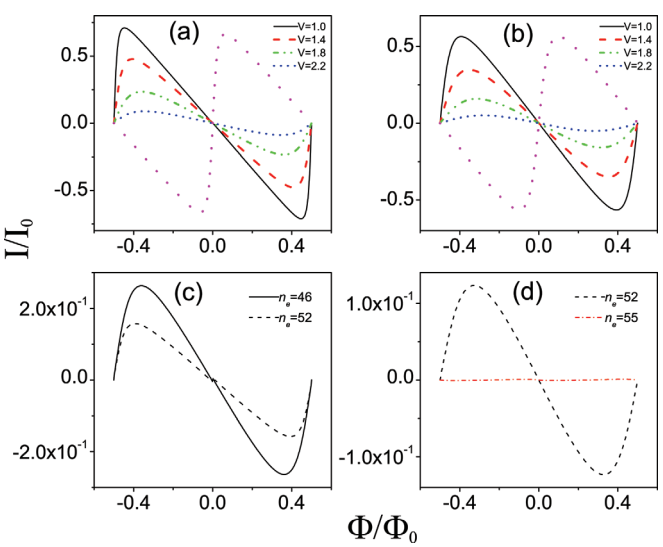

FIG. 2. (Color online) The persistent current (PC) vs the magnetic flux Φ in the FK ring, where $I_0 = (4\pi c/N\Phi_0)\sin(n_e\pi/N)$ and $N_{tot} = 89$. (a) and (b) show the PC with $n_e = 18$ (all lines except the magenta dotted one) and $n_e = 19$ (magenta dotted line) under different amplitudes of on-site potential V: (a) $K = 0.02$ and (b) $K = 0.04$. (c) and (d) plot the PC under different electron filling numbers n_e, where $V = 1.4$. (c) $K = 0.02$; (d) $K = 0.04$.

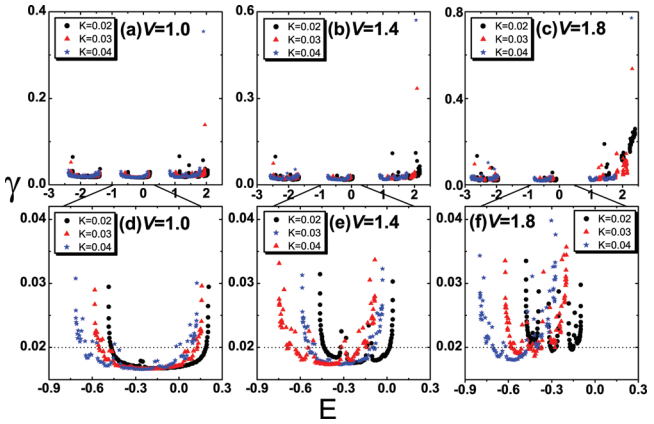

FIG. 3. (Color online) The Thouless exponents as a function of eigenenergy for the FK ring. (a), (b), and (c) illustrate the full spectral range for $N_{\text{tot}} = 377$; (d), (e), and (f) present the selected range of eigenenergies that correspond to the central bands of (a), (b), and (c), respectively.

dependent PC is like that in a diamagnet in the FK ring with even n_e, and it behaves like that in a paramagnet in a ring with odd n_e. However, the magnitude of the PC in the FK ring can be altered by tuning the electron-filling number n_e or the Fermi level. As shown in Figs. 2(c) and 2(d), if the Fermi level is in the energy sub-band, the PC is unsuppressed, and if the Fermi level approaches the edge of the sub-band, the PC is suppressed dramatically. For example, if n_e is 55, the Fermi level comes to the "top" of a sub-band, and the PC is suppressed dramatically. Interestingly, in the FK ring with $K = 0.04$, the Fermi level that is closest to $E = 0$ corresponds to $n_e = 55$, while it corresponds to $n_e = 52$ in the ring with $K = 0.02$. As a result, the PC around $E = 0$ decreases sharply in the FK ring for $K > K_c$ compared with that in the ring for $K < K_c$.

In order to understand the behavior of the PC in the FK ring clearly, we have studied the Thouless exponent. The Thouless exponent is a quantity that describes the localization of eigenstates.[10] For an eigenfunction corresponding to the eigenenergy E_i, the Thouless exponent is given by $\gamma(E_i) = (1/N)\sum_{j\neq i} \ln|E_i - E_j|$.[9] $\gamma(E_i)$ is proportional to the inverse of the localization length, i.e., $\gamma \sim 1/\xi$. If γ is about the order of $1/N$ for a finite chain of length N, the eigenstates are extended or critical. Otherwise, the eigenstates are localized. In Fig. 3, we plot γ as a function of eigenenergy for different values of V and K. There are several interesting features. First, the distribution of the Thouless exponent against the eigenenergy E_i forms a "band" structure [as shown in Figs. 3(a)–3(c)], and the value of the Thouless exponent in the sub-bands is smaller than that at the sub-band edges. With increasing V, the tail of the curve is enlarged [see the longitudinal coordinates in Figs. 3(a)–3(c)]. As we know, the Thouless exponent is proportional to the inverse of the localization length. Obviously, in the FK ring, the localization length at the vicinity of the "band" gaps is shorter than that in the "band." Therefore, the amplitude of the PC is suppressed when the Fermi level approaches the edge of the sub-band. Second, the curves are driven up by increasing the amplitude of the on-site potential V [as shown in Figs. 3(d)–3(f)]. That is to say, the localization length is shortened at a particular Fermi level by increasing V. This feature is helpful when trying to understand the diminishment of PC when V is enlarged. Finally, the Thouless exponent behaves differently for $K < K_c$ and $K > K_c$. As shown in Figs. 3(d)–3(f), the curves are smooth when $K = 0.02$, but the maps show clumping in the coordinates when $K = 0.04$. The reason is that the eigenvalue distribution changes over the transition at K_c. Moreover, in the FK ring with $V = 1.4$ and $K = 0.02$, the Thouless exponent at $E = 0$ is about 0.03; thus the localization length $\xi = 1/\gamma \sim 10^2$, which is about the order of the size of the FK ring. However, the Thouless exponent at $E = 0$ for $K = 0.04$ is almost infinite. Then the PC around $E = 0$ decreases sharply, and an electronic gap appears in the FK ring when $K > K_c$. Therefore, in the FK rings, the PC depends on the coupling constant K, the amplitude of the on-site potential V, and the Fermi level in a rather complicated manner. Large PCs can be observed when the Fermi level is in the sub-band.

This work was supported by grants from the National Natural Science Foundation of China (Grant Nos. 10904061, 50972057, 11034005, 61077023, and 11021403) and the State Key Program for Basic Research from the Ministry of Science and Technology of China (Grant No. 2010CB630705).

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