Extended and critical wave functions in a Thue-Morse chain

C. S. Ryu, G. Y. Oh, and M. H. Lee
Department of Physics, Seoul National University, Seoul 151-742, Korea
(Received 19 December 1991; revised manuscript received 26 February 1992)

We study the one-dimensional tight-binding model with site energies arranged in the Thue-Morse sequence. To show the characteristics of eigenstates, we study the trace map, wave functions, and the resistance, and perform a multifractal analysis on the wave functions. Half of all the eigenstates are represented by lattice-like wave functions, the amplitudes of which resemble the Thue-Morse sequences of lower order. These lattice-like wave functions are denoted as chaotic or extended, depending on the lattice size considered. The other half are classified into critical or extended states. We discuss the properties of the electronic spectrum. Our results show that critical states coexist with extended ones; therefore, the spectrum consists of absolutely continuous parts and singular continuous parts.

I. INTRODUCTION

Recently, there has been much interest in quasiperiodic systems[1] which are intermediate between periodic and disordered systems. The Fibonacci lattice, which is a one-dimensional (1D) version of quasicrystals, is known to have a Cantor-set spectrum and critical eigenstates. More recently, much attention has been paid to generalized Fibonacci[2,3] and other deterministic aperiodic[4] lattices. It has been shown that the Fibonacci lattice has the generic features of generalized Fibonacci lattices. The Thue-Morse (TM) lattice, which is deterministic aperiodic and not quasiperiodic, is known to have a singular continuous Fourier transform[5] and a Cantor-like phonon spectrum.[6] But little have been reported for the electronic properties of the TM lattice.

By examining the ground state and the highest excited one, Riklund *et al.*[7] claimed that the TM lattice is a link between quasiperiodic and periodic lattices. And Qin *et al.*[8] supported the claim by discussing the electronic spectrum by means of a renormalization procedure. Note that their conclusions were obtained only by showing that the wave functions (the integrated density of states) are more like those (that) of a periodic lattice than those (that) of a quasiperiodic one. On the other hand, La Rocca[9] performed a multifractal analysis on the spectrum and suggested that the spectrum contains absolutely continuous parts (extended states) plus point singularities (localized states). It is well known that periodic (disordered) systems have extended (localized) states and absolutely continuous (point) spectra. Thus it seems that there are some discrepancies between the above results and that a clear understanding of the eigenstate of the TM lattice has not been given yet. It is the purpose of this paper to examine the properties of the electronic state in a 1D tight-binding model with the site energies given by the TM sequence.

II. THE MODEL AND THE METHODS

The TM lattice can be generated in many ways.[7] One of the simplest ways to generate it is with successive substitutions $A \rightarrow AB$ and $B \rightarrow BA$. Repeated substitutions will give the following sequences.

$$A\,\underline{B} \rightarrow AB\,\underline{BA} \rightarrow ABBA\,\underline{BA\,AB} \rightarrow ABBABA\,AB\,\underline{BA\,ABABBA} \rightarrow \cdots .$$

The nth order TM lattice of the length $N=2^n$ consists of 2^{n-1} A and B atoms. It is interesting to note that the nth TM lattice is composed of the $(n-1)$th lattice and its complement (underlined part) which is obtained by exchanging A and B. Here, we consider the tight-binding on-site model

$$t\psi_{k+1}+t\psi_{k-1}+V_k\psi_k=E\psi_k , \tag{1}$$

where the site energy $V_k=V_A$ (V_B) if the kth atom is A (B) and the hopping matrix element t is set to unity. Equation (1) can be rewritten as

$$t\psi_{k+1}+t\psi_{k-1}+V'_k\psi_k=E'\psi_k , \tag{2}$$

where $V'_A=(V_A-V_B)/2=-V'_B$ and $E'=E-(V_A+V_B)/2$. We can obtain the spectrum of Eq. (2) by shifting that of Eq. (1) by $(V_A+V_B)/2$. Thus we can choose $V_A=-V_B=V$ without loss of generality. Introducing a transfer matrix, we can write Eq. (1) as

$$\begin{bmatrix}\psi_{k+1}\\ \psi_k\end{bmatrix}=\begin{bmatrix}E-V_k & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\psi_k\\ \psi_{k-1}\end{bmatrix}=\mathbf{P}_k\begin{bmatrix}\psi_k\\ \psi_{k-1}\end{bmatrix} . \tag{3}$$

For the TM lattice, the trace map[10] is

$$X_{n+1}=4X_{n-1}^2(X_n-1)+1 , \tag{4}$$

where

$$X_n=\tfrac{1}{2}\mathrm{Tr}\mathbf{M}_n,\quad \mathbf{M}_n=\mathbf{M}(N)=\prod_{k=1}^{N}\mathbf{P}_k , \tag{5}$$

with initial condition

$$X_1=\tfrac{1}{2}(E^2-V^2)-1,\quad X_2=\tfrac{1}{2}(E^2-V^2)^2-2E^2+1 . \tag{6}$$

The trace X_n is even in E and V.

When we consider infinite periodic repetition of the nth TM lattice [periodic approximation (PA)], the energy E belongs to the spectrum if $|X_n|\le 1$. For periodic boundary condition, 2^n eigenstates are determined by the condition $X_n=1$. Besides the trace map, we calculate the density of states (DOS) to examine the nature of the spectrum. We use the negative-eigenvalue theorem[11] to obtain the DOS. To investigate the localization properties, we calculate wave functions and the resistance[12] R using the periodic boundary condition and the Landauer formula,[13] respectively. The resistance and wave functions are very useful to distinguish localized states from extended ones. But to discern critical states, we need more elaborate methods.

Recently, multifractal analysis[14] (MFA) has been used to investigate the self-similarity in the fluctuating regimes of localized wave functions in disordered systems[15] and that of the wave functions in quasiperiodic ones.[16] It has also been performed to examine the characteristics of the wave functions for large fields in an incommensurate[17] and a hierarchical system[18] under an electric field. We compute $\tau(q)$ which obeys

$$\tau(q)=\lim_{l\to 0}[\ln Z(q,l)/\ln l] , \tag{7}$$

where $Z(q,l)=\sum_{i=1}^{N/L}p_i^q$ and $l=L/N$. The lattice is covered with consecutive boxes of size L and p_i is the probability of finding the electron within the ith box. We use the normalized wave function and find $\tau(q)$ by plotting $\ln Z(q,l)$ versus $\ln L$ for a fixed q. Using the relations

$$\frac{d\tau(q)}{dq}=\alpha, \quad f(\alpha)=q\alpha-\tau(q) , \tag{8}$$

we can obtain the multifractal spectrum characterized by a continuous set of scaling indices α and the fractal dimensions $f(\alpha)$.

For an extended wave function, one can obtain a single point $f=\alpha=1$, which means the absence of self-similar features in the wave function. When a wave function is localized, if L is larger than the localization length, the $f(\alpha)$ spectrum consists of two points, one being $f(0)=0$ and the other $f(\infty)=1$. For a critical (self-similar or chaotic) wave function, one gets a continuous $f(\alpha)$ spectrum. But a chaotic wave function shows quite different shapes in each scale and does not yield an $f(\alpha)$ spectrum independent of L.[19] Thus the self-similarity of a wave function is confirmed by the L-independent $f(\alpha)$ spectrum.

III. RESULTS AND DISCUSSION

A. The electronic spectrum

Figure 1 shows the DOS and the inverse localization length γ equal to $\ln(R+1)/N$ for the finite TM lattice. The spectrum consists of six main bands and has a symmetry about $E=0$. The sixth (first) and the fourth (third) bands are formed by AA (BB) clusters and the other bands by isolated A or B sites.[7] As can be seen in Fig. 2, the spectra of the PA's show highly fragmented structures but less clear self-similarity than that of the spectra of the Fibonacci lattice.

The spectrum of the nth ($n\geq 3$) PA does not seem to consist of 2^n bands. This is not because another gap is too narrow to find. For $n=3$, this can be easily demonstrated by determining all intervals of E satisfying the inequality $|X_3(E)|\leq 1$. This can be explained qualitatively by the trace map. We can know from Eq. (4) that if $X_m(E)=1$, then $X_n(E)=1$ for all $n>m$. In other words, if the energy E is the eigenvalue of the mth TM lattice for the periodic boundary condition, E is also that of the higher order TM lattice than the mth one. This property plays an important role in understanding the weak self-similarity of the spectra and the lattice-like wave functions which will be mentioned later. For the third TM lattice, $X_3=1$ gives eight eigenvalues, four of which are determined by $X_2=1$ and the others by $X_1^2=0$. Thus the eigenvalues obtained from $X_1^2=0$ are doubly degenerate. Calculating the integrated density of states for the third PA to confirm the degeneracy, we can find that the second (or the fifth) band contains twice as many states as

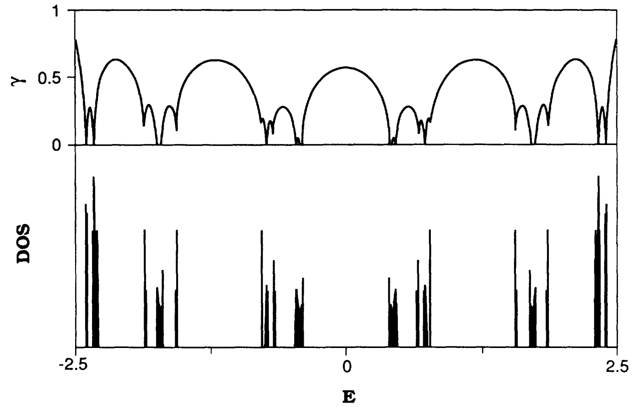

FIG. 1. The inverse localization length γ and the DOS for $V=1$ and $N=4096$. The scale of the DOS is arbitrary.

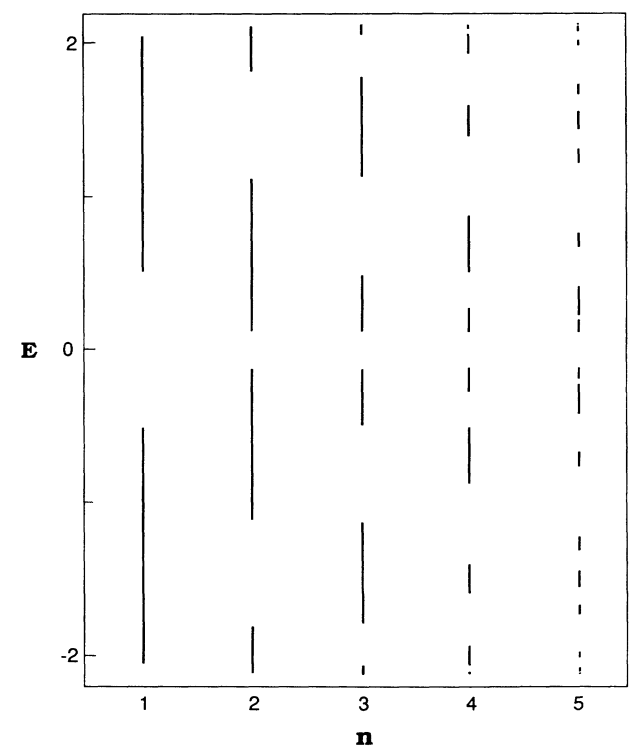

FIG. 2. The band structures of the nth PA for $V=0.5$ where $n=1$, 2, 3, 4, and 5.

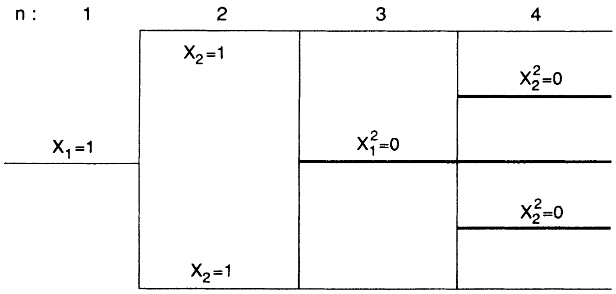

FIG. 3. Schematic representation of the eigenvalue tree for the length $N=2^n$, where $n=1$, 2, 3, and 4. Thick lines indicate doubly degenerate eigenvalues.

the other bands. From the above consideration, we obtained the eigenvalue tree as shown in Fig. 3. Note that only half of the tree is shown, since X_n is even in E. Considering the degeneracy and the constancy of eigenvalues, we find that the number of the branches of the tree,

$$b_n=b_{n-1}+2^{n-2}=2^{n-1}+2, \quad n\geq 3 , \tag{9}$$

where $b_1=2$ and $b_2=4$. Therefore the spectrum of the nth PA consists of $(2^{n-1}+2)$ bands.

B. Lattice-like wave functions

One of the electronic properties particular to the nth TM lattice is that half of all the eigenstates are described by the wave functions the amplitudes of which resemble the TM sequences of lower order. The wave function at the energy E satisfying $X_m(E)=1$ is AB-type for the $(m+1)$th lattice, $ABBA$-type for the $(m+2)$th lattice, etc., as shown in Figs. 4 and 5. These *lattice-like* wave functions can be understood in the following way. We consider the $(m+2)$th TM lattice (see Fig. 6) and an eigenvalue E satisfying $X_m(E)=1$. Since $X_n(E)=1$ for all $n>m$, $\psi_0=\psi_N=\psi_{2N}=\psi_{4N}$. Replacing V_k by $-V_k$ in the sublattice A, we can obtain the sublattices B and Γ. Since the trace map is even in V, we have $\psi_{2N}=\psi_{3N}$. The wave function in the sublattice $A(B)$ is the same to that in the sublattice $\Delta(\Gamma)$, because the site energies and the boundary condition in the sublattice $A(B)$ are the same to those in the sublattice $\Delta(\Gamma)$. Thus we find that the wave function for the length 2^{m+2} is $ABBA$-type, that is, the second TM lattice-like. Any lattice-like wave function can be explained in this way. Extending the arguments, we find that the wave function at the energy E for $N=2^{m+\ell}$ is the ℓth TM lattice-like one if $X_m(E)=1$. In other words, for the nth TM lattice, there are 2^{n-2} AB-type, 2^{n-3} $ABBA$-type, . . . , four $(n-2)$th TM lattice-like eigenfunctions.

In Fig. 5, the resistances, where the free-end (scattering) boundary condition is imposed, also appear to be

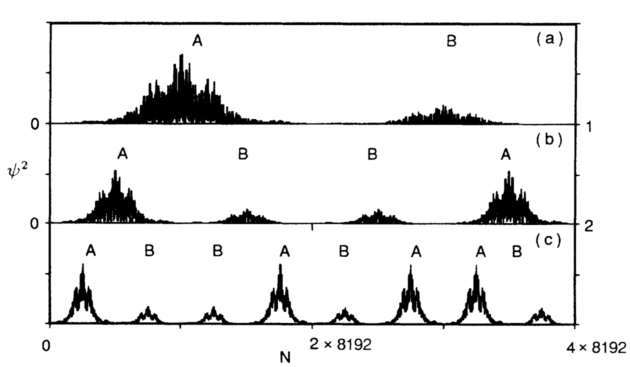

FIG. 4. Lattice-like wave functions for $V=1$ and $E=1.723\,817\,824\,669$ where $X_{12}(E)=1$. (a) AB-type, (b) $ABBA$-type, (c) $ABBA\ BAAB$-type. Note $2^{13}=8192$. The amplitudes of smaller subpatterns are averaged.

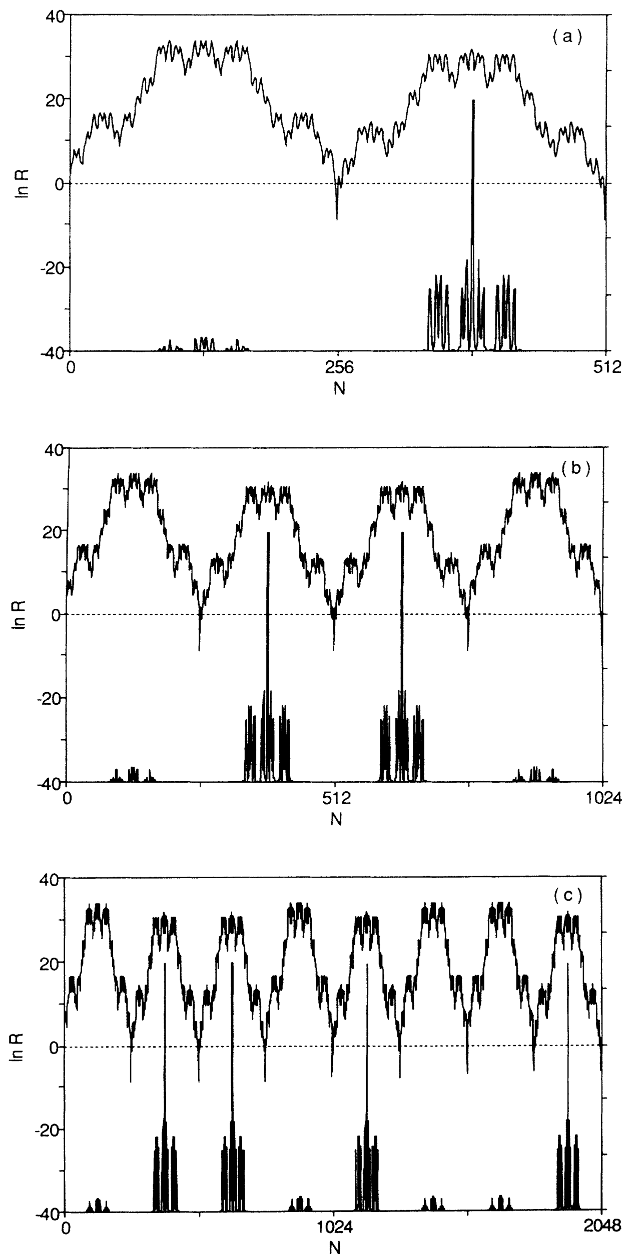

FIG. 5. Lattice-like wave functions and the resistances (upper curves) for $V=2$ and $E=1.335\,707\,112\,481\,781\,087$ where $X_8(E)=1$. (a) AB-type, (b) $ABBA$-type, (c) $ABBA\ BA\ AB$-type.

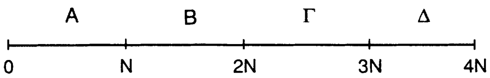

FIG. 6. The $(m+2)$th TM lattice. The lattice is divided into four sublattices A, B, Γ, and Δ of the same length $N=2^m$.

AB-type, $ABBA$-type, etc. Finally, we obtained the wave functions for other boundary conditions. Successive applications of Eq. (3) yield

$$\begin{bmatrix} \psi_N \\ \psi_{N-1} \end{bmatrix} = \mathbf{M}(N-1) \begin{bmatrix} \psi_1 \\ \psi_0 \end{bmatrix} . \tag{10}$$

For the fixed-end boundary condition, $\psi_0=\psi_N=0$. To yield non-trivial solution, $a=[\mathbf{M}(N-1)]_{11}$ must be zero. The condition $a=0$ determines all the eigenvalues for the fixed-end boundary condition. Figures 7(a) and 7(b) show the lattice-like features of the wave functions for the fixed-end boundary condition and with initial condition $\psi_0=1, \psi_1=3$ respectively. We have shown the lattice-like features of the wave functions for not only periodic but also fixed-end and open boundary condition, and those of the resistances for scattering one.

Next, we examine the characteristics of these lattice-like wave functions. The wave functions with $E=\pm 1 \pm \sqrt{1+V^2}$ satisfying $X_2(E)=1$ spread most evenly, two of which are the ones that Riklund *et al.*[7] have studied. Note that there is no energy E satisfying $X_1(E)=X_2(E)=1$ and Eq. (4) holds for $n \geq 2$. All the eigenvalues besides the above four ones are doubly degenerate. The wave functions with $E=1+\sqrt{1+V^2}$ are shown in Fig. 8. Considering that A part of the amplitude is negligibly small [see Fig. 8(b)], we can find the wave function to be the seventh lattice-like. We regard these states as extended ones. In Fig. 9, the geometrically averaged resistance $\langle R \rangle$ is shown for another seventh lattice-like state. It has been reported that the average resistance of critical states shows many coupled oscillations without uniform convergence.[20] Thus $\langle R \rangle$ displaying not fast but uniform convergence, shows that the ℓth lattice-like wave functions with large ℓ (or $n \gg m$) can also be considered to be extended. Since the quantity $\ell=n-m$ indicates the degree of spatial extension, it may be called the *degree of extension.* For a TM chain with springs, Axel *et al.*[6] proved that points in a dense subset of the phonon spectrum give rise to extended states and studied the example of the extended ones. The example corresponds to the extended state of the energy E satisfying $X_1(E)^2=0$ [therefore $X_3(E)=1$] in our case.

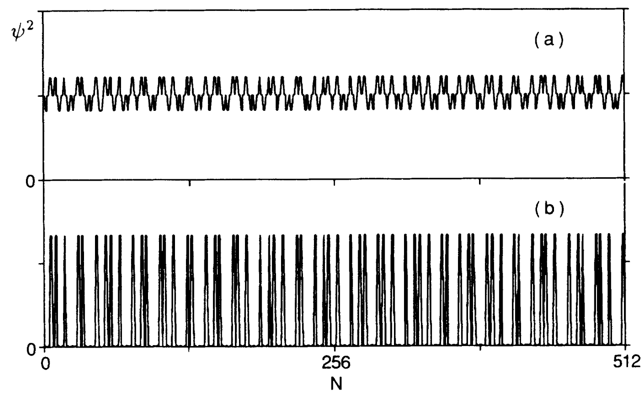

FIG. 8. Extended wave functions. (a) $V=0.1$ and $E=2.004\,987\,562\,112\,09$. (b) $V=4$ and $E=5.123\,105\,625\,617\,660\,55$. The wave functions are the seventh lattice-like ones.

If the $A(B)$ parts of the amplitudes of AB-type wave functions are much larger than the $B(A)$ parts of those, the wave functions may be considered to be localized[10] [see Fig. 5(a)]. But they are not localized since the localized state is very insensitive to changed boundary conditions.[21] In this case, the larger the lattice becomes, the more the wave function becomes extended. If the AB-type wave functions are localized, they remain localized with new energies changed by the increase of the system size. But they evolve into the $ABBA$-type wave functions and so on. Similar consideration of the wave function of Fig. 10(a) shows that the wave function is not localized. In generalized Fibonacci lattice, the existence of localized states has been reported.[3] But some of the results are not

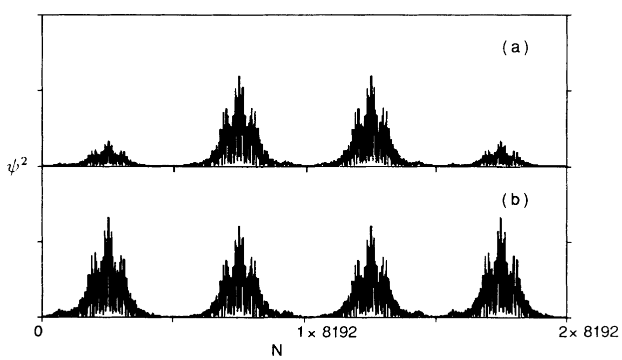

FIG. 7. (a) $ABBA$-type wave function for the fixed-end boundary condition, where $V=1$ and $E=1.723\,817\,824\,668\,993\,174$. (b) $ABBA$-type wave function with $\psi_0=1$ and $\psi_1=3$, and where $V=1$ and $E=1.723\,817\,824\,669$. The amplitudes of smaller subpatterns are averaged.

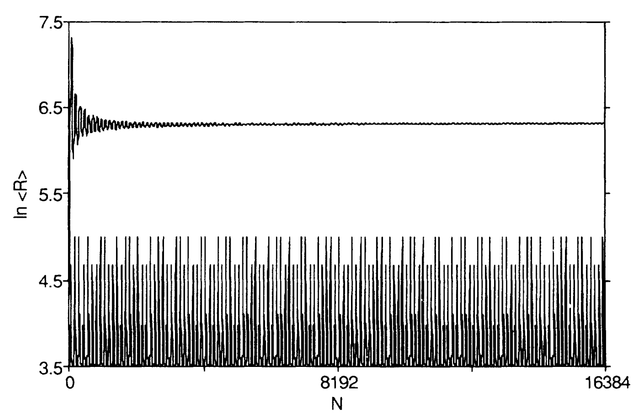

FIG. 9. An extended wave function. A seventh lattice-like wave function and the average resistance (upper curve) for $V=1$ and $E=2.401\,967\,743\,500\,58$ where $X_7(E)=1$. The amplitudes of smaller subpatterns are averaged.

valid, the insensitivity of localized states being considered.[22]

The lattice-like wave functions with weak degree of extension (small ℓ) are neither extended nor localized in the usual sense. These wave functions, of course, become more extended-like as the lattice size increases; when n goes to $n+1$, the ℓth lattice-like wave function becomes the $(\ell+1)$th one. But the appearance of 2^{n-1} new AB-type wave functions maintains the ratio between various types of lattice-like wave functions. Thus we can find the lattice-like wave functions with weak degree of extension at any large N. Since successive iterations of the trace

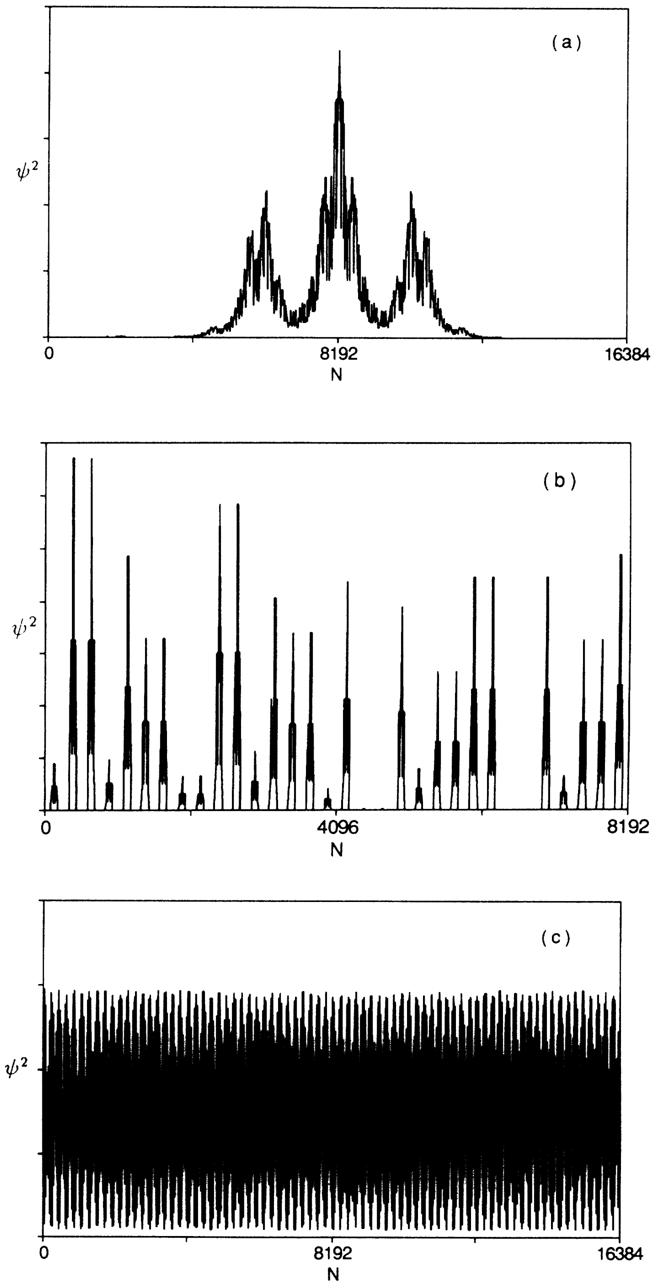

FIG. 10. Wave functions at the eigenenergies appearing for the first time. (a) A chaotic wave function for $V=1$ and $E=1.723\,847\,756\,906\,832$ where $X_{14}(E)=1$. (b) A chaotic wave function for $V=2$ and $E=1.335\,707\,112\,481\,780\,997$ where $X_{13}(E)=1$. (c) An extended wave function for $V=1$ and $E=1.730\,070\,706\,869\,8$ where $X_{14}(E)=1$. The amplitudes of smaller subpatterns are averaged. Three wave functions evolve into AB-type lattice-like ones as N increases.

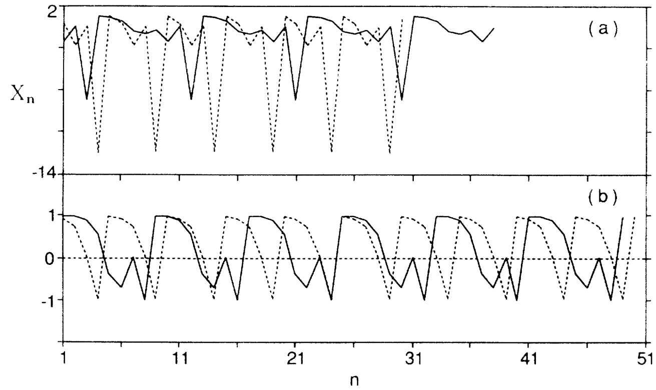

FIG. 11. Trace X_n vs n. (a) Five-cycle orbit: $V=0.7$, $E=1.756\,670\,883\,151\,046\,245$ (dotted line). Nine-cycle orbit: $V=1.22$, $E=0.818\,361\,652\,276\,616\,781$ (solid line). (b) Five-cycle orbit: $V=0.000\,12$, $E=1.963\,857\,402\,804\,679\,756$ (dotted line). Eight-cycle orbit: $V=0.0025$, $E=1.996\,268\,618\,926\,149\,129$ (solid line). The lines are guides to the eye.

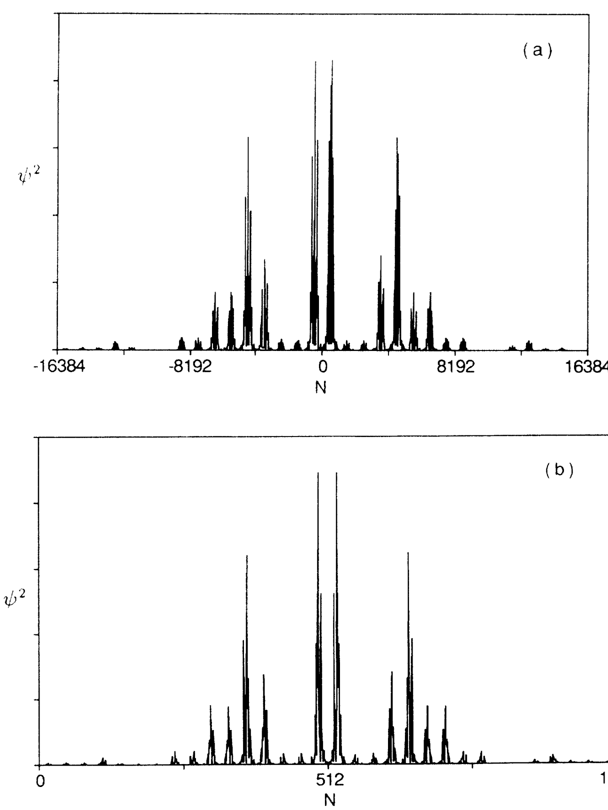

FIG. 12. A self-similar wave function where $V=0.7$ and $E=1.756\,670\,883\,151\,046\,245$. The self-similarity can be shown in the display of the different portions of the same wave function. The amplitudes of smaller subpatterns are averaged.

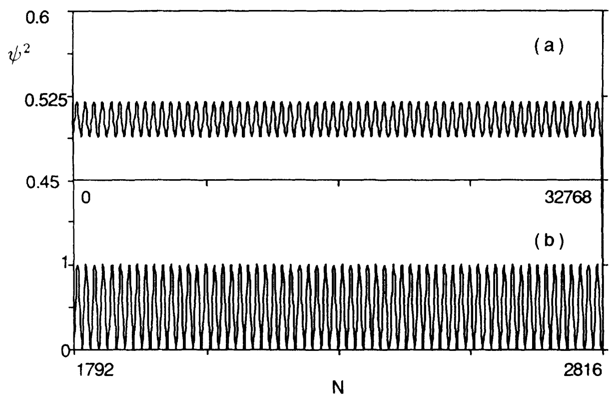

FIG. 13. An extended wave function for $V=0.000\,12$ and $E=1.963\,857\,402\,804\,679\,756$. The peaks in (a) are modulated as shown in (b) at smaller length scales. The amplitudes of smaller subpatterns are averaged.

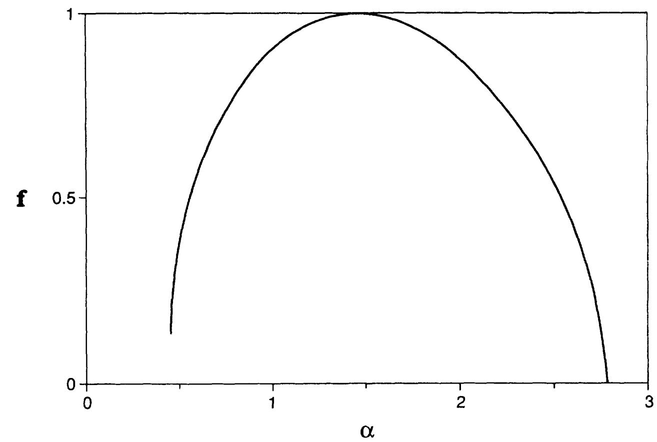

FIG. 14. The $f(\alpha)$ spectrum for the wave function shown in Fig. 12. q ranges from -5 to 64.

map yield aperiodic orbits before $X_m(E)=1$ for most energies, we consider these lattice-like wave functions to be chaotic. In conclusion, the lattice-like wave functions with strong degree of extension (large ℓ) are extended and the ones with weak degree of extension (small ℓ) chaotic. And they do not depend on boundary conditions. The lattice-like states are due to resonant tunnelings which arise from the symmetry of the TM lattice.

C. Self-similar and extended wave functions

Chaotic are most of the other half of all the eigenstates which are given by $X_n(E)=1$ and appear for the first time. Some chaotic wave functions are shown in Fig. 10. Simple calculation shows that there can not exist two-cycle orbit. We were able to identify five-cycle, eight-cycle, and nine-cycle orbit for the trace map as shown in Fig. 11. The wave functions of five-cycle orbits are shown in Figs. 12 and 13. We performed an MFA on the wave function shown in Fig. 12 and obtained a continuous $f(\alpha)$ spectrum, as shown in Fig. 14.

An MFA on the wave function shown in Fig. 13 yields similar results as have been previously found for extended wave functions in incommensurate systems.[23] Multifractal features are found at very small length scales ($L<16$) but are not maintained at larger length scales. We obtained $f=\alpha=1$ for L greater than 16 and therefore consider this wave function to be extended. We also obtained similar results for the wave function shown in Fig. 10(c). These extended wave functions, of course, evolve into AB-type lattice-like wave functions. But it is very difficult to see lattice-like features since both A and B parts spread very evenly. Details of the nature of these extended states will be presented in the future.

IV. CONCLUSION

We have studied the tight-binding model with site energies arranged in the TM sequence and obtained several electronic properties independent of V. The spectrum shows highly fragmented structure and less clear self-similarity than that of the spectrum of the Fibonacci lattice. For the TM lattice of the nth order, we have found that 2^{n-1} eigenstates generated in the TM lattice of lower order are described by the lattice-like wave functions. The lattice-like wave functions are mostly chaotic and they become more extended-like as n increases. We have shown that the lattice-like wave functions with strong degree of extension can be regarded as extended ones. Most of the other 2^{n-1} eigenfunctions are chaotic and a few of them are self-similar or extended. We have discussed the absence of localization in the TM lattice.

Our results show that critical states coexist with extended ones, which means that the spectrum consists of the absolutely continuous parts and singular continuous parts. The coexistence of critical and extended states has been reported in some of generalized Fibonacci lattices.[3,22,24] Our results support the claim that the TM lattice is intermediate between periodic and quasiperiodic systems. More detailed investigations on the spectrum will be reported later.

ACKNOWLEDGMENTS

This work was supported in part by the Center for Theoretical Physics, Seoul National University and in part by the Basic Science Research Institute Program through the Ministry of Education of Korea.

[1]M. Kohmoto, B. Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1987) and references therein.

[2]G. Gumbs and M. K. Ali, Phys. Rev. Lett. **60**, 1081 (1988); M. Holzer, Phys. Rev. B **38**, 1709 (1988); J. Q. You and Q. B. Yang, J. Phys.: Condens. Matter **2**, L2093 (1990).

[3]G. Gumbs and M. K. Ali, J. Phys. A **21**, L517 (1988); M. Severin and R. Riklund, Phys. Rev. B **39**, 10 362 (1989); J. Q. You, J. R. Yan, T. Xie, X. Zeng, and J. X. Zhong, J. Phys.: Con-

dens. Matter **3**, 7255 (1991).

[4]J. M. Luck, Phys. Rev. B **39**, 5834 (1989).

[5]Z. Cheng, R. Savit, and R. Merlin, Phys. Rev. B **37**, 4375 (1988).

[6]F. Axel and J. Peyrière, J. Stat. Phys. **57**, 1013 (1989).

[7]R. Riklund, M. Severin, and Y. Liu, Int. J. Mod. Phys. B **1**, 121 (1987).

[8]M. G. Qin, H. R. Ma, and C. H. Tsai, J. Phys.: Condens. Matter **2**, 1059 (1990).

[9]G. C. La Rocca, Solid State Commun. **70**, 115 (1989).

[10]F. Axel, J. P. Allouche, M. Kléman, M. Mendès-France, and J. Peyrière, J. Phys. (Paris) Colloq. **47**, C3-181 (1986).

[11]P. Dean, Rev. Mod. Phys. **44**, 127 (1972).

[12]A. D. Stone, J. D. Joannopoulos, and D. J. Chadi, Phys. Rev. B **24**, 5583 (1981).

[13]R. Landauer, Philos. Mag. **21**, 863 (1970).

[14]T. C. Halsey, M. H. Jensen, L. P. Kadanoff, I. Procaccia, and B. I. Shraiman, Phys. Rev. A **33**, 1141 (1986).

[15]L. Pietronero, A. P. Siebesma, E. Tosatti, and M. Zannetti, Phys. Rev. B **36**, 5635 (1987).

[16]S. N. Evangelou, J. Phys. C **20**, L295 (1987); H. E. Roman, Phys. Rev. B **36**, 7173 (1987); H. Hiramoto and M. Kohmoto, *ibid.* **40**, 8225 (1989).

[17]C. S. Ryu, G. Y. Oh, and M. H. Lee, J. Phys.: Condens. Matter (to be published).

[18]G. Y. Oh, C. S. Ryu, and M. H. Lee, Phys. Rev. B **45**, 6400 (1992).

[19]T. Tokihiro, Phys. Rev. B **40**, 2889 (1989).

[20]Y. J. Kim, M. H. Lee, and M. Y. Choi, Phys. Rev. B **40**, 2581 (1989).

[21]D. J. Thouless, Phys. Rep. **13**, 93 (1974).

[22]G. Y. Oh, C. S. Ryu, and M. H. Lee, unpublished.

[23]A. P. Siebesma, L. Pietronero, Europhys. Lett. **4**, 597 (1987); M. Johansson and R. Riklund, Phys. Rev. B **42**, 8244 (1990).

[24]M. Kolář and M. K. Ali, Phys. Rev. A **39**, 6538 (1989).