Energy Spectrum and Conductance of a Two-Dimensional Quasicrystal

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A model of a two-dimensional Fibonacci lattice is presented. Numerical calculations show that there is a transition as a function of strength of potential from the regime of zero spectral measure for a strong potential to the regime of finite measure for a weak potential. The conductance fluctuates with the system size and in the strong-potential regime the fluctuation is of the order of e^2/h, just like the universal conductance fluctuation in a mesoscopic random system.

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There has been much recent interest in electronic states in quasiperiodic systems. A typical example in one dimension is a tight-binding Hamiltonian where the potential or the hopping matrix element is arranged in a Fibonacci sequence—a diagonal or an off-diagonal Fibonacci chain. The Fibonacci chain was originally proposed by two groups[1,2] and has been studied very intensively by many authors.[3-8] On the basis of analytical as well as numerical studies, it is now commonly believed that the energy spectrum is a Cantor set and wave functions are critical, namely neither extended nor localized.

A prototype of two-dimensional quasicrystals is the famous Penrose tiling. Several types of tight-binding Hamiltonians on the Penrose tiling were studied by several groups.[9-11] The existence of confined states, which are special localized states whose amplitudes are nonzero only on finite clusters, was pointed out by Semba and Ninomiya[12] and independently by Kohmoto and Sutherland.[11] We have investigated the energy spectrum and wave functions numerically by use of a series of periodic tilings which tends to the perfect Penrose tiling.[10] The numerical results indicate that the spectrum is singular continuous, and most of the wave functions other than the confined states are critical.

In this Letter we present a two-dimensional Fibonacci lattice (2DFL) which is a direct extension of the 1DFL. We found that there is a transition as a function of potential. The energy spectrum of the 2DFL is always singular continuous. The transition takes place between two regimes where the spectral measures are different. In one regime where the potential is weak the spectral measure is finite, while in the other regime the spectral measure is zero. We also found that conductance of the 2DFL fluctuates when the system size is varied in microscopic scale, one lattice spacing. Interestingly enough, in the strong-potential regime the fluctuation of the conductance is of the order of e^2/h, just like the universal conductance fluctuation found by Stone and Lee.[13,14]

The Fibonacci sequence is the series $\{\tau,1,\tau,\tau,1,\ldots\}$ which is generated by the recursion relation, $\tau\rightarrow\{\tau,1\}$, $1\rightarrow\tau$ with the initial condition $\{\tau\}$. At the lth stage of the recursion the length of the sequence is the lth Fibonacci number F_l.

We consider a Schrödinger equation on the square lattice:

$$-\psi_{n+1,m}-\psi_{n-1,m}-\psi_{n,m+1}-\psi_{n,m-1}+V_{n,m}\psi_{n,m}=E\psi_{n,m}, \quad (1)$$

where the potential $V_{n,m}$ is arranged according to the Fibonacci sequence in both directions. A particularly simple case is a separable potential

$$V_{n,m}=V_n^{(1)}+V_m^{(2)} \quad (2)$$

where

$$V_n^{(i)}=\begin{cases}V^{(i)} \text{ for } n \text{ a } \tau \text{ site},\\ 0 \text{ for } n \text{ a } 1 \text{ site}.\end{cases}$$

For the separable potential an eigenfunction is a product $\psi_{n,m}=\phi_n^{(1)}\phi_m^{(2)}$ and its eigenvalue is a sum $E=E^{(1)}+E^{(2)}$, where $\phi_n^{(i)}$ is an eigenfunction of the 1D Schrödinger equation

$$-\phi_{n+1}^{(i)}-\phi_{n-1}^{(i)}+V_n^{(i)}\phi_n^{(i)}=E^{(i)}\phi_n^{(i)}. \quad (3)$$

In what follows we use a one-parameter Hamiltonian, $V^{(1)}=-V^{(2)}=V$. The densities of states of a finite lattice of 34×34 sites are shown in Fig. 1 for $V=0.25$, 1, and 4. Note that the integrated density of states when $V=4$ is a typical devil's staircase. Since the energy spectrum of the 1DFL is a Cantor set it is clear that the energy spectrum of the 2DFL is also singular continuous.

For a singular continuous spectrum its measure can be either finite or zero. To address the question we did the band calculations for periodic systems changing the size of the unit cells, $F_l\times F_l$. We calculated the total bandwidth $B(l)$ from $l=3$ to $l=12$. Kohmoto, Kadanoff, and Tang[1] have found that in the 1DFL the total bandwidth gets narrower and narrower and that the critical index defined by

$$B(l)\propto B_0F_l^{-\delta^{(d)}(V)}, \quad (4)$$

where d is the dimension of the system, changes continuously from zero at $V=0$. Figure 2 shows the critical in-

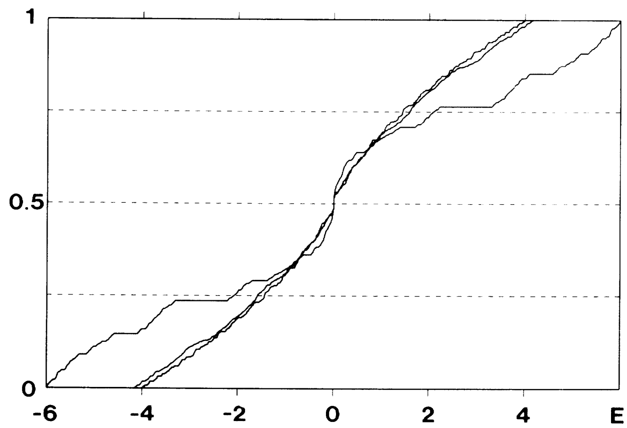

FIG. 1. Integrated density of states of a square Fibonacci lattice (34×34 sites). The potentials are $V=0.25$, 1, and 4 in the units of the transfer energy.

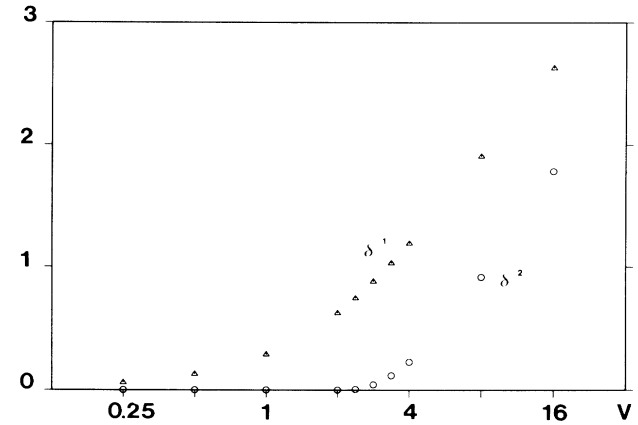

FIG. 2. Critical indices δ in 1D (triangles) and 2D (circles) as functions of potential V. The spectral measure in the 2D system is finite for V less than $2^{1.25}=2.38$.

dices for the 1DFL and 2DFL. It is clearly seen that there is a transition from the region of finite measure, $\delta^{(2)}(V)=0$, to the zero measure, $\delta^{(2)}(V)>0$. We have also confirmed that there is no gap in the spectra for weak potentials, $V=0.25$, 0.5, and 1, independent of the system size. The critical value estimated from the numerical calculation is $V_c \cong 2^{1.25}=2.38$.

The order of the critical value V_c can be understood in the following way. For large V there is an asymptotic relation between the critical indices in 1D and 2D, $\delta^{(2)}=\delta^{(1)}-1$. Now define the decreasing ratio of the bandwidth $\rho=\lim(B_{l+1}/B_l)$; then $\delta^{(1)}=-\log\rho/\log\tau$. Estimating ρ by $B_2/B_1 \cong 2/V$, we get $V_c \cong 2\tau=3.24$. The numerical result shows that this value is surprisingly close to the condition of $\delta^{(1)}=1$. Of course the bands in the 2D lattice start to overlap in the critical region leading to a correction to the asymptotic relation between $\delta^{(1)}$ and $\delta^{(2)}$.

Since the wave functions are products of those in 1D, they are critical. Conductance is sensitive to the exotic behavior of the singular continuous spectrum and the critical wave functions. The 2DFL is a very convenient system to study the conductance since the transfer-matrix method can be utilized.

We consider a strip of the 2DFL whose width is M and length is N. We use the transfer-matrix method in the N direction. Let a column vector be $\Psi_n=(\psi_{n,1}, \psi_{n,2}, \ldots, \psi_{n,M})^{\mathrm{T}}$; then the transfer matrices are defined as

$$\begin{pmatrix} \Psi_{n+1} \\ \Psi_n \end{pmatrix} = T_n \begin{pmatrix} \Psi_n \\ \Psi_{n-1} \end{pmatrix}, \tag{5}$$

where T_n is a $2M \times 2M$ matrix given by

$$T_n = \begin{pmatrix} H_n - E1 & -1 \\ 1 & 0 \end{pmatrix}. \tag{6}$$

H_n is the Hamiltonian of the isolated nth chain and E is the energy under consideration. The quantity we need is a product of the transfer matrices, $T(n)=T_nT_{n-1} \cdots T_2T_1$. It is easy to see that any positive integer is uniquely expressed by a sum of Fibonacci numbers, $n=F_{l_1}+F_{l_2}+\ldots+F_{l_m}$ ($l_i+2 \le l_{i+1}$). From the generation rule of the Fibonacci sequence the product of the transfer matrices is expressed as

$$T(n)=P_{l_1}P_{l_2}\cdots P_{l_m} \tag{7}$$

where P_l is the product of the transfer matrices for the lth Fibonacci sequence, $P_l=T_{F_l}T_{F_l-1}\ldots T_2T_1$. The advantage of the transfer-matrix method is that there is a recursion relation[1]

$$P_{l+1}=P_{l-1}P_l. \tag{8}$$

Thus we can calculate the product $T(n)$ very efficiently.

The transfer matrices are symplectic; eigenvalues are in pairs (e_i, e_i^{-1}), $i=1,2,\ldots,M$. The localization length λ is defined by[15,16]

$$\lambda=2N/\ln(e_{\min}), \tag{9}$$

where $e_{\min}$ is the minimum eigenvalue of $T(N)T(N)^\dagger$ greater than unity. This length is frequently used to discuss the localization problem and shows very unusual behavior in this system as we will show below. Since the band is symmetric for our choice of the potential, we fix the energy at the center of the band at $E=0$.

Examples of raw data of the localization length are shown in Fig. 3 for $V=4$. As the widths of the strips, M, we used $F_6=13$, $F_7=21$, $F_8=34$, $F_9=55$, and $F_{10}=89$ and N was varied from 1 to 400. The data show that λ tends to a constant value for a long strip, $N \gg M$. In Fig. 4 we plot the average of the localization length normalized by the width M, $\Lambda=\langle\lambda\rangle/M$, where the angular brackets mean the average over $N=301-400$.

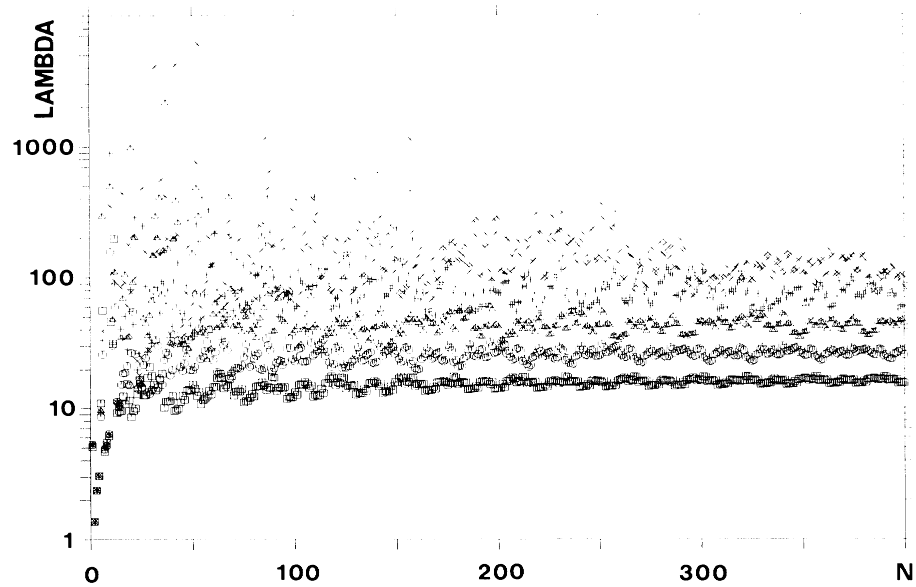

FIG. 3. Raw data of the localization length for strips whose widths are 13 (squares), 21 (octagons), 34 (triangles), 55 (pluses), and 89 (crosses).

We see that for a strong potential ($V \geq 4$) the average Λ is well defined (the standard deviation is small) and independent of the width of the strip. It means that the wave functions are critical, namely, the localization length goes to infinity as $M,N \rightarrow \infty$. For a weak potential ($V < 2$), of course, there is no localization ($\lambda \gg N \gg M$). The standard deviations are of the same order of magnitude as the mean values, showing very exotic behavior of the wave functions.

The localization length λ of 2D samples ($M \sim N$) fluctuates very rapidly. An interesting question is whether a real physical quantity shows such a fluctuation. We studied the conductance of the 2DFL with use of a multichannel Landauer formula.[17] The formula we used is the Pichard expression[18] for the dimensionless conductance g, $G = (e^2/h)g$,

$$g = \mathrm{tr}\left(\frac{2}{TT^{\dagger} + (TT^{\dagger})^{-1} + 2}\right). \tag{10}$$

The conductance fluctuates very rapidly with the length of the strip, i.e., conductivity is not well defined. The mean values $\langle g \rangle$ and the variances $\langle (\Delta g)^2 \rangle$ are listed in Table I [the average is over $N = M - (2M-1)$]. The most striking fact is that the variances for strong potentials ($V > V_c$) are of the order of unity. Note that when $V = 16$ the standard deviations are larger than the mean values and do not depend on the system size, suggesting that the fluctuation is intrinsic.

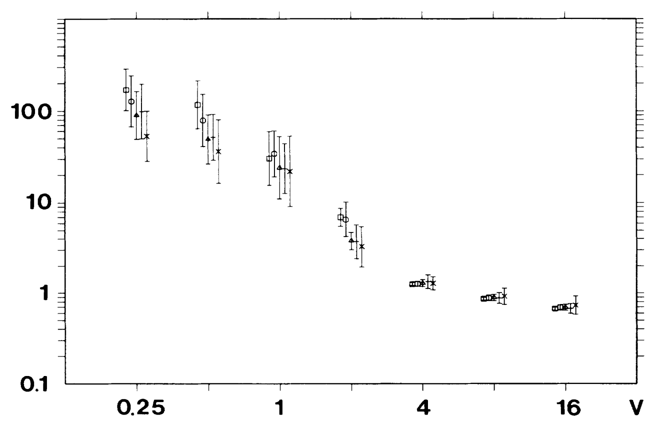

FIG. 4. Average of the localization length normalized by the width of the strips. The average is over $N = 301-400$ and the bars denote the standard deviations. Symbols as in Fig. 3.

Stone and Lee[13,14] proposed a universal fluctuation of the conductance for random systems of mesoscopic scales. Since the present system is deterministic, the mechanism of the conductance fluctuation is different from that in the random system. However, the two sys-

TABLE I. Conductance, g, of two-dimensional Fibonacci lattices.

Potential	$M = 55$		$M = 89$	
V	$\langle g \rangle$	$\langle (\Delta g)^2 \rangle$	$\langle g \rangle$	$\langle (\Delta g)^2 \rangle$
0.25	28.46	5.127	44.54	11.28
1	12.45	4.334	17.83	9.310
4	1.759	1.301	1.908	1.887
16	0.5845	1.042	0.770	1.026

tems have a common feature. Wave functions are critical and typically show power-law decay. Imry[18] proposed a general mechanism for the universal fluctuation of the conductance. He pointed out that if the eigenvalues of $\log(TT^{\dagger})$ have a random distribution of Dyson's orthogonal ensemble[19] then the variance is 0.296.

Kohmoto, Sutherland, and Tang[4] showed that depending on energy the matrix map defined by Eq. (8) has a cyclic or a chaotic trajectory in the 1D system. In 2D we have more degrees of freedom and it is natural to expect that the trajectories of the matrix map are chaotic. Thus we are led to the idea that we may treat the matrices $T(n)$ as if they were a set of random matrices. We looked at the distribution of the eigenvalues and observed that Imry's idea of the conductance fluctuation gives a consistent picture for the present case, although the distribution is not an ideal orthogonal ensemble.

We would like to stress that intrinsic fluctuations of various physical quantities in a *macroscopic* system may be a characteristic feature of a quasiperiodic system. Other examples than the conductance are periodic oscillations in the specific heat and the susceptibility of the 1D XY model.[20] The final point we want to make is that the consequences of the transition from zero spectral measure to a finite one are still to be investigated. For example, the size of our numerical study is not large enough to draw a definitive conclusion whether there is a sharp transition in the localization length or the conductance. We leave this as an interesting future problem.

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[1]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).

[2]S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. D. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).

[3]M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 145 (1984).

[4]M. Kohmoto, B. Sutherland, and C. Tang, to be published.

[5]J. P. Lu, T. Odagaki, and J. L. Birman, Phys. Rev. B **33**, 4809 (1986).

[6]M. Fujita and K. Machida, Solid State Commun. **59**, 61 (1986).

[7]F. Nori and J. Rodriguez, Phys. Rev. B **34**, 2207 (1986).

[8]T. Ninomiya, J. Phys. Soc. Jpn. **55**, 3709 (1986).

[9]T. C. Choy, Phys. Rev. Lett. **55**, 2915 (1985).

[10]H. Tsunetsugu, T. Fujiwara, K. Ueda, and T. Tokihiro, J. Phys. Soc. Jpn. **55**, 1420 (1986).

[11]M. Kohmoto and B. Sutherland, Phys. Rev. Lett. **56**, 2740 (1986).

[12]K. Semba, Master's thesis, University of Tokyo, 1985 (unpublished); and T. Ninomiya, private communication.

[13]A. D. Stone, Phys. Rev. Lett. **54**, 2692 (1985).

[14]P. A. Lee and A. D. Stone, Phys. Rev. Lett. **55**, 1622 (1985).

[15]A. MacKinnon and B. Kramer, Z. Phys. B **53**, 1 (1983).

[16]J. L. Pichard and G. Sarma, J. Phys. C **14**, L127 (1981).

[17]P. W. Anderson, D. J. Thouless, E. Abrahams, and D. S. Fisher, Phys. Rev. B **22**, 3519 (1980).

[18]Y. Imry, Europhys. Lett. **1**, 249 (1986).

[19]F. J. Dyson and M. L. Mehta, J. Math Phys. (N.Y.) **4**, 701 (1963).

[20]Th. M. Nieuwenhuizen, J. Phys. (Paris), Colloq. **7**, C3-311 (1986).