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Conductance of a Penrose tiling

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The conductance of a tight-binding model on a Penrose tiling is calculated as a function of Fermi energy by the multichannel Landauer formula. The conductance shows spiky fine structures. The behavior of the conductance is compared with the density of states of the corresponding system. It is also found that the dependence of the conductance on the system size is anomalous and analogous to the universal conductance fluctuation.

The discovery of fivefold symmetry by Shechtman, Blech, Gratias, and Cahn[1] sparked off intensive investigation of a new state of matter, quasicrystals. Typical examples of the quasicrystals in low dimensions are a Penrose tiling in two dimensions and a Fibonacci chain in one dimension. Concerning electronic states, the quasicrystals have two fundamental properties:[2] lack of translational symmetry and existence of self-similarity. The former has a tendency to cause wave-function localization. The latter results in the property that every patch in a lattice occurs infinitely often and the distance between two neighboring patches is the same order of magnitude as its diameter. This repetition causes the wave functions to become delocalized.[3] In the Fibonacci chain competition between these two tendencies is clearly seen and there is a consensus that the energy spectrum is a Cantor set[4] and that wave functions of the eigenstates are critical,[5,6] i.e., neither extended nor localized. Analysis of eigenstates of a Penrose tiling is more difficult; however, numerical calculations of eigenstates of a Penrose tiling show similar features to the Fibonacci chain.[3] The energy spectrum also seems to be singular but does not have a simple self-similar structure of energy gaps like the one observed in the Fibonacci chain. Most of the wave functions are also critical and show a power-law decay.

In the present paper we study the conductance of the Penrose tiling. It is not trivial to define the conductance of such an aperiodic lattice. When one uses an arbitrary part of the Penrose tiling and calculates its conductance, it is difficult to make a systematic analysis because there is no natural way to attach lead lines and the rough edges will produce large scattering. To investigate the eigenstates of the Penrose tiling we used the *periodic Penrose tilings*[3,7] (PPT's) which optimally approximate the original one; the matching rule to construct the Penrose tiling is violated on only two edges independent of the size of the unit cells of the PPT's. The PPT's are very convenient systems in which to study conductance, since it has a natural way to attach the lead lines and it is free from the edge scattering due to the imposition of the periodic boundary condition in the vertical direction. We have calculated the conductance with increasing system size. It shows rapid fluctuations as a function of the Fermi energy. The fluctuations of the conductance are related to the roughness of the energy spectrum and are considered to originate from the power-law decay of the eigenfunctions. We note that the strongly localized system shows bigger fluctuations due to resonant tunneling. Here the resonance is not so sharp as in the localized system.

In a previous work we studied the two-dimensional Fibonacci lattice (2D FL) as a simpler two-dimensional quasicrystal.[8] There we found that quasiperiodic potential had a critical strength. Below the critical value, the energy spectrum has finite measure but zero measure above it. In the weak-potential regime, fluctuation of the conductance increases with the system size but it is smaller than the average of the conductance. Above the critical value, the fluctuation is on the order of unity and on the same order as the average. This example suggests the possibility of the existence of a critical energy which also separates the two regimes in the Penrose tiling and actually we will see that the character of the fluctuation changes from the low-energy to the high-energy case.

We calculate the conductance at zero temperature by using the multichannel Landauer formula,[9] $g=\mathrm{Tr}(tt^{\dagger})$, where g is a dimensionless conductance in units of e^2/h and t is the transmission matrix. When there is an underlying regular lattice (e.g., 2D FL, Anderson localization problem on a regular lattice, etc.), it is generally more convenient to use Pichard's expression[10] for the Landauer formula; $g=\mathrm{Tr}\{2/[TT^{\dagger}+(TT^{\dagger})^{-1}+2]\}$ where T is the transfer matrix at a given energy E. But in the Penrose tiling, the number of sites connected to a certain column is in general not the same as in the column. In that case, some modes of an incident wave are totally reflected independent of energy. Therefore it is impossible to define the transfer matrix and we are obliged to calculate the scattering matrix S directly.

As a scatterer, we use a unit cell of a PPT (N sites) and M sites on the adjacent line, where M is the number of the channels (shaded region in Fig. 1). Two semi-infinite square lattices with the same width M are connected on both sides as lead lines. The periodic boundary condition is imposed in the vertical direction. Therefore the system is in a cylindrical shape with finite sites in the vertical direction. The model we use is a tight-binding Hamiltoni-

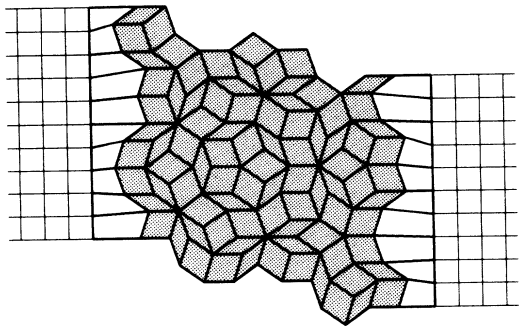

FIG. 1. Geometry of the scattering problem. $N=76$, $M=10$.

an with an s-orbital placed on the *center* of each rhombus and where the transfer energy is a constant (-1) for nearest-neighbor pairs. Since the atomic configuration is not bipartite, the energy spectrum is asymmetric.

In the lead lines, the wave function with energy E can be expanded into plane waves (open channels) and exponentially decaying functions (closed channels). They have parallel and perpendicular wave numbers k_x and k_y which satisfy the following relation:

$$E=-2(\cos k_x+\cos k_y),\quad 0\leqq \mathrm{Re}k_x<\pi,\quad k_y=2\pi n/M \qquad (n=0,1,\ldots,M-1).$$

A real k_x corresponds to an open channel and a complex k_x to a closed channel. Let M_0 be the number of open channels. The S matrix relates amplitudes of the $2M_0$ incident plane waves to those of the $2M_0$ scattering plane waves

$$\begin{pmatrix} b_L \\ b_R \end{pmatrix} \equiv S \begin{pmatrix} a_L \\ a_R \end{pmatrix} \equiv \begin{pmatrix} r & t' \\ t & r' \end{pmatrix} \begin{pmatrix} a_L \\ a_R \end{pmatrix},$$

where a and b are the amplitudes of the incident and scattering waves and the subscripts L and R indicate the left and the right lead lines. The S matrix is composed of transmission matrices t,t' and relfection matrices r,r'. For given a_L and a_R, we solve the Schrödinger equation, $H\psi_i=E\psi_i$ at $N'\equiv N+M$ sites of the scatterer and at adjacent $2M$ sites in the lead lines on both sides (bold tetragons in Fig. 1). The unknown variables are N' amplitudes at the sites inside the scatterer, $2M_0$ amplitudes for the outgoing plane waves (b_L and b_R), and $2(M-M_0)$ amplitudes for exponentially decaying modes. Therefore the number of equations is sufficient to obtain b_L and b_R in terms of a_L and a_R.

We calculated conductance of Penrose tilings as a function of Fermi energy using five different unit cells of PPT's.[11] The size of the scatterers is $N=76$, 199, 521, 1364, and 3571, and the numbers of the channels are $M=10$, 16, 26, 42, and 68, respectively. Typical results are shown in Fig. 2. We immediately notice spiky fine structures. The structures are not simply due to the finiteness of the scattering sites; when a part of regular lattice is used as a scatterer, it has larger conductance and smaller fluctuation. These structures are due to the resonant tunneling; however, in an ordinary metallic system resonances are broadened.[12] These narrow widths are expected on the basis of our previous work[3] indicating that most of the wave functions in the Penrose tiling show power-law decay because for such a type of wave functions it is hard to permeate into the lead lines. Overlapped with these fine fluctuations, there are global structures depending on energy; the conductance is large in the low-energy region and shows some large dips.

The energy dependence of the conductance is related to the density of states (DOS). Figure 3 shows the DOS of the PPT's without lead lines. On the unit cells of the PPT's, the periodic and antiperiodic boundary conditions can be imposed. We obtain four eigenvalues corresponding to Γ, X, Y, and M points in the Brillouin zone for each band. We suppose that there is no level crossing and approximate the band by a square one between the minimum and the maximum. We then obtain the DOS curves shown in Fig. 3. At lower energies many bands overlap, while at higher energies there are many tiny gaps whose number is comparable as the number of the bands itself. As a result, the DOS curve looks smoother in the lower-energy region than in the higher-energy region. This means that wave functions at lower energies are extended more than at higher energies. Clearly there is correspondence between the DOS and the conductance.

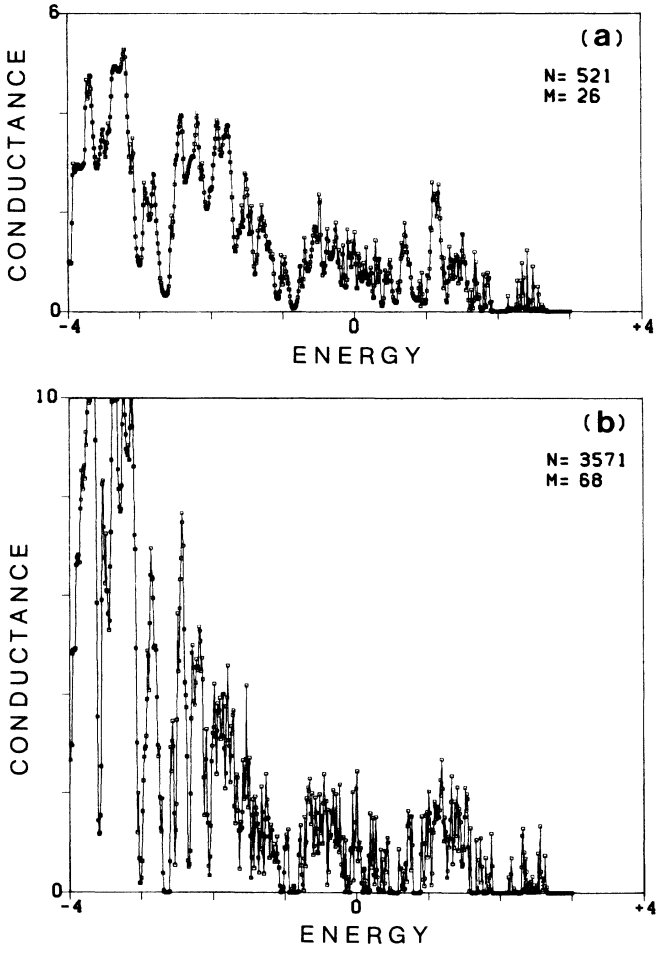

FIG. 2. Conductances in units of e^2/h of Penrose tilings as a function of Fermi energy at every 0.01. The case of $E=2$ is not calculated.

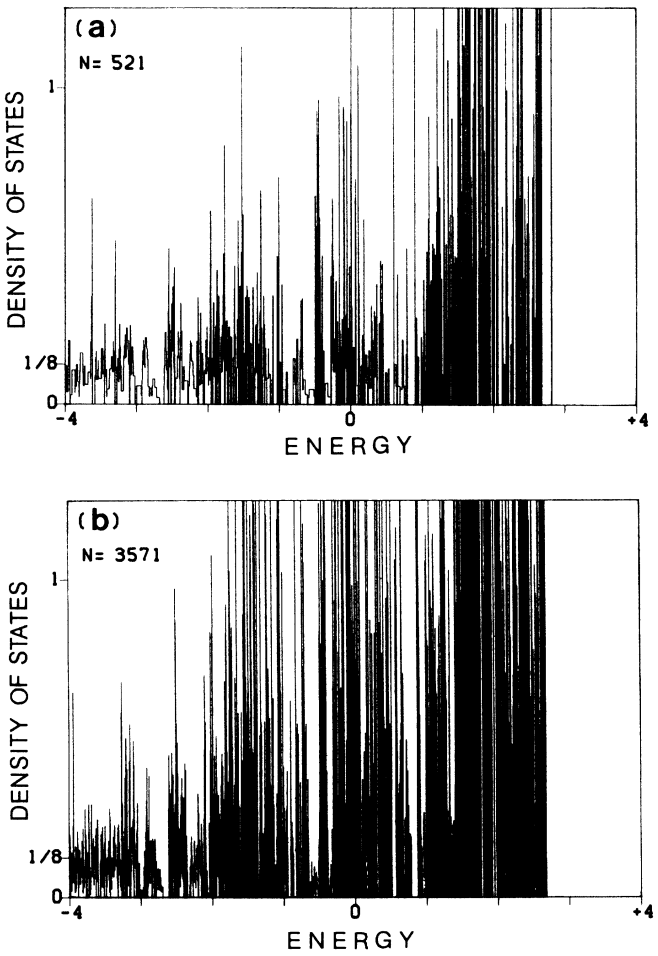

FIG. 3. Density of states of periodic Penrose tilings.

The conductance is also smoother at low energies.. There are several outstanding gaps in the DOS. At the gaps, the conductance is nearly zero, as it should be. But dips corresponding to very narrow gaps disappear due to the finite size of the scatterer.

The size dependence of the conductance varies with energy. We divide the total energy region into five subregions separated by large gaps in the DOS. The averages and the standard deviations of the conductance in each region are plotted in Fig. 4. In the region A for example, the standard deviation is smaller than the average and the average increases with the size of the scatterer. In regions D and E the standard deviations are order of unity and on the same order as or greater than the averages, and both exhibit only weak system dependence. Therefore even in the macroscopic system the conductance is not well defined. This is similar to the universal conductance fluctuation.[12] This similarity is due to the power-law behavior of wave functions. We note that the behavior of the conductance in low- and high-energy regions resemble those of the 2D FL in weak and strong potential cases.

Thouless numbers[13] $\delta E/\Delta E$ are also calculated (Fig. 5). Here δE is the difference between the maximum and the minimum of four eigenenergies at Γ, X, Y, and M points, and ΔE is distance between two neighboring states defined

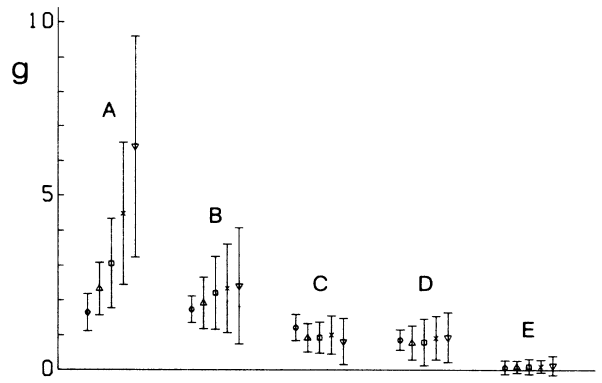

FIG. 4. Averages and standard deviations of the conductances in five energy regions; $E=$ (A) -4.00 to -2.69, (B) -2.61 to -0.95, (C) -0.82 to 0.78, (D) 0.88 to 1.92, (E) 1.98 to 3.00. Five systems are used: ○, $M=10$, $N=76$; △, $M=16$, $N=199$; □, $M=26$, $N=521$; ×, $M=42$, $N=1364$; ▽, $M=68$, $N=3571$. The unit of g is e^2/h.

by the average of these four points. The Thouless number represents sensitivity to the boundary condition and is a measure of the conductance. The smoothness of the DOS manifests itself in ΔE and δE is the measure of the degree how the wave functions are extended. It is readily seen that the overall features are very similar to those in Fig. 2.

In conclusion, we have computed systematic approximations to the conductance of a Penrose tiling using the Landauer formula and a sequence of unit cells of the periodic Penrose tilings, the properties of which approach those of the perfect Penrose tiling. We have observed rich structure in the dependence of the conductance on the Fermi energy and an anomalous unit-cell size dependence, similar to the phenomenon of the universal conductance fluctuation in mesoscopic systems. This behavior is related to the singular behavior of the density of states and the wave functions of the quasicrystals. We believe such anomalous behavior may be reflected in the fluctuation of the conductance as a function of temperature at sufficiently low temperatures.

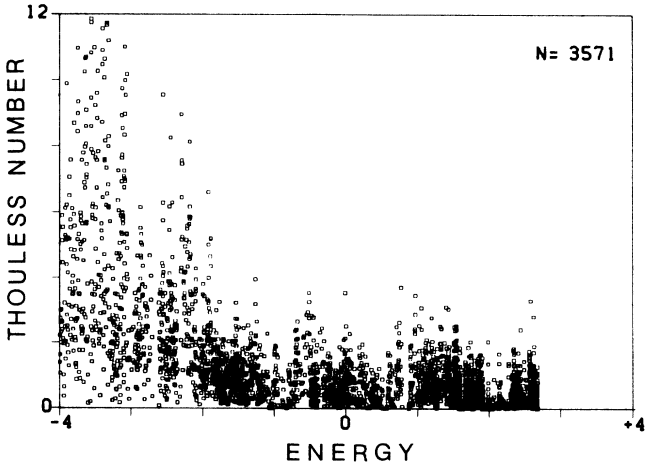

FIG. 5. Thouless number of a Penrose tiling with $N=3571$ for all eigenenergies.

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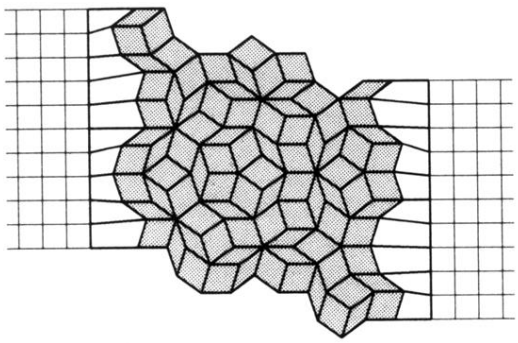

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