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Electronic Transmission and Switch Effect in *k*-Component Fibonacci Nanowires

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We present the electronic transport in the *k*-component Fibonacci (KCF) nanowires, in which *k* different incommensurate intervals are arranged according to a substitution rule. For the KCF nanowires with an identical *k*, by increasing the length of the nanowire, the minima in transmission extend gradually into the band gap over which the transmission is blocked. Meanwhile more transmission peaks appear. For finite KCF nanowire, by increasing the number of different incommensurate intervals *k*, the width of electronic band gap is enlarged. Moreover, when the value of *k* is sufficiently large, the transmission is shut off, except at a few resonant energies. These properties make it possible to use the KCF nanowires as switching devices. Furthermore, a dimensional spectrum of singularities associated with the transmission spectrum demonstrates that the electronic propagation in the KCF nanowire shows multifractality. These investigations open a unique way to control quantum transport in nanodevices.

Keywords: Quasiperiodic Nanowires, Electronic Transmission, Multifractal, Switch Effect, Dimensional Spectrum.

1. INTRODUCTION

With the development of micro-fabrication technology, the feature size of microelectronic devices may reach several tens of nanometers.[1–2] It becomes very important to manipulate the electron transport on nanometer scale, where quantum interference plays an essential role. The electronic behavior in nanostructures can be described by Landauer–Büttiker theory.[3–5] Based on the Landauer–Büttiker theory, Pouthier et al. obtained a localization–delocalization transition of electron through a set of metallic clusters randomly attached to an adsorbed nanowire when the incident energy of electron coincides with the antiresonances of a cluster.[6] Actually, the localization–delocalization transition of electrons was first predicted by Dunlap et al. in one-dimensional (1D) random-dimer (RD) model in 1990.[7] Physically, electronic delocalization in RD-like systems originates from the internal structural symmetry (or inverse symmetry) of the impurity cluster.[7–9] And electronic transmission in symmetric metallic nanowires shows some novel characteristics.[10] Recently the systematic tuning of electronic band structure of atomic-scale gold wires has been demonstrated by controlling the density of impurity atoms.[11] Now that the electron behaviors in nanowires depend critically upon the distribution of atoms, it is interesting to investigate the electron transport in nanowires with various configurations, such as periodic, quasiperiodic, and even other aperiodic structures.

One of the well-known examples in 1D quasiperiodic systems is the Fibonacci sequence. Since Merlin et al. reported the first realization of Fibonacci superlattices,[12] much attention has been paid to the exotic wave phenomena of Fibonacci systems in X-ray scattering spectra,[13] optical transmission spectra,[14, 15] and propagation modes of acoustic waves on corrugated surfaces.[16] To the best of our knowledge, there seems to have been no work on the electron transport in nanowire with 1D aperiodic structure which contains more than two incommensurate intervals. In this work, we present the electronic transport in the *k*-component Fibonacci (KCF) nanowires, which contain *k* incommensurate intervals A_i $(i = 1, 2, \ldots, k)$ and can be generated by the substitution rules $A_1 \rightarrow A_1A_k$, $A_k \rightarrow A_{k-1}, \ldots, A_i \rightarrow A_{i-1}, \ldots, A_2 \rightarrow A_1$. The KCF sequence can be periodic $(k = 1)$, quasiperiodic $(1 < k < 6)$, and multifractal between quasiperiodicity and disorder $(k \geq 6)$. Based on the transfer matrix method, the electronic transmission in the KCF nanowires is calculated, which illustrates a rich structure. Moreover, a dimensional spectrum of singularities associated with the transmission spectrum demonstrates that the electron propagation in the KCF nanowire shows multifractality. These investigations open a unique way to control quantum transport in nanodevices.

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2. THE THEORETICAL MODEL

Firstly we give a description of the k-component Fibonacci structures (KCFS).[17, 18] Consider the substitution S acting on an alphabet of k elements $A_1, A_2, \ldots, A_i, \ldots, A_k$ according to the rule: $S(A_1 \to A_1A_k, A_k \to A_{k-1}, \ldots, A_i \to A_{i-1}, \ldots, A_2 \to A_1)$. Thereafter, these k elements are arranged in a KCF sequence. On the other hand, the KCFS can also be described as a limit of the generations of sequence $G_n^{(k)}$. Let $G_n^{(k)} = S^n A_1$, it follows $G_0^{(k)} = A_1$, $G_1^{(k)} = A_1A_k$, $G_2^{(k)} = A_1A_kA_{k-1}, \ldots, G_{k-1}^{(k)} = A_1A_kA_{k-1}\ldots A_3A_2$, and in general, $G_n^{(k)} = G_{n-1}^{(k)} + G_{n-k}^{(k)}$. It has been rigorously proven that the KCFS are quasiperiodic when $1 < k < 6$, while for $k \geq 6$, the KCFS are nonquasiperiodic, yet they still ordering.

Now consider the electron behavior in a host monatomic chain, where a cluster of KCF is inserted. Assuming the host chain is composed of atom A_1 only, in the on-site model, atoms $A_1, A_2, \ldots, A_i, \ldots, A_k$ have the energies of $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_i, \ldots, \varepsilon_k$, respectively. The nearest-hopping integral is taken as the same constant V. Under tight-binding approximation, the Schrödinger equation for a spinless electron in 1D KCF chain can be written in the matrix form of

$$\begin{pmatrix} C_{j+1} \\ C_j \end{pmatrix} = \begin{pmatrix} (E-\varepsilon_j)/V & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} = P_j \begin{pmatrix} C_j \\ C_{j-1} \end{pmatrix} \quad (1)$$

where ε_j depends on the atom which occupies the jth site, P_j is the transfer matrix that correlates the adjacent site amplitudes C_j and $C_{j\pm1}$. The whole chain contains three parts: the KCF cluster, its left part, and its right part. The amplitudes of wave functions can be described as $C_j = e^{ikj} + re^{-ikj}$ for the left part of the KCF cluster and $C_j = te^{ikj}$ for right part of the KCF cluster. Here r and t are the reflection and the transmission amplitudes of KCF cluster, respectively.

If the cluster of KCF occupies the sites from $h+1$ to $h+m$, the total transfer matrix across the KCF cluster can be expressed as $\bar{P} = P_{h+m-1} \cdot P_{h+m-2} \ldots P_h$. For a given $\bar{P}$, the reflection amplitude r and transmission amplitude t can be written as

$$r = -\xi^{2h} \frac{\alpha^T \Gamma \bar{P} \alpha}{\alpha^T \Gamma \bar{P} \alpha^*}, \quad \text{and} \quad t = \xi^{-m} \frac{2i \sin k}{\alpha^T \Gamma \bar{P} \alpha^*} \quad (2)$$

respectively. Here

$$\xi = e^{ik}, \Gamma = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \alpha = \begin{pmatrix} \xi \\ 1 \end{pmatrix}$$

and α^T is the transpose of α.

On the other hand, multifractal analysis is a tool for characterizing the nature of a positive measure in a statistical sense.[18–20] If a positive measure is covered with boxes of size θ and $p_i(\theta)$ is denoted as the probability in the ith box, an exponent (singularity strength) α_i can be defined as $p_i(\theta) \sim \theta^{\alpha_i}$. We count the number of boxes $N(\alpha)d\alpha$ where the probability p_i has singularity strength between α and $\alpha + d\alpha$, then $f(\alpha)$ can be loosely defined as the fractal dimension of set of boxes with singularity strength α. In the case of transmission spectrum, the transmission coefficient is a positive quantity and the energy space is a support. The weight of transmission coefficient in the transmission spectrum can be defined as $p_i = |T_i|^2/(\sum_{i=1}^N |T_i|^2)$, where T_i is the transmission coefficient of electron with incident energy $E_i = \varepsilon_a - 2V + i\Delta$, and Δ denotes pace length. Due to the energy ranges from $\varepsilon_a - 2V$ to $\varepsilon_a + 2V$, N is set as $N = 4V/\Delta$. The partition function can then be expressed as

$$Z(q) = \sum_{i=1}^{N} p_i^q, \quad Z'(q) = dZ/dq = \sum_{i=1}^{N} p_i^q \ln p_i \quad (3)$$

where the parameter q provides a 'microscope' for exploring the singular measure in different regions. For $q > 1$, $Z(q)$ amplifies the more singular regions of p_i, while for $q < 1$ it accentuates the less singular regions. For $q = 1$ the measure $Z(1)$ replicates the original measure. The $f(\alpha)$ curve of any finite sample is therefore available at a local level, i.e., for a given energy space. The values of α and $f(\alpha)$ are given by

$$\alpha = -\frac{Z'(q)}{Z(q)\ln N}, \quad f(\alpha) = \frac{1}{\ln N}\left(\ln Z(q) - \frac{qZ'(q)}{Z(q)}\right) \quad (4)$$

Besides, the generalized dimension D_q provides an alternative description of singular measure. It is defined as

$$D_q = [1/(q-1)] \lim_{\theta \to 0} \{\ln \textstyle\sum_i [p_i(\theta)]^q / \ln \theta\} \quad (5)$$

D_q corresponds to scaling exponents for the qth moments of the measure.

3. THE NUMERICAL CALCULATIONS

Based on the above analysis, we can carry out numerical calculations of electron transport. Figure 1 gives the transmission coefficient T as a function of electron energy for the three-component Fibonacci nanowires ($k = 3$) with the generations $G_8^{(3)}$, $G_{10}^{(3)}$, $G_{15}^{(3)}$, and $G_{25}^{(3)}$, respectively. It is obvious that in the case of a very small number of atoms, there is no total reflection, although there exist some regions of minimum transmission. When the number of atoms becomes large, the minima in transmission become extended gradually into the band gap where the transmission is blocked. Generally, with increasing the number of atoms in the nanowire, more and more transmission zones diminish gradually, and some of them approach zero transmission. In this way, a one-dimensional electronic band gap is realized. Meanwhile, more transmission peaks emerge. Most interestingly, some transmission peaks locate in between the band gaps. This property suggests potential applications in quantum interference devices.

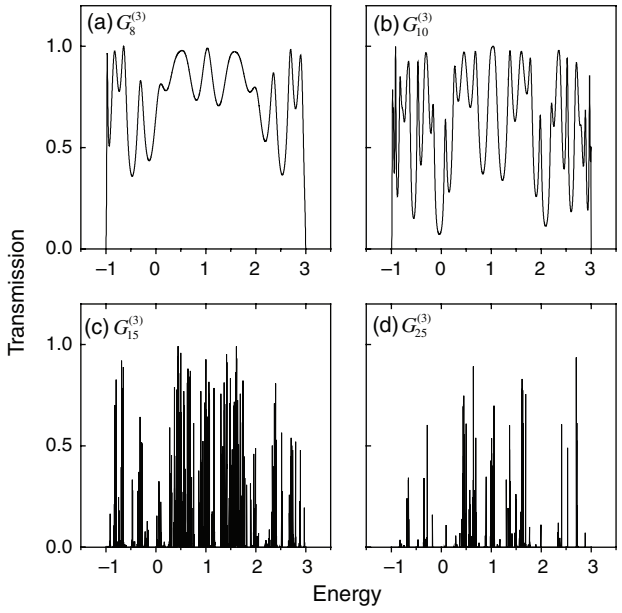

Fig. 1. Transmission coefficient T as a function of electron energy for the three-component Fibonacci structures with the following generations: (a) $G_8^{(3)}$, (b) $G_{10}^{(3)}$, (c) $G_{15}^{(3)}$, and (d) $G_{25}^{(3)}$, respectively, where $\varepsilon_1 = 1.2$, $\varepsilon_2 = 1.0$, $\varepsilon_3 = 0.8$ and $V = 1.0$.

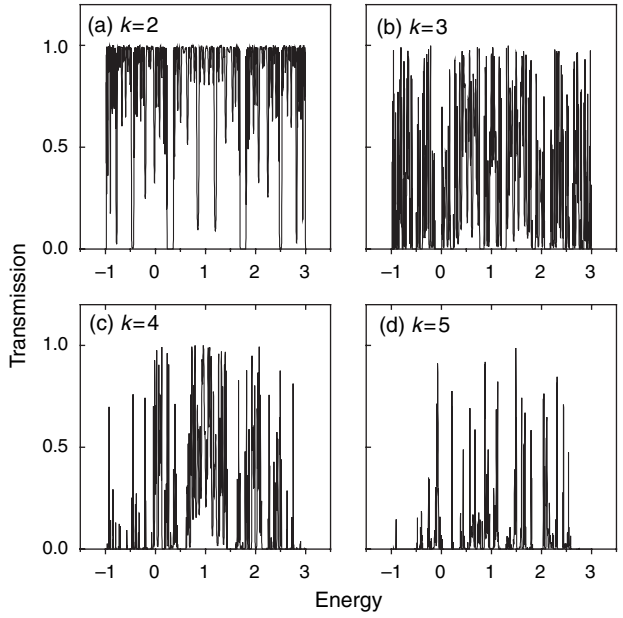

Fig. 2. Transmission coefficient T as a function of energy for the k-component Fibonacci structures with different numbers of incommensurate intervals k. The values of k, the generations, and the numbers of atoms l are as follows: (a) $k = 2$, $G_{12}^{(2)}$, and $l = 233$, (b) $k = 3$, $G_{15}^{(3)}$, and $l = 277$, (c) $k = 4$, $G_{17}^{(4)}$, and $l = 250$, (d) $k = 5$, $G_{19}^{(5)}$, and $l = 245$.

It is enlightening to compare the behaviors of the electron transport through KCF nanowires with different numbers of incommensurate intervals k. The calculations are performed on the transmission of different KCF nanowires with almost identical numbers of atoms. Figure 2 illustrates the transmission spectra for four KCF nanowires with different k. It can be seen that with increasing k, the band gaps are easily observed. It follows that the total transmission over the spectral region decreases gradually and much wider band gaps appear when k increases in the KCF nanowires. Moreover, when the value of k is sufficiently large, the transmission is basically shut off, except at a few energies where resonant tunneling takes place. It seems that if we consider the KCF nanowires for discrete logic applications, sufficient noise margins and sharp transitions between logic levels might be easily achieved, due to the fact that the 'on' and 'off' states are evident enough as shown in Figures 2(c) and (d). From this point of view, we suggest that the KCF structure might be a good candidate for use in the structural design of high-performance quantum devices for digital applications.

In order to understand the behavior of electrons in the KCF nanowire clearly, the electronic wave function has been studied. The wave function of election can be obtained by using the triangular matrix.[21] Figure 3 presents the wave functions in the KCF nanowire with $G_{15}^{(3)}$ when the electron is close to or far away from the resonant energies. It is obvious that the wave function is almost extended (shown in Fig. 3(a)) if the electron energy is close to the resonant energy E_1. In other words, electron with the energy E_1 can propagate through the whole nanowire $G_{15}^{(3)}$. Meanwhile, localized and intermediated wave functions can be observed when the electronic energy is far away from the resonant energy, as shown in Figures 3(c) and (d), respectively. Therefore, in the KCF nanowire, the transmission coefficient is almost not

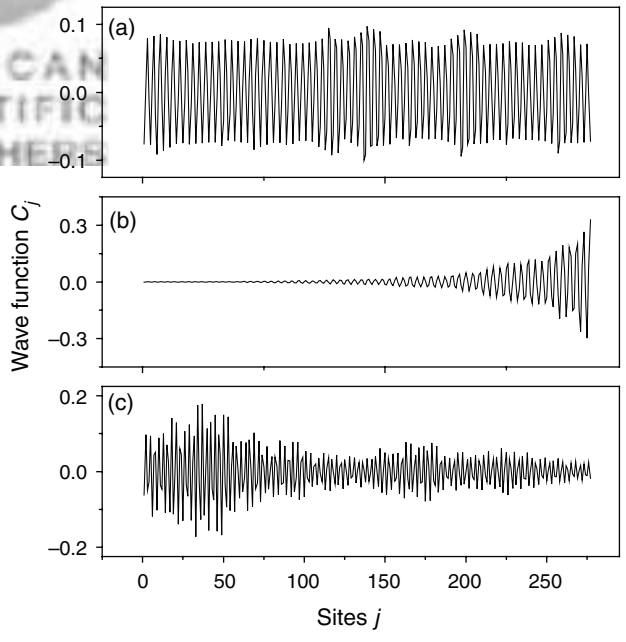

Fig. 3. Wave functions of the electron in the KCF nanowire $G_{15}^{(3)}$. The electronic state is almost extended when (a) $E_1 \approx 1.02993270$. The electron state is localized when (b) $E_2 \approx 1.22242510$. And the intermediate state is shown in (c) $E_3 \approx -0.36080077$.

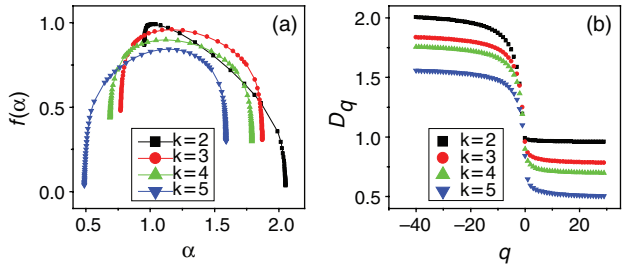

Fig. 4. (a) $f(\alpha)$ spectra and (b) plot of the generalized dimension D_q as a function of q, for the transmission distributions of the KCF nanowires where $k = 2, 3, 4, 5$, respectively.

suppressed if there is an extended electronic state. However, if the electronic state is intermediated or localized, transmission coefficient is significantly decreased.

Now we illustrate the multifractality of the transmission spectra shown in Figures 2(a)–(d). We have calculated the $f(\alpha)$ spectra and the generalized dimension according to Eqs. (3)–(5) (as shown in Fig. 4). The quantity $f(\alpha)$ is commonly the dimension of the set of energy E in the transmission spectrum. There are several physical meanings.

(i) The abscissa α_0 of the summit of the $f(\alpha)$ curve, which corresponds to $q = 0$, is the strength of a generic singularity. When k increases, the fractal dimension of the support $f(\alpha_0)$ decreases correspondingly due to the width of the electronic band gap is enlarged.

(ii) The extremes $\alpha_{\min}$ and $\alpha_{\max}$, which represent the minimum and the maximum of the singularity exponent α. By increasing k in the KCF nanowires, the value of $\Delta\alpha = \alpha_{\max} - \alpha_{\min}$ also gradually increases. This implies that the electron transmission measure of the KCF nanowires approaches the behavior of a random system when k increases.

(iii) The dimension of the set of transmission peaks $f(1)$ represents the dimension of the set of energy for which the local singularity exponent α is less than unity.

As shown in Figure 4(a), when k increases, $f(1)$ decreases evidently. Therefore, different KCF nanowires exhibit different transmission distributions. On the other hand, the generalized dimension D_q characterizes the nonuniformity of the measure. The plots of D_q versus q in Figure 4(b) correspond to the plots of $f(\alpha)$ versus α in Figure 4(a). For some special values of q, one can take D_q as the dimension of a special set.

(1) D_0 for $q = 0$ is the dimension of the support as mentioned above, $D_0 = f(\alpha_0) < 1$.

(2) For $q = 1$, $f(\alpha(1)) = \alpha(1) = D_1$. The distance of D_1 to unity is a faithful measure of how singular the transmission measure is. Figure 4(b) shows $D_1 < D_0 < 1$. So the transmission distribution of the KCF nanowires is definitely a fractal measure.

(3) D_2 for $q = 2$ is the correlation dimension. We have $D_2(k) < D_2(k')$ in the KCF if $k > k'$.

It has been demonstrated that when k becomes larger, there are fewer transmission peaks in the transmission spectrum of the KCF nanowire and the electronic band gaps are definitely enlarged. The above scaling analysis indicates that the transmission spectra of the KCF $(1 < k < 6)$ are singular continuous and possess multifractality.

4. SUMMARY

In summary, we have presented electronic transmission and switch effect in KCF nanowires. Electronic band gap structure is realized for the KCF nanowires with an identical k by increasing the length of the nanowire. For finite KCF nanowire, by increasing the number of different incommensurate intervals k, the width of electronic band gap is enlarged. Moreover, a dimensional spectrum of singularities associated with the transmission spectrum demonstrates that the electron propagation in the KCF nanowire shows multifractality. These investigations open a unique way to control quantum transport in nanodevices.

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