Electron transmission in a one-dimensional quasicrystal

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(Received 7 July 1986)

The resistance of a one-dimensional quasicrystal has been calculated at zero temperature by using the Landauer formula. Our result shows that two kinds of electron-energy regions exist. One corresponds to localized states with the resistance exponentially increasing with sample length and the other one corresponds to extended states or resonant tunneling states with finite resistance R. The localization length $L_c(k)$ has also been computed as a function of k, and it shows a self-similar structure for local regions of electron energy.

Recently, quasicrystals or nonperiodic lattices with long-range order have attracted wide attention as new ordered and condensed materials, which seem to be the intermediate cases between the truly random and periodic lattices and possess rather unusual mathematical structures.[1-3] In this article, we shall study the problem of single-electron transmission in a one-dimensional (1D) quasicrystal. Based on our knowledge, it has not yet been fully studied.[4] In the following, we shall use the iterating method to generate a quasicrystal, even though the construction of a 1D quasicrystal with two different spacings by projecting method has been explicitly discussed previously.[5] Denoting a and b as the two basic lengths, one can generate a quasicrystal by the following iterating rule:

$$\begin{aligned} a &\rightarrow f(a,b)\ , \\ b &\rightarrow g(a,b)\ , \end{aligned} \tag{1}$$

where $f(a,b)$ and $g(a,b)$ are sequences consisting of the elemental codes a and b. For example, suppose the two sequences are $f(a,b)=ab$ and $g(a,b)=a$. One can generate the following sequences, starting from element b, by Eq. (1):

b
a
ab
aba
$abaab$
$abaababa$
. . . .

As the iterating number N goes to infinity, we obtain an infinitely long quasicrystal with Fibonacci sequence. A trivial example is $f(a,b)=g(a,b)$. This situation reduces into a periodic lattice. A specific class of quasicrystals with $g(a,b)=a$ can be explicitly expressed by an iterating equation which generates the Nth sequence from $(N-1)$th and $(N-2)$th sequences. Denoting Q_N as Nth quasicrystal sequence, the iterating equation for the case of $g(a,b)=a$ is

$$Q_N=f(Q_{N-1},Q_{N-2})\ , \tag{2}$$

where f is the same function of sequence as defined in Eq. (1). The Fibonacci sequence discussed above belongs to this class, and from Eq. (2) its iterating equation reduces to

$$Q_N^f=Q_{N-1}^f Q_{N-2}^f \tag{3}$$

with $Q_1^f=b$ and $Q_2^f=a$. We shall consider the Fibonacci sequence only; other sequences described by Eq. (2) should yield no qualitatively different results. The electronic properties of a single electron in 1D random and periodic lattices are well known; the electron exhibits localized behavior in a random lattice except for some discrete resonant states.[6] In a periodic lattice the allowed electron states are extended. For a 1D quasicrystal, the behavior of a single electron seems to be in between those of random and periodic cases. Due to the nonperiodic and long-range order property of the crystal, we expect that the unusual feature should appear in the electron-transmission coefficient.

For simplicity, we shall consider an electron moving in a 1D quasicrystal along which the δ-function potentials are located at the lattice sites x_i and with strength V. It can be described by the following Schrödinger equation:

$$-\frac{d^2}{dx^2}\psi(x)+\sum_{i=1}^{f_N} 2V\delta(x-x_i)\psi(x)=k^2\psi(x)\ , \tag{4}$$

where $k=(2E)^{1/2}$ and E is the energy of the tunneling electron, $f_N=f_{N-1}+f_{N-2}$ is the Fibonacci number, with $f_0=f_1=1$, and the unit of $m=\hbar=1$ has been used. The solution of Schrödinger equation in the region of $x_n<x<x_{n+1}$ can be expressed as

$$\psi_n(x)=A_n e^{ik(x-x_n)}+B_n e^{-ik(x-x_n)}\ . \tag{5}$$

By matching the wave function at $x=x_n$, we obtain

$$\begin{bmatrix} A_{n+1} \\ B_{n+1} \end{bmatrix} = \begin{bmatrix} \left(1+\frac{V}{ik}\right)e^{ik\Delta_n} & \frac{V}{ik}e^{-ik\Delta_n} \\ -\frac{V}{ik}e^{ik\Delta_n} & \left(1-\frac{V}{ik}\right)e^{-ik\Delta_n} \end{bmatrix} \begin{bmatrix} A_n \\ B_n \end{bmatrix}$$

$$= t_n \begin{bmatrix} A_n \\ B_n \end{bmatrix} \tag{6}$$

where $\Delta_n = x_{n+1} - x_n$ can be either a or b according to the sequence. Denoting

$$T^N = \prod_{n=1}^{f_N} t_n \ , \tag{7}$$

as the transfer matrix of Nth Fibonacci sequence, we obtain the iterating equation from Eq. (3),

$$T^N = T^{N-1}T^{N-2} \tag{8}$$

with $T^1 = t_b$ and $T^2 = t_a$. Following Kohmoto *et al.*[7,8] and defining $X_N = \mathrm{Tr}(T^N)/2$, Eq. (8) can be cast into a nonlinear mapping

$$X_N = 2X_{N-1}X_{N-2} - X_{N-3} \ . \tag{9}$$

A conserved quantity λ^2 can be found[7,9] as

$$\lambda^2 = \tfrac{1}{8}\mathrm{Tr}(T^N, T^{N-1})$$

$$= -1 + X_N^2 + X_{N-1}^2 + X_{N-2}^2 - 2X_N X_{N-1} X_{N-2} \tag{10}$$

here $(T^N, T^{N-1}) = T^N T^{N-1} - T^{N-1}T^N$. In fact, λ^2 depends on k but not on N. Replacing (X_{N-2}, X_{N-1}, X_N) by (X, Y, Z) in Eq. (10) and setting $\lambda^2 = \text{const}$, the above equation determines a 2D surface in space (X, Y, Z). If an initial point (X_0, X_1, X_2) is chosen on the surface, then the following iterating points (X_{N-2}, X_{N-1}, X_N) generated by Eq. (9) will be on the same surface.

For δ-function potentials, one should choose

$$T^0 = \begin{bmatrix} e^{ik(a-b)} & 0 \\ 0 & e^{-ik(a-b)} \end{bmatrix}$$

in order to satisfy Eq. (8), namely $T^2 = T^1 T^0$. Therefore, the initial point (X_0, X_1, X_2) can be expressed as

$$\begin{aligned} X_0 &= \cos[(1-\gamma)k] \ , \\ X_1 &= \cos(k) + (V/k)\sin(k) \ , \\ X_2 &= \cos(k\gamma) + (V/k)\sin(k\gamma) \ , \end{aligned} \tag{11}$$

which is a function of k, where $b = 1$ and $a = \gamma$ have been chosen. For a periodic case $\gamma = 1$, $X_0 = 1$ and $X_1 = X_2$, the initial points are always on the $\lambda^2 = 0$ surface; the regions that $|X_1| > 1$ correspond to energy gaps while $|X_1| < 1$ correspond to energy bands.[10] For a quasicrystal $\gamma \neq 1$, we have

$$\lambda^2 = \frac{V^2}{k^2}\sin^2[(1-\gamma)k] \ , \tag{12}$$

where only the points (X_0, X_1, X_2) with $k = k_n = n\pi/(1-\gamma)$ touches the $\lambda^2 = 0$ surface and they belong to the discrete set of tunneling states in k space. This is different from the tight-binding model where λ^2 is independent to electron energy[7,8] or k. There exist two kinds of k regions. One corresponds to those points (X_0, X_1, X_2) from which the iterating points escape to infinity as N becomes large; namely $X_N \to \infty$ as $N \to \infty$. We shall call these points escaping points, while the other kind of points do not escape to infinity as nonescaping points.

We have performed a numerical calculation for the iteration of Eq. (8) up to $N = 100$ which corresponds to a long chain with the length about 10^{21} in the unit of a or b. The dimensionless resistance of the Fibonacci sequence with δ-function potentials has been calculated by using the Landauer formula[11] $R_N = |T_{12}^M|^2$, where T_{12}^N is the off-diagonal element of transfer matrix T^N. To convince ourselves we first calculated the resistance $R = R_{100}$ as a function of k for the periodic lattice by setting $\gamma = 1$. In comparison with the analytic band structure, the resistance R and $|X_1|$ vs k have been plotted in Fig. 1. It is easy to see that the resistance is infinitely large at the gap regions which correspond to $|X_1| > 1$ and it oscillates rapidly and has finite value in the conduction bands which correspond to $|X_1| \leq 1$. The smooth upper limit for the resistance in the band region shown in Fig. 1 is caused by the reflection at the two ends of a finite chain. For quasicrystals $\gamma \neq 1$, the resistance R changes quickly as a function of k and shows that two kinds of electron energy regions exist, namely $R \sim C$ and $R \sim e^{\alpha L}$, where C is k dependent and has finite value even for the crystal length $L \to \infty$. The regions for $R \sim C$ originate from the nonescaping points (X_0, X_1, X_2) which form a Contor set in k space;[7] these states correspond to the resonance tunneling in a 1D random lattice.[6] On the other hand, the regions that $R \sim e^{\alpha L}$ for a long chain can be recognized as escaping points (X_0, X_1, X_2) which form a coset of a Contor set in k space. In the following we shall choose $\gamma = 0.6180339\ldots \simeq (\sqrt{5}-1)/2$. In Fig. 2, we show

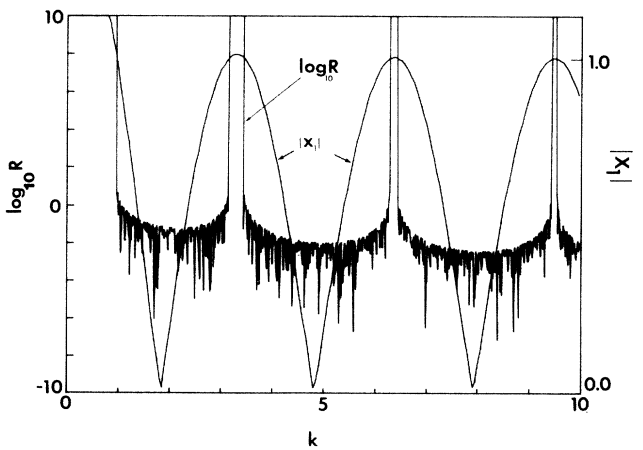

FIG. 1. The quantities $\log_{10}(R)$ with the resistance $R = R_{100}$ and $|X_1|$ are plotted as functions of k for periodic lattices, where the spacings are $a = b = 1$ and the potential strength $V = 0.5$.

$\ln(R+1)$ vs length L generated from the Fibonacci sequence at different values of k which belong to the escaping point set. The dots with large N in Fig. 2, which correspond to several different lengths using the iterating equation, are closely located on a straight line. For example, the last dots at right on line 1 and line 2 are, respectively, for $N=24$ and 39. This implies the resistance for the escaping points exponentially increasing with the sample length L.

The exponential dependence of R on L reminds us of the electron transmission in a random lattice, where the electron collides with randomly distributed scatterers and the ensemble-averaged resistance has the exponential behavior[12] $R=e^{\alpha L}-1$. Here α is the linear resistivity or the inverse of localization length. In fact, the reason for the exponential dependence $R\sim e^{\alpha L}$ in a quasicrystal is different from that of a random phase average. This will become transparent in the following analysis. Taking the logarithm on both sides of Eq. (9) and using the notation $Y_N=\ln(X_N)$, we have

$$Y_N=\ln[2\exp(Y_{N-1}+Y_{N-2})-\exp(Y_{N-3})] . \tag{13}$$

As discussed by Kohmoto *et al.*,[7] once $|X_{l-1}|>1$ and $|X_l|>1$, $Y_N=\ln|X_N|$ will grow exponentially with N as long as $N>l$. For an escaping point and sufficiently large N, $Y_N\gg 1$, and the above equation can be approximated as

$$Y_N\simeq Y_{N-1}+Y_{N-2} . \tag{14}$$

This is the same equation satisfied by the Fibonacci number f_N. Let $Z_N=Y_N/Y_{N-1}$, Eq. (14) becomes

$$Z_N\simeq 1+\frac{1}{Z_{N-1}} . \tag{15}$$

Z_N converges to the fixed point σ of Eq. (15), namely

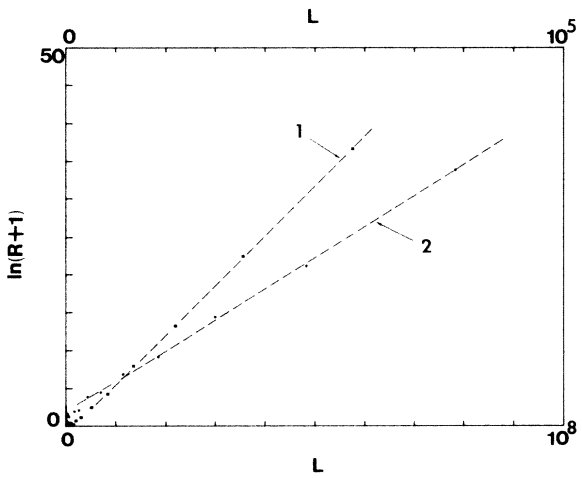

FIG. 2. The quantity $\ln(R+1)$ is plotted at several different lengths L (dots along line 1 are for $k=2.2$ and line 2 are for $k=2.0$). The last dot at right on line 1 is for $N=24$ and on line 2 is for $N=39$. Here the ratio of spacings $a/b=\gamma=0.6180339\ldots\simeq(\sqrt{5}-1)/2$ with $b=1$ and the potential strength $V=0.5$. The upper length scale is for $k=2.2$ and the lower one is for $k=2.0$.

$Z_N\to\sigma$ as $N\to\infty$, here $\sigma=(\sqrt{5}+1)/2$ is the golden mean value. Therefore, we obtain the asymptotic behavior for an escaping point

$$\frac{\ln X_N}{\ln X_{N-1}}=\sigma \tag{16}$$

as $N\to\infty$. Defining M to be an integer number such that for $N\geq M$ the above equation begins approximately valid, we obtain

$$\begin{aligned} X_{M+S}&\simeq X_{M+S-1}^{\sigma} \\ &\simeq X_M^{(\sigma^S)} . \end{aligned} \tag{17}$$

The associated sample length $L=L_{M+S}$ for the Fibonacci sequence is

$$\begin{aligned} L_{M+S}&=f_{M+S-1}a+f_{M+S-2}b \\ &=L_{M+S-1}\left[1+\frac{f_{M+S-3}a+f_{M+S-4}b}{f_{M+S-2}a+f_{M+S-3}b}\right] . \end{aligned} \tag{18}$$

Let $\sigma_N=f_N/f_{N-1}$ and $\gamma=a/b$. Equation (18) becomes

$$\begin{aligned} L_{M+S}=L_{M+S-1}[&1+1/\sigma_{M+S-2}(1+\gamma/\sigma_{M+S-3}) \\ &\times(1+\gamma/\sigma_{M+S-2})^{-1}] \end{aligned}$$

and using an asymptotic expression for $\sigma_N\simeq\sigma$ as $N\gg 1$ the above equation reduces to

$$\begin{aligned} L_{M+S}&\simeq L_{M+S-1}\left[1+\frac{1}{\sigma}\right]=L_{M+S-1}\sigma , \\ &\simeq L_M\sigma^S . \end{aligned} \tag{19}$$

Eliminating σ from Eqs. (17) and (19) we obtain

$$X_{M+S}\simeq X_M^{(L_{M+S}/L_M)} . \tag{20}$$

From the expression of transfer matrix

$$T^N=\begin{bmatrix} \sqrt{1+R_N}e^{i\phi_N} & \sqrt{R_N}e^{i\theta_N} \\ \sqrt{R_N}e^{-i\theta_N} & \sqrt{1+R_N}e^{-i\phi_N} \end{bmatrix}$$

and the definition of X_N, $|X_{M+S}|^2$ can be shown to have the form

$$|X_{M+S}|^2=(R_{M+S}+1)\cos^2(\phi_{M+S}) . \tag{21}$$

By Eqs. (20) and (21) we finally have

$$R_{M+S}\simeq\exp\left[\frac{L_{M+S}}{L_c(M)}-2\ln|\cos(\phi_{M+S})|\right]-1 , \tag{22}$$

with the localization length

$$L_c(M)\simeq\frac{L_M}{2\ln|X_M|} . \tag{23}$$

The exponential dependence of $R=R_{M+S}$ on $L=L_{M+S}$ is rigorously valid for large L. The term $2\ln|\cos\phi_{M+S}|$ in Eq. (22) usually makes a small deviation from the straight line for $\ln(R+1)$ vs L as shown in Fig. 2.

The numerical calculation of the localization length

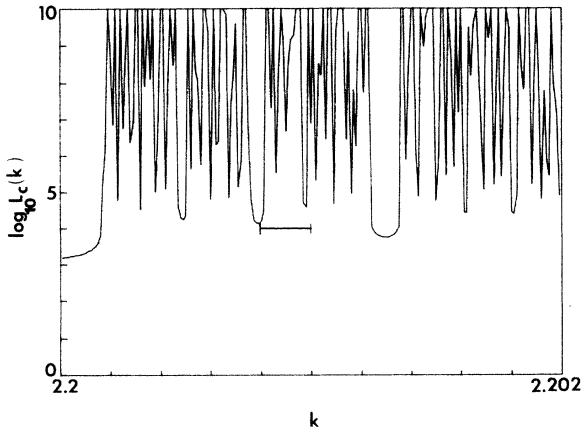

FIG. 3. The quantity $\log_{10}[L_c(k)]$ is plotted as function of k for the Fibonacci sequence with $\gamma = 0.6180339\ldots \simeq (\sqrt{5}-1)/2$ and $b=1$. The potential strength $V=0.5$.

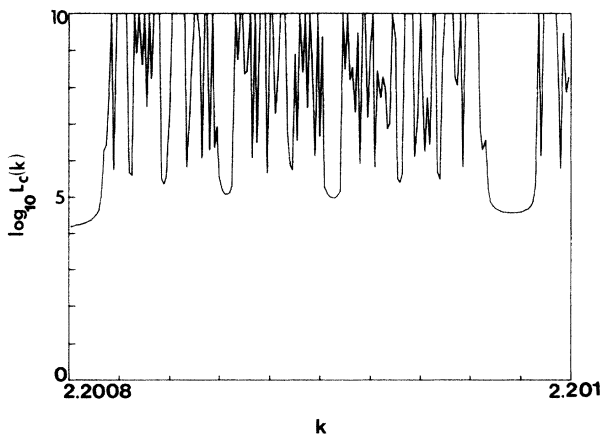

FIG. 4. The quantity $\log_{10}[L_c(k)]$ is plotted as function of k for a narrow region which is indicated by a bar in Fig. 3.

$L_c(k)$ defined as $L_{100}/\ln(R_{100}+1)$ has been carried out, which is a sensitive function of k. In Fig. 3, we plot $L_c(k)$ vs k in the neighborhood of $k=2.2$. In Fig. 4 the same quantity is plotted with a finer scale in k space which corresponds to the region indicated by the horizontal bar in Fig. 3. 200 calculated points have been shown in Figs. 3 and 4, but the detailed structures of the regions with many peaks and valleys are not shown clearly here. Values of $L_c(k)$ larger than 10^{10} have been cut off from the figures. Comparing the smooth regions of $L_c(k)$ in Figs. 3 and 4 clearly shows a self-similarity in local k space.

In conclusion, we have examined and given the qualitative picture of single-electron transmission through a 1D quasicrystal with the Fibonacci sequence at zero temperature. It states that two kinds of energy regions exist. One corresponds to localized states with the resistance $R \sim e^{\alpha L}$ and the other one corresponds to extended or tunneling states with finite R. The exponential dependence of R on L has been analytically studied, as we have shown that it has a quite different origin as in the case of a random phase average for a 1D disordered lattice.[12] Numerical simulation shows that self-similarity appears in the localization length $L_c(k)$. This property, embedded by the structure of quasicrystals, should also appear in other physical quantities like the transmission coefficient for electromagnet waves.

We would like to thank Professor S. C. Moss for helpful discussions. This work is partly supported by a grant from the Texas Advanced Technological Research Program.

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