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Persistent currents in k-component Fibonacci mesoscopic rings threaded by a magnetic flux

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Abstract

On the basis of the tight-binding model, we have studied the energy spectra and persistent currents (PCs) in one-dimensional k-component Fibonacci (KCF) mesoscopic rings threaded by a magnetic flux. The KCF structures, which contain k basic units, can be periodic (if $k = 1$), quasiperiodic (if $1 < k < 6$), and intermediate cases between quasiperiodicity and disorder (if $k \geqslant 6$). It is shown that the flux-dependent eigenenergies form 'band' structure in the KCF rings. The subbands possess the hierarchical characteristic with self-similarity if $1 < k < 6$, while if $k \geqslant 6$, there is no obvious self-similarity in the subbands. In fact, the energy spectra ultimately determine the behaviour of the PCs in the mesoscopic KCF rings. On one hand, the PC depends on the total energy bandwidth: the narrower the bandwidth, the smaller the PC. On the other hand, the parity effect of electrons is disimilar in different KCF rings. As k increases, there is less likelihood of observing a dramatic change in currents of several orders of magnitude when one electron is added to or removed from the KCF rings. If k is large enough, the current behaviour may approach some features of disordered systems.

1. Introduction

In the past few decades, much attention has been paid to the mesoscopic system, where quantum coherence can drastically affect the equilibrium properties. One of the interesting phenomena is the persistent current (PC) in mesoscopic rings threaded by a magnetic flux. Since Büttiker *et al* first discussed the quantum interference effect in one-dimensional (1D) metal loops in 1983 [1] there has been a lot of theoretical and experimental work on this subject [2–12]. Study on the magnitude of PCs is still in progress. In the early experiment carried out by Lévy *et al* [2], the PC measured in 10^7 copper rings was in agreement with the theoretical prediction. However, the experimental observation made by Chandrasekhar *et al* [3] indicated that the PC in a single Au ring is one or two orders of magnitude larger than the value predicted by the nonintertacing-electron theory. To explain this discrepancy, Kirczenow [4] proposed a model with electron scattering by grain boundaries. Later, Ben-Jacob *et al* [5] gave a theoretical analysis considering both electron–electron interactions and grain boundaries. All of these

authors obtained the same order of magnitude for the PCs as those observed experimentally in [3]. More recently, with the development of fabrication techniques, more mesoscopic-scale experiments on PCs have been reported and introduced new challenges to the theoretical work, such as the sign of the PC near zero field and the correlation of the PC with the phase coherence time [6–11].

Generally speaking, the disorder of the system and the electron–electron interaction are two important factors influencing the magnitude of the PC. It has been theoretically shown that disorder reduces the magnitude of the PC [13–15], but in correlated disordered rings, the PC is not reduced if the Fermi level is just at the unscattered state energy level; instead, it displays free-electron behaviour regardless of the disorder [16]. Meanwhile, the electron–electron interaction is also complicated. Some reports [17, 18] have indicated that both long- and short-range electron–electron interactions decrease the PC, while other authors [19–21] have claimed that the amplitude of the PC is enhanced due to the Coulomb interaction. More realistically, the 'spinful' system and also two- and three-dimensional models have been taken into account [22–25]. In addition, the importance of the many-channel effect and the geometrical influence have been recently reported on [26, 27]. However, previous studies concentrate most on either periodic or disordered systems. Only few studies [28] are based on the structures between periodic and disordered ones.

One of the well-known examples in 1D quasiperiodic systems is the Fibonacci sequence. The Fibonacci sequence can be produced by repeating the substitution rules $A \to AB$ and $B \to A$, in which the ratio of the values of the two different elements A and B is equal to the golden mean $\tau = (\sqrt{5}+1)/2$. Since Merlin *et al* [29] reported the first realization of Fibonacci superlattices, many works have been carried out on the exotic wave phenomena of Fibonacci systems in x-ray scattering spectra [30, 31], Raman scattering spectra [32, 33], optical transmission spectra [34–36], and in propagation modes of acoustic waves on corrugated surfaces [37–39]. It should be noted that the above work is based on the 1D Fibonacci chain structures, which do not have the ring geometry that we will show in the following text.

In this paper, we have investigated the energy spectra and PCs in mesoscopic rings with N sites arranged according to k-component Fibonacci (KCF) sequences, which contain k basic units A_i ($i = 1, 2, \ldots, k$) and can be generated by the substitution rules $A_1 \to A_1A_k$, $A_k \to A_{k-1}, \ldots, A_i \to A_{i-1}, \ldots, A_2 \to A_1$. The KCF structure can be periodic (if $k = 1$), quasiperiodic (if $1 < k < 6$), and intermediate cases between quasiperiodicity and disorder (if $k \geqslant 6$). The energy spectra of KCF rings threaded by a magnetic flux are calculated on the basis of the tight-binding approximation, and the PC behaviours are also discussed.

2. The theoretical model and the numerical method

Firstly let us give a brief introduction to the k-component Fibonacci structures (KCFS). Consider the substitution S acting on an alphabet of k elements $A_1, A_2, \ldots, A_i, \ldots, A_k$ according to the rules

$$S\begin{pmatrix} A_1 \to A_1A_k, \\ A_k \to A_{k-1}, \\ \vdots \\ A_i \to A_{i-1}, \\ \vdots \\ A_2 \to A_1 \end{pmatrix}. \tag{1}$$

Thereafter, these k elements are arranged in a KCF sequence. For example, the three-component Fibonacci (3CF) structure ($k = 3$) consists of three kinds of element A_1, A_2,

and A_3. Based on the substitution rules S: $A_1 \to A_1A_3$, $A_3 \to A_2$, and $A_2 \to A_1$, these three kinds of element are in sequence as $A_1A_3A_2A_1A_1A_3A_1A_3A_2\ldots$. On the other hand, the KCFS can also be described as a limit of the generation of sequence $C_n^{(k)}$. Let $C_n^{(k)} = S^n A_1$; thus,

$$\begin{aligned} C_0^{(k)} &= A_1, \\ C_1^{(k)} &= A_1A_k, \\ C_2^{(k)} &= A_1A_kA_{k-1}, \\ &\vdots \\ C_{k-1}^{(k)} &= A_1A_kA_{k-1}\ldots A_3A_2, \end{aligned} \tag{2}$$

and in general

$$C_n^{(k)} = C_{n-1}^{(k)} + C_{n-k}^{(k)} \qquad (n \geqslant k).$$

Define the number of elements in the generation $C_n^{(k)}$ as $F_n^{(k)}$. It follows that $F_n^{(k)}$ satisfies $F_n^{(k)} = F_{n-1}^{(k)} + F_{n-k}^{(k)}$ with $F_n = n + 1$ $(n = 0, 1, \ldots, k-1)$, while we denote the number of A_i $(i = 1, 2, \ldots, k)$ in $C_n^{(k)}$ as $N_n^{(k)}(A_i)$. The ratios of these numbers are expressed as $\eta_i = \lim_{n\to\infty}[N_n^{(k)}(A_i)/N_n^{(k)}(A_1)]$. It turns out that the set $\{\eta_i\}$ satisfies

$$\begin{aligned} &\eta_k^k + \eta_k = 1, \\ &1{:}\eta_k = \eta_k{:}\eta_{k-1} = \cdots = \eta_i{:}\eta_{i-1} = \cdots = \eta_3{:}\eta_2. \end{aligned} \tag{3}$$

Therefore all these ratios $\eta_i = \eta_k^{k-i+1}$ $(1 < i \leqslant k)$ are irrational numbers between zero and unity except $\eta_1 = 1$. It has been rigorously proven [40] that the KCFS are quasiperiodic when $1 < k < 6$; while for $k \geqslant 6$, the KCFS are nonquasiperiodic, but they are still ordered.

Now consider the electronic behaviour in one-dimensional (1D) KCF mesoscopic rings threaded by a magnetic flux, which contain k kinds of site A_i $(i = 1, 2, \ldots, k)$ and in total N sites arranged according to the KCF sequences. Under the tight-binding approximation [10, 15, 41] with the on-site model, the Schrödinger equation for a spinless electron in a 1D aperiodic mesoscopic ring can be written as

$$t_{l+1}\psi_{l+1} + t_l\psi_{l-1} + v_l\psi_l = E\psi_l \tag{4}$$

where l is the site index, t_l is the hopping integral, and the site energy v_l depends on the site. We define $v_l = v_i = -v + \frac{2v}{k-1}(i-1)$, if the lth site is A_i. Equation (4) can be expressed in the matrix form

$$\begin{pmatrix} \psi_{l+1} \\ \psi_l \end{pmatrix} = T_{l+1,l} \begin{pmatrix} \psi_l \\ \psi_{l-1} \end{pmatrix} \tag{5}$$

where the transfer matrix

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

Here, we simply define $t_l = -1$ and take it as the energy unit.

Because a magnetic flux Φ threaded through the ring will lead to the twisted boundary condition for the wavefunctions of the electrons [1], the equation for the global transfer matrix has the form

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = \overline{M} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \equiv \mathrm{e}^{\mathrm{i}\,2\pi\Phi/\Phi_0} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{6}$$

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

Define the trace of $\overline{M}$ as $\chi = \frac{1}{2}\operatorname{tr}\overline{M}$; the flux-dependent energy of an electron $E_n(\Phi)$ in the mesoscopic ring can be obtained from

$$\chi = \cos(2\pi\Phi/\Phi_0). \tag{7}$$

The PC in the ring contributed from the nth energy level is expressed as

$$I_n(\Phi) = -c\frac{\partial E_n(\Phi)}{\partial\Phi} = -c\frac{\partial E_n}{\partial\chi}\frac{\partial\chi}{\partial\Phi} = \frac{2\pi c}{\Phi_0}\frac{\sin(2\pi\Phi/\Phi_0)}{\partial\chi/\partial E_n}. \tag{8}$$

At zero temperature, the number of electrons in the spinless fermion system N_e is equal to the highest occupied level labelled by the index m. Therefore, the energy of the system follows

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

and the total PC in the system satisfies

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

The response of the PCs to the magnetic flux can be described by the charge stiffness, which is defined as

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

On the basis of equations (5)–(11), we can carry out the numerical calculations of the energy spectra and the PCs in the KCF mesoscopic rings.

3. The three-component Fibonacci mesoscopic ring

Firstly we discuss the case of the 3CF ring. According to the above theoretical model, the PCs are ultimately determined by the flux-dependent energy spectra of the system. Figure 1 shows the energy spectrum of the 3CF ring with generation $C_{14}^{(3)}$ ($k = 3$) when the magnetic flux $\Phi/\Phi_0 = 0.25$ and $v = 0.3$, i.e. the three kinds of site energy are $v_1 = -0.3$, $v_2 = 0$ and $v_3 = 0.3$. There are in total $F_{14}^{(3)} = 277$ eigenenergies (as shown in figure 1) which form four subbands, and each subband consists of $F_{11}^{(3)} = 88$, $F_9^{(3)} = 41$, $F_{11}^{(3)} = 60$, and $F_{11}^{(3)} = 88$ eigenenergies. Furthermore, each subband is composed of a four-band structure. For example, the inset of figure 1 shows the structure in the first subband. In fact, the energy spectrum of the 3CF structure is a Cantor-like set with self-similarity, which is quite similar to the optical phonon dispersion spectrum of the 3CF multilayer [42].

On the basis of the energy spectrum, the behaviour of the PC in the mesoscopic ring can be obtained from equations (8) and (10). It is shown that the site energy and the electron-filling number in the system play an important role in the PCs. Figure 2 plots the PC in the 3CF ring with $N = F_{14}^{(3)} = 277$ for several site energies in two cases with the electron-filling number $N_e = 138$ and 139. The maximum PC of the periodic model, i.e., $I_0 = (4\pi c/N\Phi_0)\sin(N_e\pi/N)$, is taken to be the unit of current. According to figure 2, it is obvious that when $v = 0$, the flux-dependent current is just the case for the free electron [13], and the PC has a sudden transition at the point of $\Phi/\Phi_0 = 0$ (for even N_e) or $\Phi/\Phi_0 = 0.5$ (for odd N_e). Meanwhile, if v increases, the PC is suppressed and becomes a continuous function around the point of $\Phi/\Phi_0 = 0$. Increasing v means that the quasiperiodicity in the structure becomes stronger; then the dependence of the energy level on the flux becomes smoother. Therefore the current contribution coming from these energy levels will decrease according to

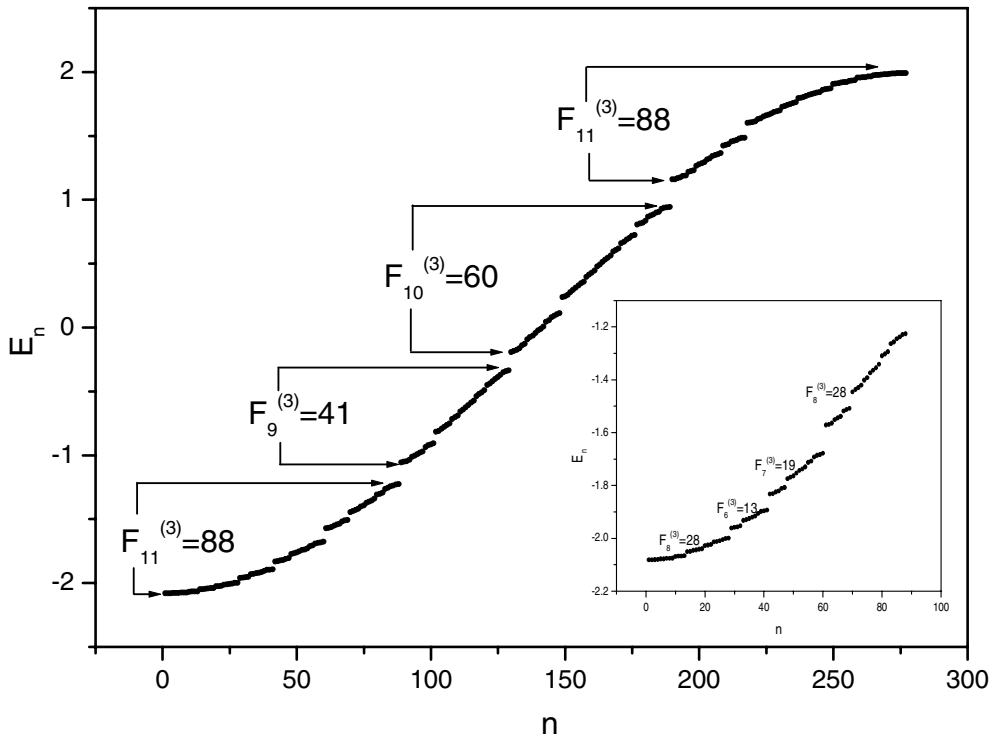

Figure 1. The flux-dependent energy spectrum of the 3CF ring, where $N = F_{14}^{(3)} = 277$, $v = 0.3$, and $\Phi/\Phi_0 = 0.25$. The inset shows the affiliation rule.

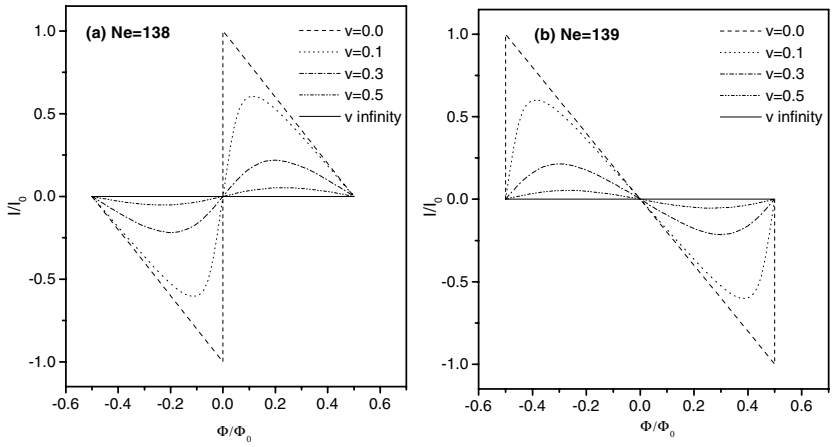

Figure 2. I/I_0 for the PC versus the magnetic flux in the 3CF ring with even and odd electron-filling number (N_e) under different site energies v, where the total number of sites $N = F_{14}^{(3)} = 277$. (a) $N_e = 138$; (b) $N_e = 139$.

equation (8). Consequently, the total current will decrease. This property is similar to that in the disordered system [13–15].

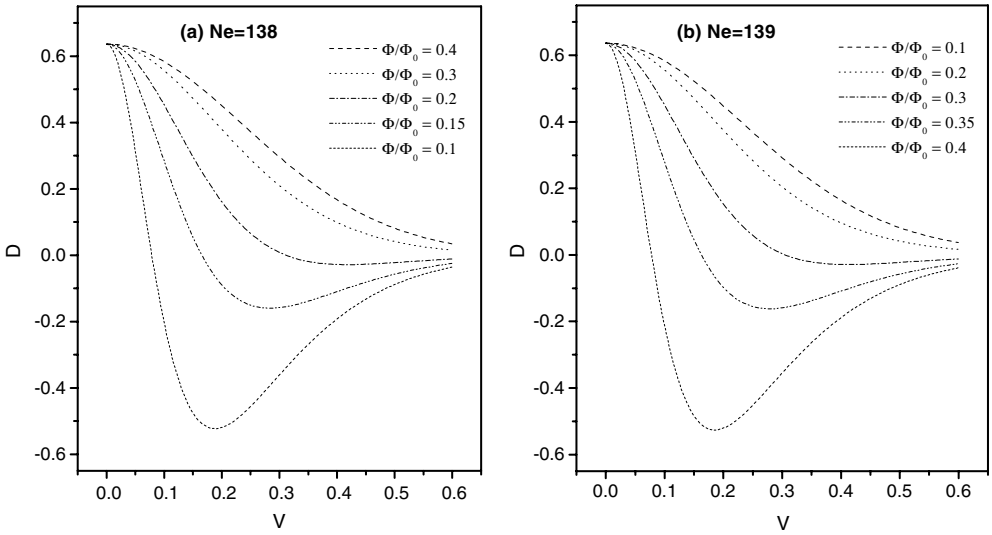

Figure 3. The charge stiffness D versus the site energy v in the 3CF ring with even and odd N_e under different magnetic fluxes, where $N = F_{14}^{(3)} = 277$. (a) $N_e = 138$; (b) $N_e = 139$.

It is interesting to consider the sign of the PC, i.e., whether the PC shows diamagnetic or paramagnetic behaviour near zero field. From the theoretical point of view, the dominant contribution to the total current always comes from the highest occupied energy level. Therefore, at the zero-temperature limit, the sign of the PC is determined by the electron filling number N_e. In the ring with an even number of electrons, the dependence of currents on magnetic flux (as shown in figure 2(a)) is like that for a paramagnet, whereas in a ring with an odd number of electrons, the flux-dependent PC (as shown in figure 2(b)) behaves like that in a diamagnet. (This property is also called the parity effect.) However, due to the Fermi distribution at finite temperature, electrons can occupy the upper level and, consequently, the sign of the PC will be changed [15]. In a real experiment, roughly speaking, the sign of the PC is random, dependent on the number of electrons in the isolated ring and the specific realization of the random potential [2, 3]. For example, diamagnetic responses of the PC were observed in copper rings [2] and in an array of gold rings [8]. However, paramagnetic behaviour of the PC was shown in gold rings made by Chandrasekhar *et al* [3]. Recent studies suggest that the sign and also the magnitude of the PC are affected by the phase coherence time τ_φ which is related to the internal (or external) noise [7] and the interaction between conduction electrons and impurities in the mesoscopic rings [11]. However, further experimental and theoretical work needs to be done to determine the sign of the PC near zero field.

In order to address the response of the PCs to the magnetic flux, the charge stiffness D is also calculated on the basis of equation (11). Figure 3 gives the charge stiffness in the 3CF ring with $N = F_{14}^{(3)} = 277$, where $N_e = 138$ and 139. It can been seen that D approaches 0.636 as $v \to 0$, which corresponds to the free-electron case. In the system with an even number of electrons (such as that in figure 3(a)), with v increasing, the response of the PC to the applied magnetic flux becomes more and more retarded in the cases of $0.3 < \Phi/\Phi_0 < 0.5$; while in the cases of $0 < \Phi/\Phi_0 \leqslant 0.3$, the charge stiffness depends greatly on the magnetic flux. The absolute value of D will approach zero when v is large enough for all magnetic flux. The behaviour of D in the system with an odd number of electrons (such as that in figure 3(b)) is similar to the case for the system with an even number of electrons, except that Φ/Φ_0 has a shift of $1/2$ (due to the parity effect).

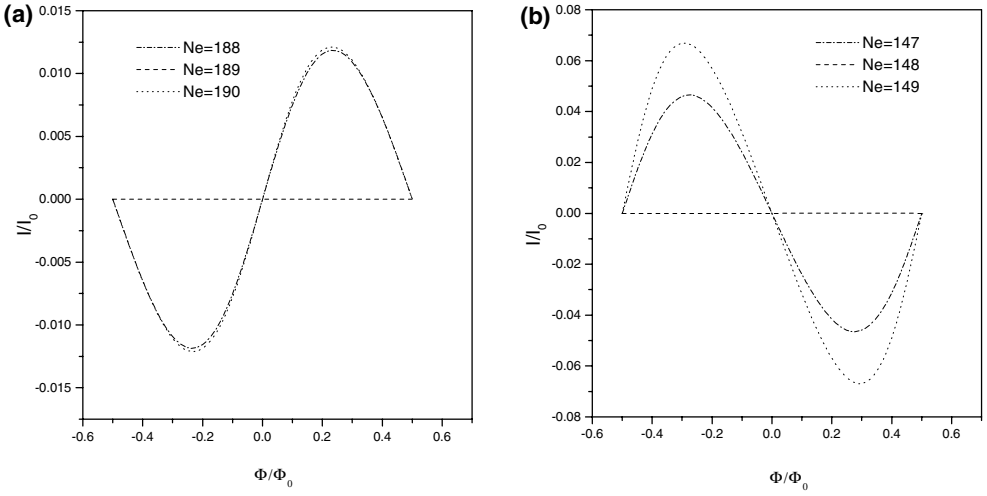

Figure 4. The change of I/I_0 for the PCs in the 3CF ring in the vicinity of the energy gap, where $N = F_{14}^{(3)} = 277$ and $v = 0.3$. (a) $N_e = 188$, 189, and 190. $\Delta E = 0.215$; (b) $N_e = 147$, 148, and 149. $\Delta E = 0.127$.

Additionally, the PC will dramatically change when the Fermi level of the system nears the energy gap. It is seen from figure 1, where $N_e = 189$, that electrons are filled just to the top of one energy band, above which there is the largest gap ($\Delta E = 0.215$). If one more electron is added, the Fermi energy reaches the bottom of another band. Figure 4(a) demonstrates that the PC varies dramatically if one electron is added ($N_e = 190$) or removed ($N_e = 188$). The magnitude of the maximum PC is $I/I_0 \sim 2.7 \times 10^{-8}$ in the ring with $N_e = 189$. But the magnitude of the current reaches $I/I_0 \sim 0.012$ (normal value) in the rings with $N_e = 190$ and 188. On the other hand, if electrons are filled to the top of the band near a smaller gap, the change in the PC will decrease. For example, in the ring with $N_e = 148$ (the nearest gap $\Delta E = 0.127$), the maximum of the currents has $I/I_0 \sim 1.0 \times 10^{-4}$, while the current takes on the normal magnitude of about 5.0×10^{-2} if the one electron is added or removed (as shown in figure 4(b)). Generally, the wider the energy gap, the larger the change in the PC. This can be understood because the PC is proportional to the slope of the flux-dependent energy level, and at the top of one subband, the energy level is much smoother than the others. Therefore the PC becomes much lower when the Fermi level is on the top of the band, and if there is a subtle change in the electron number of the system, the current will increase by several orders of magnitude.

4. The k-component Fibonacci mesoscopic rings

Figures 5(a)–(f) show the flux-dependent energy spectra of the KCF mesoscopic rings ($k = 2$, 3, 4, 5, 6, and 10) when $v = 0.4$ and $\Phi/\Phi_0 = 0.25$. The insets show the corresponding energy gaps $\Delta E = E_{n+1} - E_n$. In the case of $1 < k < 6$, the KCF structure is quasiperiodic, and the energy eigenvalues form $k + 1$ subbands (as shown in figures 5(a)–(c)). For example, in the four-component Fibonacci system ($k = 4$), each subband consists of $F_{11}^{(4)} = 50$, $F_8^{(4)} = 19$, $F_{10}^{(4)} = 36$, $F_9^{(4)} = 26$, and $F_{11}^{(4)} = 50$ eigenenergies. It should be noted that the five-component Fibonacci structure still possesses this property, which is much clearer in the case of the site energy $v = 0.8$ than that in figure 5(d) where $v = 0.4$. As k increases, the hierarchical characteristic becomes more obscured and there are more gaps in the energy spectra, but those gaps tend

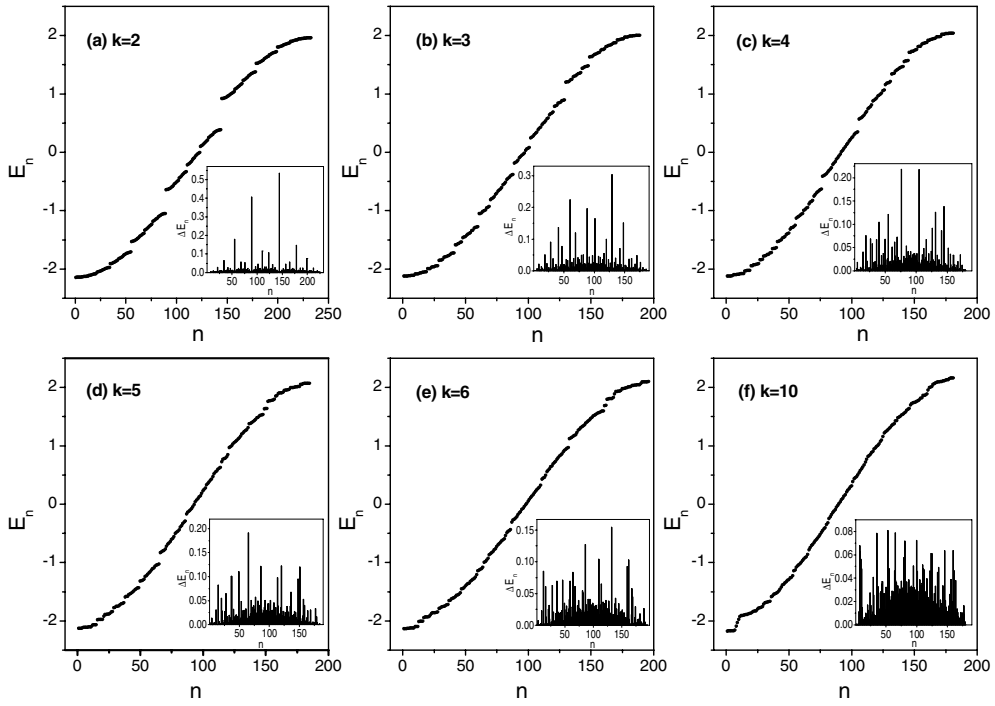

Figure 5. The flux-dependent energy spectra in KCF rings for $k = 2$, 3, 4, 5, 6, and 10, where $v = 0.4$ and $\Phi/\Phi_0 = 0.25$. The insets show the corresponding energy gaps $\Delta E = E_{n+1} - E_n$. (a) $N = F_{11}^{(2)} = 233$; (b) $N = F_{13}^{(3)} = 189$; (c) $N = F_{15}^{(4)} = 181$; (d) $N = F_{17}^{(5)} = 185$; (e) $N = F_{19}^{(6)} = 196$; (f) $N = F_{25}^{(10)} = 181$.

to be homogeneous (as shown in the insets of figures 5(e)–(f)). In fact when k is large enough, the energy spectrum of the KCF ring approaches the point spectra of disordered systems.

Now that the PC in a mesoscopic ring is completely determined by the energy spectra, it is interesting to investigate the behaviour of the PCs in several different KCF systems. It is found that, with k increasing, there is less likelihood of observing a dramatic transition of the PCs in the KCF mesoscopic rings when the electron parity is changed. Figure 6 gives the ratio of the maximum PCs in several KCF rings ($2 \leqslant k \leqslant 10$) with the electron numbers $N_e + 1$ and N_e, where $v = 0.4$. Here N_e is the electron-filling number when the Fermi level is just at the bottom of the largest energy gap in each KCF ring that we discussed. As shown in figure 6, as k increases, the ratio $I_{\max}(N_e + 1)/I_{\max}(N_e)$ reduces substantially. The reason is that the biggest energy gap in the energy spectrum of the KCF ring decreases rapidly with increasing k (see the insets of figures 5(a)–(f)). It can be expected that when k becomes large enough, the change of the electron parity may not lead to a dramatic transition of the PCs in the KCF rings.

However, when k increases, there is no obvious evolution of the absolute currents in the KCF rings. Figure 7 gives the series of curves of maximum PC $I_{\max}(\Phi)$ versus even N_e in the KCF rings for $k = 2$, 3, 4, 5, 6, and 10, where $v = 0.4$. (Here the constant $2\pi c/\Phi_0$ in equation (8) is considered as the unit.) It is easy to see that the maximum PC in the KCF ring does not decrease as k increases. For example, $I_{\max}(k = 2) > I_{\max}(k = 6) > I_{\max}(k = 3)$. This implies that the PCs may not reduce in the KCF rings although the strength of the disorder enhances in the structures with k increasing. This phenomenon may be similar to the result for correlated disordered rings [16]. On the other hand, according to equation (8),

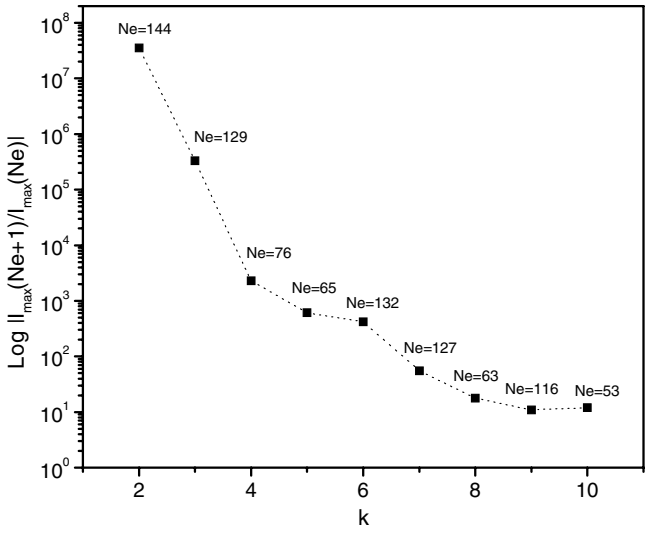

Figure 6. The ratio of the maximum persistent currents $I_{max}(N_e + 1)/I_{max}(N_e)$ in KCF rings ($2 \leqslant k \leqslant 10$), where $v = 0.4$. N_e is the electron-filling number when the Fermi level is just at the bottom of the largest energy gap in each KCF ring. The number of sites N is as same as that in figure 5 for $k = 2$, 3, 4, 5, 6, and 10; while for $k = 7$, $N = F_{21}^{(7)} = 211$; for $k = 8$, $N = F_{22}^{(8)} = 184$; and for $k = 9$, $N = F_{24}^{(9)} = 201$.

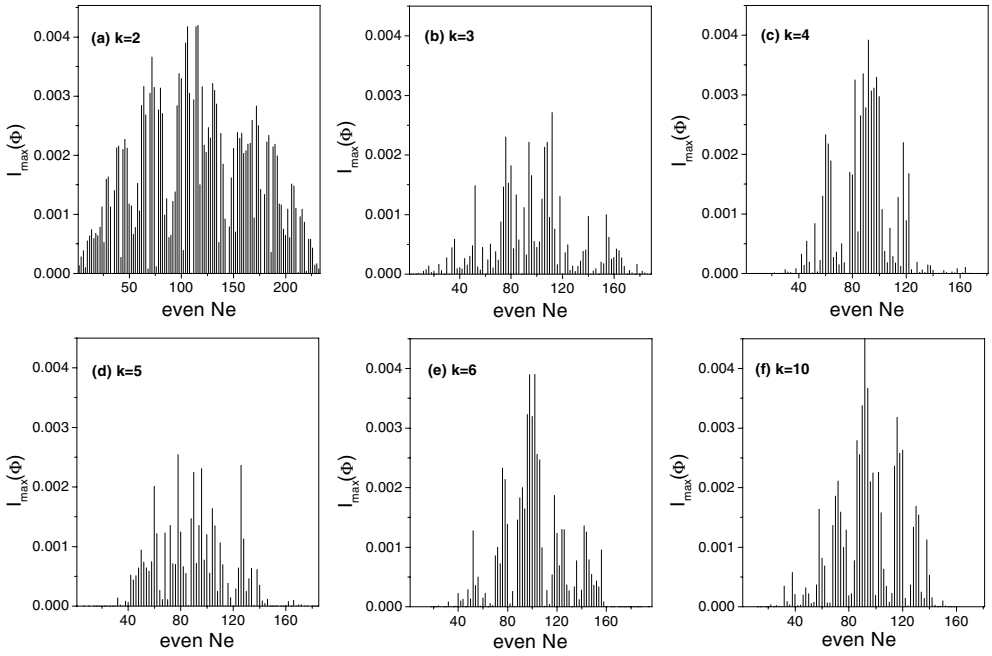

Figure 7. The maximum magnitude of the absolute PCs $I(\Phi)$ at even N_e for $k = 2$, 3, 4, 5, 6, and 10, where $v = 0.4$. (a) $N = F_{11}^{(2)} = 233$; (b) $N = F_{13}^{(3)} = 189$; (c) $N = F_{15}^{(4)} = 181$; (d) $N = F_{17}^{(5)} = 185$; (e) $N = F_{19}^{(6)} = 196$; (f) $N = F_{25}^{(10)} = 181$.

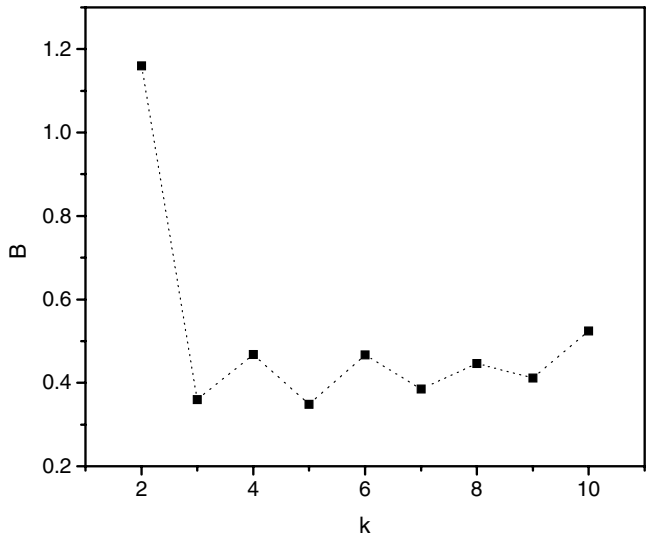

Figure 8. The total bandwidth $B = \sum_n |E_n(\Phi/\Phi_0 = 0) - E_n(\Phi/\Phi_0 = 0.5)|$ in KCF rings ($2 \leqslant k \leqslant 10$), where $v = 0.4$. The number of sites N is as same as that in figure 6.

the PC depends on the slope of the flux-dependent energy level. Roughly, those slopes are related to the bandwidth in the energy spectrum. Figure 8 shows the total bandwidth $B = \sum_n |E_n(\Phi/\Phi_0 = 0) - E_n(\Phi/\Phi_0 = 0.5)|$ for $2 \leqslant k \leqslant 10$, where $v = 0.4$. It seems that in principle, the narrower the total bandwidth, the smaller the magnitude of the overall PC.

5. Summary

We have investigated the energy spectra and the PCs in one-dimensional KCF mesoscopic rings threaded by a magnetic flux. The KCF structures can be periodic (if $k = 1$), quasiperiodic (if $1 < k < 6$), and intermediate cases between quasiperiodicity and disorder (if $k \geqslant 6$). In the cases of $1 < k < 6$, the electron eigenenergies $E_n(\Phi)$ form a 'band' structure with self-similarity; while in the cases of $k \geqslant 6$, the hierarchical characteristic becomes more obscured. In fact, the difference in energy spectra gives rise to the variety of PCs in the KCF rings. The 3CF system has been given as an example to clarify how the site energy and the electron-filling number influence the PC. And it is found that there is no uniform evolution in the absolute PC in different KCF rings when k increases. Generally, the narrower the bandwidth, the smaller the PC. However, with k increasing, there is less likelihood of observing a dramatic transition of the PCs in the KCF mesoscopic rings when the electron parity is changed. We can expect that when k becomes large enough, the behaviour of the PC in the KCF ring will approach the disordered cases.

Acknowledgments

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