RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 40, NUMBER 10 1 OCTOBER 1989

Multifractal wave functions on a Fibonacci lattice

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(Received 31 July 1989)

Wave functions on a Fibonacci lattice are analyzed from the multifractal point of view. An entropy function $[f(\alpha)]$ which represents the distribution of a particle probability density is obtained exactly for the state at the center of the spectrum. Numerical calculations for other states are also presented. A finite-size scaling analysis shows that the ordered critical wave functions are multifractals.

The energy spectrum of a Schrödinger operator is classified into three types: absolutely continuous, singular continuous, and dense point.[1] Extended states correspond to an absolutely continuous spectrum and localized states correspond to a dense-point spectrum. For a periodic system all states are extended due to the Bloch theorem. Extended and localized states can exist for random systems. The localization problem in random systems is still one of the most important problems in condensed-matter physics.[2] However, as far as we know, there is no random system with a purely singular continuous spectrum. It is important to understand properties of wave functions which correspond to a singular continuous spectrum.

The one-dimensional tight-binding model or discrete Schrödinger equation on a Fibonacci lattice which allows an exact renormalization-group (RG) equation was proposed by Kohmoto, Kadanoff, and Tang[3] and Ostlund *et al.*[4] It is a quasiperiodic system. Although there is no rigorous proof, it is conjectured to have a purely singular continuous spectrum. This rather remarkable property is confirmed by various studies.[5-9] The energy spectrum is a self-similar Cantor set with zero Lebesgue measure. It was shown that the spectrum is a fractal with continuous scaling indices.[9] The wave functions are expected to be neither localized nor extended in a standard manner and we call them critical. Wave functions of this type are further classified into two types: self-similar and non-self-similar. It was shown[9] that a wave function which corresponds to a cycle of the RG map is self-similar. On the other hand, a wave function which corresponds to a bounded chaotic orbit is not self-similar. The purpose of this paper is to understand the critical wave functions quantitatively from the multifractal point of view.[10-15]

We study the off-diagonal version of the Fibonacci model:

$$t_{j+1}\psi_{j+1}+t_j\psi_{j-1}=E\psi_j\,, \tag{1}$$

where t_j's $(j=1,2,\ldots)$ take two values t_A and t_B arranged in a Fibonacci sequence T_∞ which is defined as the limit of a recursion $T_{n+1}=T_nT_{n-1}$ with $T_1=\{A\}$ and $T_2=\{AB\}$. So one has $T_3=\{ABA\}$, $T_4=\{ABAAB\}$, and so on. In order to investigate the infinite system, we take a series of finite systems T_n whose number of sites is a Fibonacci number F_n defined by $F_{n+1}=F_{n-1}+F_n$ with $F_0=F_1=1$. For a finite system T_n we take $p_j=|\psi_j|^2$ which is normalized by $\sum_{j=1}^{F_n}p_j=1$ as a probability measure and $l=l_n=1/F_n$ as a Lebesgue measure of each site. An exponent α_j is defined by $p_j=l^{\alpha_j}$ which represents the singularity of the probability measure. Now the distribution $\Omega_n(\alpha)$ characterizes the wave function, where $\Omega_n(\alpha)d\alpha$ is the number of sites whose value of α_j lies between α and $\alpha+d\alpha$. Since the number of sites F_n increases exponentially as n is increased $\{F_n\sim\tau^n=[(\sqrt{5}+1)/2]^n\}$, so does $\Omega_n(\alpha)$. Then the fundamental quantity to characterize the wave function is the entropy function defined by[11]

$$S(\alpha)=\lim_{n\to\infty}S_n(\alpha)=\lim_{n\to\infty}(1/n)\ln\Omega_n(\alpha)$$

or

$$f(\alpha)=S(\alpha)/\varepsilon\,, \tag{2}$$

where

$$\varepsilon=\lim_{n\to\infty}\varepsilon_n=-\lim_{n\to\infty}(1/n)\ln l_n=\ln\tau\,.$$

So one has a relation $\Omega(\alpha)\sim l^{-f(\alpha)}$.[10] The entropy function or $f(\alpha)$ is calculated from the partition function as

$$Z_n(q)=\sum_{j=1}^{F_n}|\psi_j|^{2q}=\sum_{j=1}^{F_n}p_j^q=\sum_{j=1}^{F_n}\exp(-qn\alpha_j\varepsilon_n)\,, \tag{3}$$

and

$$G_n(q)=(1/n)\ln Z_n(q)\,,$$
$$S_n(\alpha)=G_n(q)+q\varepsilon_n\alpha\,, \tag{4}$$
$$f_n(\alpha)=S_n(\alpha)/\varepsilon\,,$$

where $\alpha=-(1/\varepsilon_n)(d/dq)G_n(q)$ and

$$f(\alpha)=\lim_{n\to\infty}f_n(\alpha)\,.$$

An entropy function or $f(\alpha)$ is useful to characterize a wave function. An extended wave function does not have a singular probability measure and $p \sim l$, so $f(\alpha)$ is defined at a single point by $f(\alpha=1)=1$. On the other hand, a localized wave function has a nonvanishing probability only on a finite number of sites (Lebesgue measure zero). These sites have $\alpha=0$ and the other sites with probability zero have $\alpha=\infty$. So one has $f(\alpha=0)=0$ and $f(\alpha=\infty)=1$. It is extremely important to perform a careful extrapolation for finite systems.[12,16] Since, if one simply tries to calculate $f(\alpha)$ for a single finite system, one does not get the above behavior but obtains a misleading result of a smooth $f(\alpha)$ even for a localized or an extended state. We shall show that the wave functions on the Fibonacci lattice indeed have a smooth $f(\alpha)$ and consequently are neither extended nor localized in a standard manner.

In order to investigate the wave functions on the Fibonacci lattice, (1) is written as $\Psi_j=M(t_{j+1},t_j)\Psi_{j-1}$ with

$$\Psi_j=\begin{pmatrix}\psi_{j+1}\\ \psi_j\end{pmatrix},\quad \Psi_{j-1}=\begin{pmatrix}\psi_j\\ \psi_{j-1}\end{pmatrix},$$

and a transfer matrix

$$M(t_{j+1},t_j)=\begin{pmatrix}E/t_{j+1} & -t_j/t_{j+1}\\ 1 & 0\end{pmatrix}.$$

A wave function is obtained by multiplying Ψ_0 by transfer matrices successively once the energy is taken in the spectrum. There are three types of transfer matrices $M(t_A,t_A)$, $M(t_A,t_B)$, and $M(t_B,t_A)$ (note that there is no successive B's in the Fibonacci sequence). Denote the product of the first F_n transfer matrices by $M^{(n)}$, then we have a RG map

$$M^{(n+1)}=M^{(n-1)}M^{(n)}, \tag{5}$$

with $M^{(1)}=\bar{B}=M(t_A,t_A)$, and $M^{(2)}=\bar{A}=M(t_A,t_B)\times M(t_B,t_A)$.[3,4,8] Let us define $x_n=\mathrm{Tr}\{M^{(n)}\}/2$, then the energy spectrum of a periodic system consisting of T_n's is determined by a condition $|x_n|<1$. It can be shown[3] that x_n obeys a trace map

$$x_{n+1}=2x_nx_{n-1}-x_{n-2}. \tag{6}$$

The energy E enters in the initial condition and those which give bounded orbits determine the spectrum. In particular, the center of the spectrum has a six-cycle[5] and the outermost edge of the spectrum has a two-cycle.[9] Most of the bounded orbits, however, are chaotic. We shall analyze the wave functions corresponding to the above types of orbits. Note that we need a solution of the full RG map (5) to determine the wave functions.

Wave function at the center of the spectrum

When $E=0$, not only the trace map (6) but also the full RG map (5) has a six-cycle starting from

$$\bar{B}=M(t_A,t_A)=\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix},$$

and

$$\bar{A}=M(t_A,t_B)M(t_B,t_A)=\begin{pmatrix}-R & 0\\ 0 & -1/R\end{pmatrix}$$

with $R=t_B/t_A$.[8] This remarkable property allows us to determine $f(\alpha)$ exactly. Consider a finite system T_{3k+1} which consists of the first F_{3k+1} sites of the Fibonacci lattice. The wave function is determined by $\Psi_j=M_j\Psi_0$ where M_j is a product of $\bar{A}$'s and $\bar{B}$'s following the Fibonacci sequence and the bond j (between sites j and $j+1$) is always of type A. Since two successive $\bar{B}$'s are not allowed, these Ψ_j's are enough to determine the wave function ψ_j on all the sites. If one takes $\Psi_0=\binom{1}{1}$, the absolute values of Ψ_j is of the form $\binom{R^{-s}}{R^s}$ where s is an integer. Denote the number of such Ψ_j as $N_A(s,k)$ [or $N_B(s,k)$] if the last matrix in M_j is $\bar{A}$ (or $\bar{B}$). Then the partition function (3) is written as

$$Z_{3k+1}(q)=\frac{2n_A(R^{2q},k)+n_B(R^{2q},k)}{[2n_A(R^2,k)+n_B(R^2,k)]^q}, \tag{7}$$

where

$$n_A(x,k)=\sum_{s=-\infty}^{\infty}N_A(s,k)x^{-s},$$

$$n_B(x,k)=\sum_{s=-\infty}^{\infty}N_B(s,k)x^{-s},$$

and the denominator is the normalization factor of the wave function $(\sum_{j=1}^{F_{3k+1}}|\psi_j|^2)^q$. It can be shown that, if the next system $T_{3(k+1)+1}$ with $F_{3(k+1)+1}$ sites is considered, N_A and N_B obey a recursion relation

$$\begin{aligned}N_A(s,k+1)&=N_A(-s+2,k)+N_A(s+1,k)+N_A(s,k)+N_B(-s,k)+N_B(s-1,k),\\ N_B(s,k+1)&=N_A(s+2,k)+N_A(-s,k)+N_B(-s-1,k),\end{aligned} \tag{8}$$

which leads to

$$\begin{pmatrix}n_A(x,k+1)\\ n_A(x^{-1},k+1)\\ n_B(x,k+1)\\ n_B(x^{-1},k+1)\end{pmatrix}=\begin{pmatrix}x+1 & x^{-2} & x^{-1} & 1\\ x^2 & x^{-1}+1 & 1 & x\\ x^2 & 1 & 0 & x\\ 1 & x^{-2} & x^{-1} & 0\end{pmatrix}\begin{pmatrix}n_A(x,k)\\ n_A(x^{-1},k)\\ n_B(x,k)\\ n_B(x^{-1},k)\end{pmatrix}. \tag{9}$$

The maximum eigenvalue of the above matrix

$$\lambda(x)=(1/2x)\{(x+1)^2+[(x+1)^4+4x^2]^{1/2}\}, \tag{10}$$

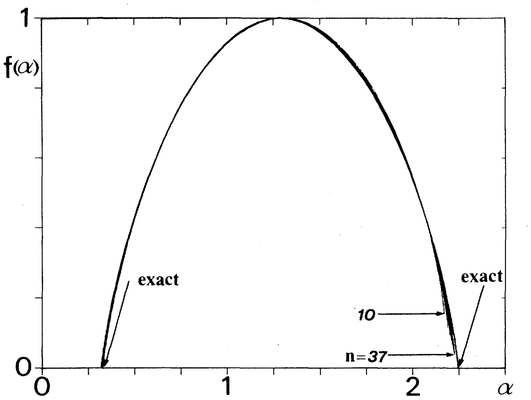

FIG. 1. $f_n(\alpha)$ for the wave function at the center of the spectrum with $R = t_B/t_A = 2$ $(n = 3k+1, k = 3,4,\ldots,12)$. The exact $f(\alpha)$ is also shown.

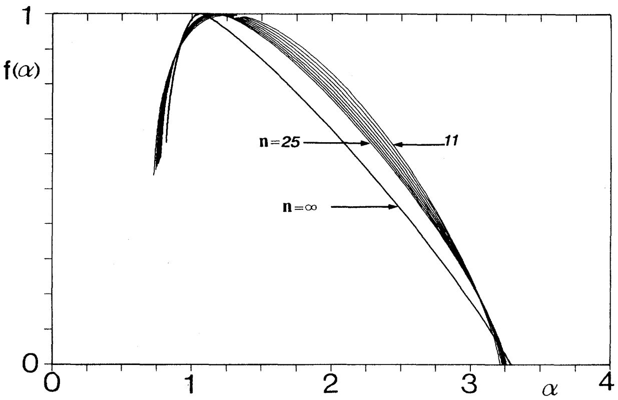

FIG. 2. $f_n(\alpha)$ for the wave function at the edge of the spectrum with $R = t_B/t_A = 2$ $(n = 2k+1, k = 5,6,\ldots,12)$. The limiting $f(\alpha)$ is also shown.

dominates the partition function (7) as $k \to \infty$, so the free energy defined in (4) is calculated as $G(q) = \frac{1}{3}\ln\{\lambda(R^{2q})/[\lambda(R^2)]^q\}$. The exact form of $f(\alpha)$ is obtained from (4) as

$$f(\alpha) = \frac{1}{3\ln\tau}\left[\ln\lambda(R^{2q}) - q\frac{d}{dq}\ln\lambda(R^{2q})\right], \qquad (11)$$

and

$$\alpha = \frac{1}{3\ln\tau}\left[\ln\lambda(R^2) - \frac{d}{dq}\ln\lambda(R^{2q})\right], \qquad (12)$$

where τ is the golden mean $(\sqrt{5}+1)/2$. The functions $f_n(\alpha)$ and $f(\alpha)$ are plotted in Fig. 1. The range of α where $f(\alpha)$ is defined is given by $[\alpha_{\min},\alpha_{\max}] = \{1/(3\ln\tau)[\ln\lambda(R^2) - \ln R^2],\ 1/(3\ln\tau)[\ln\lambda(R^2) + \ln R^2]\}$, and $f(\alpha) = 0$ for both $\alpha_{\min}$ and $\alpha_{\max}$. The minimum value $\alpha_{\min}$ corresponds to the largest square amplitude of the wave function and $\alpha_{\max}$ corresponds to the smallest one. The maximum value of $f(\alpha)$ gives the Hausdorff dimension of the support of the wave function.[10,11] This is one as it should be since the support is an interval [0,1] in our formulation.[12] The maximum occurs at $\alpha = \ln\lambda(R^2)/3\ln\tau$. It is not difficult to prove that $f(\alpha)$ is symmetric about the maximum as is seen in Fig. 1.

Wave function at the edge of the spectrum

The edge of the spectrum corresponds to a two-cycle of the trace map (6).[9] Although the trace follows the two-cycle, the matrix $M^{(n)}$ which determines the wave function does not. Instead the matrix elements grow in the full RG map (5). We determine $f(\alpha)$ numerically, since an analytical calculation of $f(\alpha)$ seems to be hard. When $R = t_B/t_A = 2$, one has $E = 2.83396$ at the edge. In determining $f(\alpha)$ from (3) and (4), we expect the finite-size correction of $f_n(\alpha)$ to be of the order $1/n$. This is checked numerically under linear extrapolation for this wave function as well as the exact wave function at the center of the spectrum. This behavior of the finite-size correction is consistent with the formal analogy between the present multifractal analysis and the canonical ensemble formalism of statistical mechanics (n corresponds to the volume of a statistical-mechanical system).

The limiting $f(\alpha)$ curve is shown in Fig. 2. In particular, we find $f = 0.633$ at $\alpha_{\min} = 0.817$ and $f = 0$ at $\alpha_{\max} = 3.29$. Notice that $f(\alpha_{\min})$ is not zero and this property is at variance with the previous wave function at $E = 0$. It seems that $f(\alpha_{\min}) \neq 0$ and $f(\alpha_{\max}) = 0$ are general properties of the critical wave function [the wave function at $E = 0$ which has $f(\alpha_{\min}) = f(\alpha_{\max}) = 0$ may be an exceptional one].

Non-self-similar wave function

The energy spectrum is a Cantor set and has a hierarchical structure. At each step of the hierarchy it is divided into three subclusters. Hence an energy in the spectrum is represented by an infinite series of 1, 0, and $\bar{1}$, where 1 corresponds to the upper subcluster, 0 to the middle one, and $\bar{1}$ to the lower one at each level of the hierarchy. For example, the center of the spectrum is represented by $\{0,0,0,0,0,\ldots\}$ and the upper edge of the spectrum is represented by $\{1,1,1,1,1,\ldots\}$. The earlier part of a series governs the local (or fine) structure of the wave function and the later part governs the global structure. A series of 1, 0, and $\bar{1}$ represents an orbit of a certain symbolic dynamical system of the trace map (6). Periodic orbits are rather rare and most of the allowed energy corresponds to a bounded chaotic orbit of the trace map. The existence of the chaotic orbits and the Cantor set spectrum can be explained by the Smale horseshoe structure or equivalently the existence of the homoclinic point of the trace map.[5] A wave function corresponding to a chaotic orbit does not seem to be self-similar.[9] We numerically investigate the scaling properties of wave function $\{1,0,1,\bar{1},0,\bar{1},0,1,\bar{1}\}$ as an example of such states. The energy is $E = 2.67029$ for $R = t_B/t_A = 2$. The wave function and its $f_n(\alpha)$ are shown in Figs. 3(a) and 3(b). Compared with the previous self-similar wave functions (see Figs. 1 and 2), $f_n(\alpha)$ does not show a monotonic convergence as n is increased. At this level of numerical data

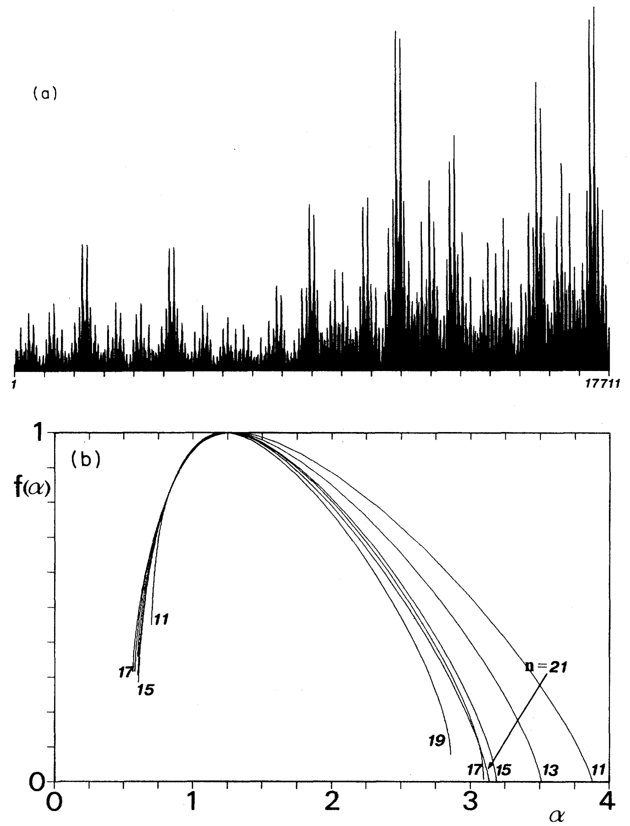

FIG. 3. (a) A non-self-similar wave function of the state $\{1,0,1,\bar{1},0,\bar{1},0,1,\bar{1}\}$ with $R=t_B/t_A=2$. (b) $f_n(\alpha)$ of the state $\{1,0,1,\bar{1},0,\bar{1},0,1,\bar{1}\}$ with $R=t_B/t_A=2$ ($n=11$–21).

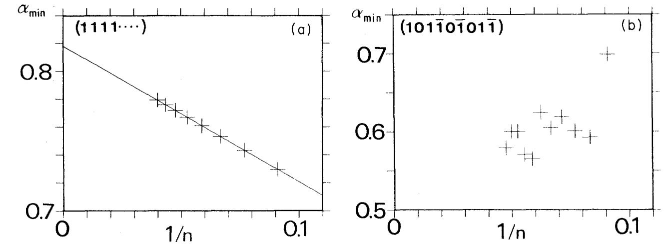

FIG. 4. Examples of the finite-size-scaling analysis of $\alpha_{\min}$. The system size is F_n, where F_n is a Fibonacci number defined by $F_{n+1}=F_{n-1}+F_n$ with $F_0=F_1=1$. (a) Wave function at the edge of the spectrum $\{1,1,1,1,\ldots\}$; (b) non-self-similar wave function $\{1,0,1,\bar{1},0,\bar{1},0,1,\bar{1}\}$.

(the maximum number of sites is $N=17711$) we do not see the convergence of $f(\alpha)$ yet. This is easily seen from the $1/n$ dependence of $\alpha_{\min}$ shown in Fig. 4. Whether a limiting $f(\alpha)$ exists for this type of wave function is still an unsolved problem.

In summary, we studied the critical wave functions on the Fibonacci lattice. An exact $f(\alpha)$ is obtained for the wave function at the center of the spectrum. This is one of the few examples in which an exact $f(\alpha)$ is calculated for a nontrivial and interesting case. For the self-similar wave function at the outermost edge of the spectrum which corresponds to a two-cycle of the trace map (6), $f(\alpha)$ is numerically determined to be a smooth curve by a careful analysis with finite-size scaling. It is clearly distinguished from localized states and extended states in which $f(\alpha)$ is defined only at finite points. So, we have a strong evidence that the ordered critical wave functions which correspond to cycles of the trace map have a smooth $f(\alpha)$. For non-self-similar wave functions which correspond to a chaotic orbit, the understanding of the scaling and the multifractal behavior is still an unsolved problem. This is a rather important one since the wave function of a disordered system at the mobility edge may have some similarities to this type of wave function.

Note added. After submission of the paper, A. Sütö (to appear in J. Stat. Phys), following S. Kotani (unpublished work), proved rigorously that the energy spectrum is singular continuous on a Fibonacci lattice. We also received a copy of an unpublished work by G. Ananthakrishna and V. Kumar in which a multifractal analysis of wave functions on a Fibonacci lattice is reported.

This work was partially supported by a Grant in Aid from the Japan Ministry of Education, Science and Culture. One of us (M.K.) was supported in part by the U.S. National Science Foundation Grant No. DMR-8615609 and the A.P. Sloan Foundation.

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