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1991 J. Phys.: Condens. Matter 3 7255

(http://iopscience.iop.org/0953-8984/3/38/003)

J. Phys.: Condens. Matter 3 (1991) 7255–7268. Printed in the UK

Generalized Fibonacci lattices: dynamical maps, energy spectra and wavefunctions

J Q You†§, J R Yan†§, Tiansheng Xie‡, Xiaobiao Zeng‡‖ and J X Zhong§

† China Centre of Advanced Science and Technology (World Laboratory), PO Box 8730, Beijing 100080, People's Republic of China

‡ Laboratory of Atomic Imaging of Solids, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110015, People's Republic of China

§ Laboratory of Modern Physics, Institute of Science and Technology, Xiangtan University, Xiangtan 411105, People's Republic of China

Received 4 February 1991, in final form 25 April 1991

Abstract. Electronic properties of the generalized Fibonacci lattices are studied using the dynamical system technique, for which the off-diagonal tight-binding model is employed. The matrix and trace maps are obtained and investigated in a unified way. It is found that the energy spectra are Cantor-like and the wavefunctions are critical at many energies. For some systems, it is also shown that there are extended and localized wavefunctions. In addition, according to the degree of spatial extension or localization, two other types of wavefunctions are further distinguished, of which one has the tendency to be extended and the other has the tendency to be localized.

1. Introduction

The physics of quasicrystals and aperiodic crystals in a broad sense has seen considerable development since the remarkable discovery of the icosahedral quasicrystals by Shechtman *et al* [1]. Recently, a class of one-dimensional (1D) quasiperiodic (aperiodic) systems, i.e. the generalized Fibonacci lattices, has become attractive to the condensed matter physicists [2–19]. Because of the development of the molecular-beam epitaxy technique, the Fibonacci layered structure was artificially manufactured [20] and it becomes possible to produce arbitrarily layered structures as well as the generalized Fibonacci layered ones. In the theoretical aspect, the studies showed [2–19] that the generalized Fibonacci systems exhibit richer physical properties than the Fibonacci structure. All this knowledge indicates that the generalized Fibonacci systems deserve investigation and the exploration of their physical properties is of real significance.

As the Fibonacci structure, the generalized Fibonacci systems are neither periodic nor random nor disordered, i.e. intermediate between the periodic crystals and the amorphous materials. Their underlying lattices are the generalized Fibonacci lattices, which are a straightforward generalization of the Fibonacci lattice. The separation of

‖ Present address: Department of Materials Science and Engineering, Cornell University, Ithaca, NY 14853, USA.

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successive lattice points of a generalized Fibonacci lattice takes value A or B and the sequence of its two kinds of tiles (building blocks) A and B is a generalized Fibonacci sequence that is generated by the recursion relation $S_{l+1} = \{S_l^n | S_{l-1}^m\}$ with $S_0 = \{B\}$ and $S_1 = \{A\}$, in which $l \geq 1$, and m and n are positive integers [2]. From the construction rule of S_l it follows that the total number F_l of tiles A and B in S_l obeys the recursion relation $F_{l+1} = mF_{l-1} + nF_l$ for $l \geq 1$ with $F_0 = F_1 = 1$. In the limit $l \to \infty$, the ratio of successive generalized Fibonacci numbers F_{l+1}/F_l tends to $\tau(m, n) = \frac{1}{2}[(n^2 + 4m)^{1/2} + n]$. The ratio F_{l+1}/F_l is an optimal rational approximation to $\tau(m, n)$. Alternatively, one can also produce the generalized Fibonacci sequences by means of the inflation rule $(A, B) \to (A^n B^m, A)$.

In their investigation of the electronic properties of the generalized Fibonacci systems, Gumbs and Ali [2, 3] derived several discrete trace maps for some generalized Fibonacci systems with specific m and n. Recently, a unified trace map for all m and n was derived by Kolář and Ali [13] for dealing with the diagonal tight-binding model on the generalized Fibonacci lattices, and independently by You *et al* [14, 15] to study the diagonal and off-diagonal tight-binding models on such aperiodic lattices. This unified trace map is the generalization of the well-known Kohmoto–Kadanoff–Tang (KKT) trace map [21] that was widely used to investigate the physical properties of the Fibonacci system [22–30]. In this paper, we study in some detail the following off-diagonal tight-binding Schrödinger equation:

$$t_{n+1}\psi_{n+1} + t_n\psi_{n-1} = E\psi_n \tag{1.1}$$

where ψ_n is the wavefunction at the nth site for an electron state with energy E and the hopping matrix element t_n takes two values t_A and t_B arranged according to the generalized Fibonacci sequences. Here the motivations are twofold. First, the off-diagonal model on the generalized Fibonacci lattices is more complicated and was investigated less as compared with the diagonal version of the tight-binding equation (1.1)

$$\psi_{n+1} + \psi_{n-1} + V_n\psi_n = E\psi_n \tag{1.2}$$

where $\{V_n\}$ form the generalized Fibonacci sequences with two kinds of site energies V_A and V_B. Second, there are some mistakes in the existing literature, which are misleading to the understanding of the physical properties of the generalized Fibonacci systems.

2. Dynamical maps and constants of motion

In the matrix form, (1.1) can be written as

$$\mathbf{\Psi}_{n+1} = \mathbf{M}(n+1, n)\mathbf{\Psi}_n \tag{2.1}$$

where $\mathbf{\Psi}_n$ is a column vector $(\psi_n, \psi_{n-1})^t$ and the transfer matrix is

$$\mathbf{M}(n+1, n) = \begin{pmatrix} E/t_{n+1} & -t_n/t_{n+1} \\ 1 & 0 \end{pmatrix}. \tag{2.2}$$

The wavefunction at an arbitrary site N is given by

$$\mathbf{\Psi}_{N+1} = \mathbf{M}^{(N)}\mathbf{\Psi}_1 \tag{2.3}$$

where

$$\mathbf{M}^{(N)} = \mathbf{M}(N+1, N)\mathbf{M}(N, N-1)\ldots\mathbf{M}(2, 1) \tag{2.4}$$

is successive multiplications of the transfer matrices.

If $N = F_l$, then $\mathbf{M}_l = \mathbf{M}^{(F_l)}$ generates the wavefunction at the generalized Fibonacci number site. From the construction rule of the generalized Fibonacci sequences one obtains that the transfer matrix $\mathbf{M}_l$ satisfies the following recursion relation for the transfer matrices:

$$\mathbf{M}_{l+1} = \mathbf{M}_{l-1}^{m}\mathbf{M}_l^{n} \tag{2.5}$$

with initial conditions

$$\mathbf{M}_1 = \mathbf{M}(A, A) \tag{2.6a}$$

$$\mathbf{M}_2 = \mathbf{M}(A, B)[\mathbf{M}(B, B)]^{m-1}\mathbf{M}(B, A)[\mathbf{M}(A, A)]^{n-1} \tag{2.6b}$$

in which the four types of transfer matrices are

$$\mathbf{M}(A, A) = \begin{pmatrix} E/t_A & -1 \\ 1 & 0 \end{pmatrix} \tag{2.7a}$$

$$\mathbf{M}(B, B) = \begin{pmatrix} E/t_B & -1 \\ 1 & 0 \end{pmatrix} \tag{2.7b}$$

$$\mathbf{M}(A, B) = \begin{pmatrix} E/t_A & -t_B/t_A \\ 1 & 0 \end{pmatrix} \tag{2.7c}$$

and

$$\mathbf{M}(B, A) = \begin{pmatrix} E/t_B & -t_A/t_B \\ 1 & 0 \end{pmatrix}. \tag{2.7d}$$

It can be easily verified that $\mathbf{M}_1$ and $\mathbf{M}_2$ are unimodular, i.e. $\det \mathbf{M}_1 = \det \mathbf{M}_2 = 1$, in which det denotes the determinant of a matrix. These initial conditions are different from those chosen by Gumbs and Ali [3]. As a matter of fact, the initial conditions chosen by them are only suitable to the Fibonacci lattice with $(m, n) = (1, 1)$.

From the theory of matrices, the Nth power of the 2×2 unimodular matrix $\mathbf{M}_l$ is given by [31]

$$\begin{aligned}\mathbf{M}_l^N &= \begin{pmatrix} a_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l) & b_l\mathcal{U}_{N-1}(x_l) \\ c_l\mathcal{U}_{N-1}(x_l) & d_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l) \end{pmatrix} \\ &= \mathcal{U}_{N-1}(x_l)\mathbf{M}_l - \mathcal{U}_{N-2}(x_l)I \end{aligned} \tag{2.8}$$

where

$$\mathbf{M}_l = \begin{pmatrix} a_l & b_l \\ c_l & d_l \end{pmatrix}$$

$x_l = \frac{1}{2}\mathrm{Tr}\,\mathbf{M}_l = \frac{1}{2}(a_l + d_l)$, in which Tr denotes the trace of a matrix, and $\mathcal{U}_N(x_l)$ is the Nth Chebyshev polynomial of the second kind

$$\mathcal{U}_N(x_l) = \frac{\sin[(N+1)\cos^{-1}(x_l)]}{\sin[\cos^{-1}(x_l)]} \tag{2.9}$$

which satisfies the recursion relation

$$\mathcal{U}_N(x_l) = 2x_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l). \tag{2.10}$$

Using (2.10) one can verify (2.8) by mathematical induction.

From (2.5) and (2.8) we have

$$x_{l+1} = \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_{l-1}^m\mathbf{M}_l^n) = \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})g_{l+1} - \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-2}(x_{l-1})x_l$$
$$- \mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-1}(x_{l-1})x_{l-1} + \mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-2}(x_{l-1}) \tag{2.11}$$

where

$$g_{l+1} = \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_{l-1}\mathbf{M}_l) = \tfrac{1}{2}(a_la_{l-1} + b_lc_{l-1} + c_lb_{l-1} + d_ld_{l-1}). \tag{2.12}$$

Since $\mathrm{Tr}(\mathbf{M}_l\mathbf{M}_{l+1}) = \mathrm{Tr}(\mathbf{M}_l\mathbf{M}_{l-1}^m\mathbf{M}_l^n) = \mathrm{Tr}(\mathbf{M}_{l-1}^m\mathbf{M}_l^{n+1})$, it follows by using (2.8) that

$$g_{l+2} = \mathcal{U}_n(x_l)\mathcal{U}_{m-1}(x_{l-1})g_{l+1} - \mathcal{U}_n(x_l)\mathcal{U}_{m-2}(x_{l-1})x_l - \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})x_{l-1}$$
$$+ \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-2}(x_{l-1}). \tag{2.13}$$

Equations (2.11) and (2.13) constitute a unified trace map for the generalized Fibonacci lattices. A similar result was obtained recently by Kolář and Ali [13]. For the off-diagonal model, the initial conditions for this unified trace map are

$$x_1 = \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_1 = \tfrac{1}{2}(E/t_A) \qquad x_2 = \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_2 \qquad g_3 = \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_1\mathbf{M}_2). \tag{2.14}$$

From (2.5) it follows that

$$(\mathbf{M}_{l-2}^{-1})^m = \mathbf{M}_{l-1}^n\mathbf{M}_l^{-1} \tag{2.15}$$

where the inverse of the unimodular matrix $\mathbf{M}_l$ is

$$\mathbf{M}_l^{-1} = \begin{pmatrix} d_l & -b_l \\ -c_l & a_l \end{pmatrix}. \tag{2.16}$$

By taking the trace of (2.15) we have

$$\mathcal{U}_{m-1}(x_{l-2})x_{l-2} - \mathcal{U}_{m-2}(x_{l-2}) = \mathcal{U}_{n-1}(x_{l-1})h_{l+1} - \mathcal{U}_{n-2}(x_{l-1})x_l \tag{2.17}$$

where

$$h_{l+1} = \tfrac{1}{2}(d_la_{l-1} - b_lc_{l-1} - c_lb_{l-1} + a_ld_{l-1}). \tag{2.18}$$

Since $g_{l+1} + h_{l+1} = 2x_lx_{l-1}$, we then obtain, from (2.11) and (2.17), another unified trace map for the generalized Fibonacci lattices

$$x_{l+1} = \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})\{2x_lx_{l-1} - [\mathcal{U}_{m-2}(x_{l-1})/\mathcal{U}_{m-1}(x_{l-1})$$
$$+ \mathcal{U}_{n-2}(x_{l-1})/\mathcal{U}_{n-1}(x_{l-1})]x_l$$
$$- [\mathcal{U}_{n-2}(x_l)/\mathcal{U}_{n-1}(x_l)]x_{l-1} - [\mathcal{U}_{m-1}(x_{l-2})/\mathcal{U}_{n-1}(x_{l-1})]x_{l-2}$$
$$+ [\mathcal{U}_{m-2}(x_{l-2})/\mathcal{U}_{n-1}(x_{l-1})$$
$$+ \mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-2}(x_{l-1})/\mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})]\}. \tag{2.19}$$

This trace map was derived by You and Yang [14], and an analogous trace map was also obtained by Kolář and Ali [13]. The initial conditions for the off-diagonal model are

$$x_1 = \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_1 = \tfrac{1}{2}(E/t_A) \qquad x_2 = \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_2 \tag{2.20a}$$

and

$$x_3 = {}^{\mathcal{Q}}U_{n-1}(x_2){}^{\mathcal{Q}}U_{m-1}(x_1)g_3 - {}^{\mathcal{Q}}U_{n-1}(x_2){}^{\mathcal{Q}}U_{m-2}(x_1)x_2 - {}^{\mathcal{Q}}U_{n-2}(x_2){}^{\mathcal{Q}}U_{m-1}(x_1)x_1 + {}^{\mathcal{Q}}U_{n-2}(x_2){}^{\mathcal{Q}}U_{m-2}(x_1) \tag{2.20b}$$

in which (2.20*b*) is obtained directly from (2.11). When $m = n = 1$ in particular, (2.19) is reduced to the well-known KKT trace map for the Fibonacci lattice [21]

$$x_{l+1} = 2x_l x_{l-1} - x_{l-2}. \tag{2.21}$$

The unified trace map (2.19) is the generalization of the KKT trace map. In the next section, we will use it to obtain the energy spectra of the generalized Fibonacci lattices.

Since the 2×2 real transfer matrix $\mathbf{M}_l$ is unimodular, it may be specified by only three numbers and then the matrix map (2.5) can be considered as a 6D dynamical system. The unified trace map (2.19) and that expressed by (2.11) and (2.13) are obtained by introducing the trace of the matrix $\mathbf{M}_l$. These trace maps are two reduced 3D dynamical systems and can be regarded as the projections of the full 6D dynamical map onto two 3D orbits. In addition, it can be derived that

$$I_{l+1} = {}^{\mathcal{Q}}U^2_{m-1}(x_{l-1})I_l \qquad l \geqslant 2 \tag{2.22}$$

where

$$I_l = \tfrac{1}{4}[\mathrm{Tr}(\mathbf{M}_l^{-1}\mathbf{M}_{l-1}^{-1}\mathbf{M}_l\mathbf{M}_{l-1}) - 2] = g_{l+1}^2 + x_l^2 + x_{l-1}^2 - 2g_{l+1}x_l x_{l-1} - 1 \tag{2.23}$$

in which

$$g_{l+1} = \frac{2x_{l+1} + {}^{\mathcal{Q}}U_n(x_l){}^{\mathcal{Q}}U_{m-2}(x_{l-1}) + {}^{\mathcal{Q}}U_{n-2}(x_l){}^{\mathcal{Q}}U_m(x_{l-1})}{2{}^{\mathcal{Q}}U_{n-1}(x_l){}^{\mathcal{Q}}U_{m-1}(x_{l-1})}. \tag{2.24}$$

When $m = 1$, $I_l = I$, i.e. the quantity I_l is independent of l. Now (2.23) serves as the constant of motion. This kind of invariant was obtained by Holzer [5] and Dotera [6]. In this case, the trace map (2.19) and that given by (2.11) and (2.13) can be further reduced to 2D dynamical maps. As $m > 1$, there is no invariant of the form (2.23) for the dynamical motion. The quantity I_l now acts as the pseudoinvariant. When ${}^{\mathcal{Q}}U_{m-1}(x_{l-2}) = 0$ in particular, then $I_l = 0$ and this surface plays as the role of an attractor [10, 13]. Recently, Suzuki [32] obtained a different kind of invariant in the case of $m = 1$: $J = (-1)^l\mathrm{Tr}(\mathbf{P}\mathbf{M}_{l-1}\mathbf{M}_l\mathbf{M}_{l-1}^{-1}\mathbf{M}_l^{-1})$, in which $\mathbf{P} \in \mathbf{M}(2, C)$ with $\mathrm{Tr}\,\mathbf{P} = 0$. However, for the generalized Fibonacci lattices with $m > 1$, whether there is any invariant or not is still an unsolved problem.

3. Energy spectra

The energy spectra of the off-diagonal tight-binding models on the generalized Fibonacci lattices are determined by the behaviour of the unified trace map (2.19) or that represented by (2.11) and (2.13). Here we only use the trace map (2.19). Merely by studying it, one can obtain the energy spectra of the generalized Fibonacci off-diagonal models.

A generalized Fibonacci lattice can be approximated by a sequence of periodic lattices with progressively larger unit cells of size F_l as defined by the optimal rational approximations to $\tau(m, n)$. According to the Bloch theorem, one has

$$\Psi_{F_l+1} = \exp(\mathrm{i}KF_l)\Psi_1 \tag{3.1}$$

where K is the wave vector and F_l the size of the unit cell. From (2.3) and (3.1) we thus have

$$\Psi_{F_l+1} = \mathbf{M}_l\Psi_1 = \exp(\mathrm{i}KF_l)\Psi_1 \tag{3.2}$$

which yields

$$\cos(KF_l) = \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_l = x_l. \tag{3.3}$$

From (3.3) we then obtain the conditions for bands and gaps in the energy spectrum

$$\text{bands: } |x_l| \leqslant 1 \tag{3.4a}$$

$$\text{gaps: } |x_l| > 1. \tag{3.4b}$$

The energy spectrum of the off-diagonal model on a generalized Fibonacci lattice is obtained in the limit $l \to \infty$.

Energy spectra are presented, as examples, in figures 1(*a*)–(*d*) for the periodic systems with periods $F_l = mF_{l-2} + nF_{l-1}$ for $l \geqslant 2$ with $F_0 = F_1 = 1$, in which $(m, n) = (1, 1), (1, 2), (2, 1)$ and $(3, 1)$, respectively. The two kinds of hopping matrix elements are chosen to be $t_A = 1$ and $t_B = 2$. One can see that each spectrum consists of F_l bands and $F_l - 1$ gaps at the lth iteration. As l gets larger, more gaps appear. In the limit $l \to \infty$, it can be concluded that the gaps are densely populated in the energy spectra. Another feature of the energy spectra is that the spectra are self-similar, which is clearly demonstrated in figures 1(*a*)–(*d*). The self-similarity and the dense distribution of the energy gaps mean that the energy spectra of the generalized Fibonacci lattices are Cantor-like.

For each of the energy spectra shown in figures 1(*a*)–(*d*) we can derive a family tree of energy bands (see figures 2(*a*)–(*d*)). In figure 2(*a*) the production rule is $(A, B) \to (AB, A)$, i.e. an A-band generates an A-band and a B-band, while a B-band becomes an A-band. In figures 2(*b*)–(*d*) the production rules are $(A, B) \to (ABA, A)$ $(A, B) \to (BAB, A)$ and $(A, B) \to (BABB, A)$, respectively. It can be easily derived that the total number of energy bands (A-bands and B-bands) at the lth generation of each family tree is $F_l = mF_{l-2} + nF_{l-1}$ for $l \geqslant 2$ with $F_0 = F_1 = 1$. This conclusion matches the observation from figures 1(*a*)–(*d*) that each energy spectrum is composed of F_l bands at the lth iteration. According to the family trees of bands, one can index any band in the energy spectra. However, other kinds of family trees of bands can also be introduced, yielding the indexing scheme non-unique. For instance, the production rule for figure 1(*b*) can also be chosen as $(A, B) \to (AAB, A)$ or $(A, B) \to (BAA, A)$. In addition, one can choose the production rule $(A, B) \to (BAB, AB)$ to construct a different type of family tree of energy bands (see figure 3), since the total number of bands at the lth generation is still $F_l = F_{l-2} + 2F_{l-1}$, in which $l \geqslant 2$ and $F_0 = F_1 = 1$.

4. Wavefunctions

From (2.3) and (2.4), namely by successive multiplications of the transfer matrices, one can obtain numerically the wavefunctions of the generalized Fibonacci systems. Here

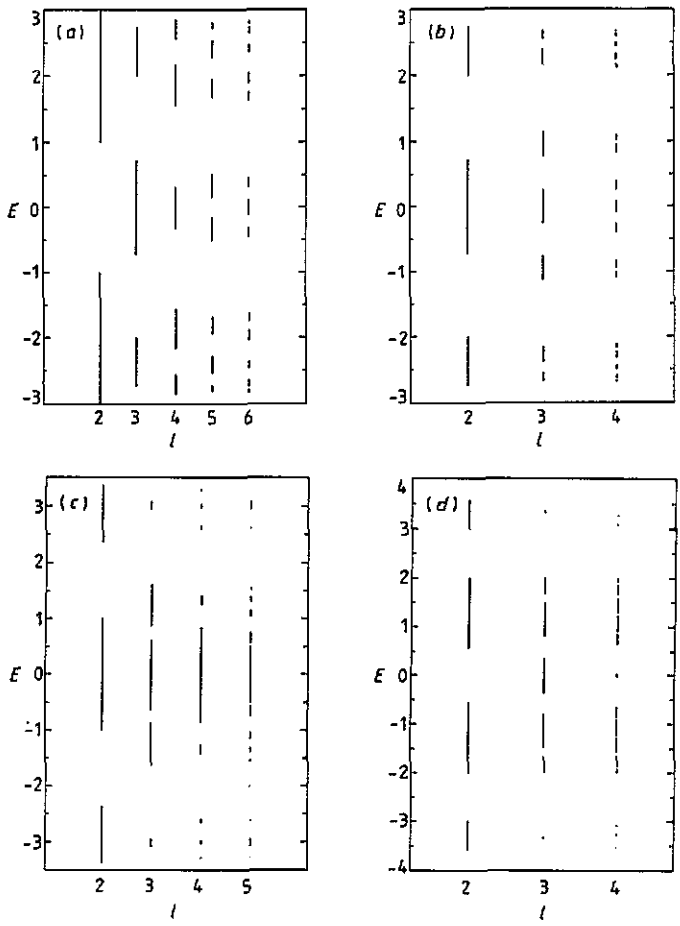

Figure 1. Energy spectra of the off-diagonal tight-binding models with $t_A = 1$ and $t_B = 2$. The systems are periodic approximations to the generalized Fibonacci lattices, of which the unit cells are of size $F_l = mF_{l-2} + nF_{l-1}$ for $l \geq 2$ with $F_0 = F_1 = 1$. (*a*) $m = 1, n = 1, l = 2, 3, 4, 5$ and 6; (*b*) $m = 1, n = 2, l = 2, 3$ and 4; (*c*) $m = 2, n = 1, l = 2, 3, 4$ and 5; (*d*) $m = 3, n = 1, l = 2, 3$ and 4. The energy spectra for the generalized Fibonacci lattices are given by the limit $l \to \infty$.

the two kinds of hopping matrix elements are chosen to be $t_A = 1$ and $t_B = 2$. In the calculation of the wavefunctions, we also monitor the quantity x_l and make sure that the chosen energies are the allowed energies of the considered systems, i.e. the condition $|x_l| \leq 1$ is satisfied for the chosen energies. In section 4.1 we present the wavefunctions at $E = 0$, while the wavefunctions at $E \neq 0$ are investigated in section 4.2.

4.1. Wavefunctions at E = 0

Four systems with $(m, n) = (1, 1), (1, 2), (2, 1)$ and $(3, 1)$ are studied, which are composed of 1597, 1393, 1365 and 1159 sites, respectively. Figures 4–7 are their wavefunctions numerically calculated at $E = 0$. For the sake of clarity, the wavefunction against 683 sites are plotted in figure 6. One can see from figures 4 and 5 that the wavefunctions are

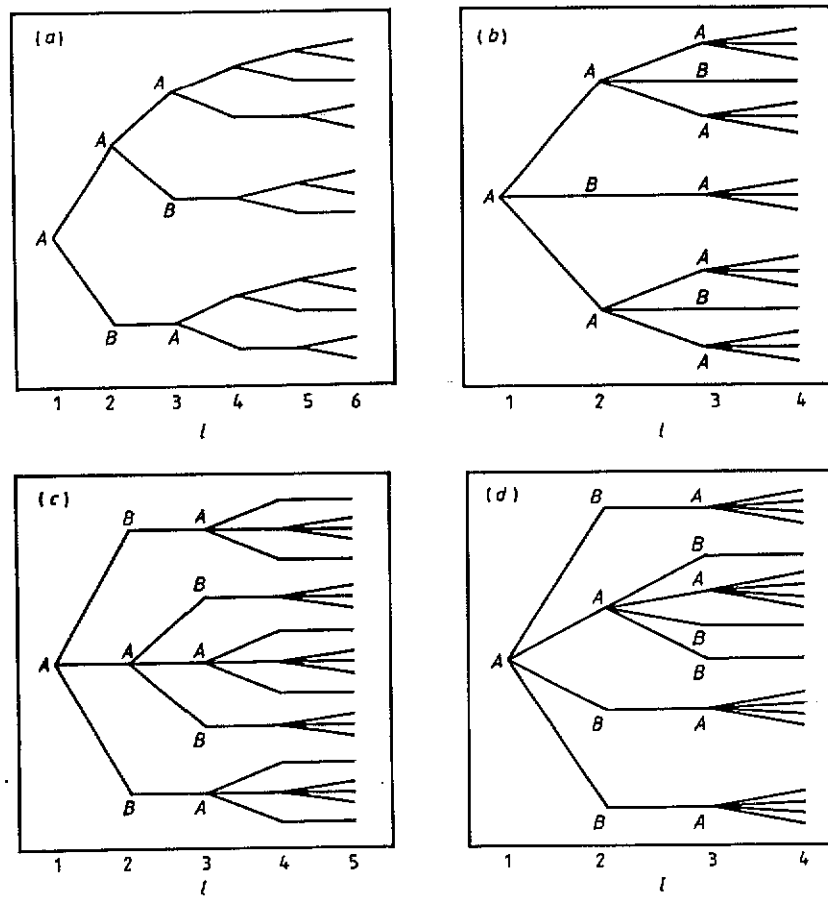

Figure 2. Family trees of energy bands for the energy spectra shown in figures 1(*a*)–(*d*), for which the production rules are chosen as (*a*) $(A, B) \rightarrow (AB, A)$, (*b*) $(A, B) \rightarrow (ABA, A)$, (*c*) $(A, B) \rightarrow (BAB, A)$ and (*d*) $(A, B) \rightarrow (BABB, A)$, respectively.

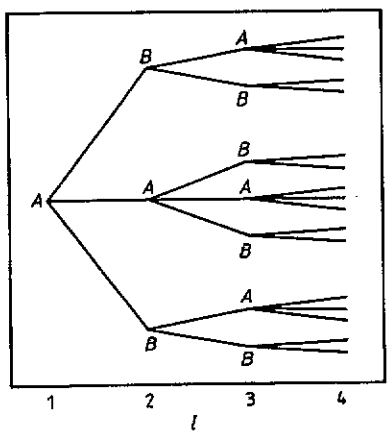

Figure 3. Family tree of energy bands for the energy spectrum shown in figure 1(*b*), which is here constructed by a different type of production rule $(A, B) \rightarrow (BAB, AB)$.

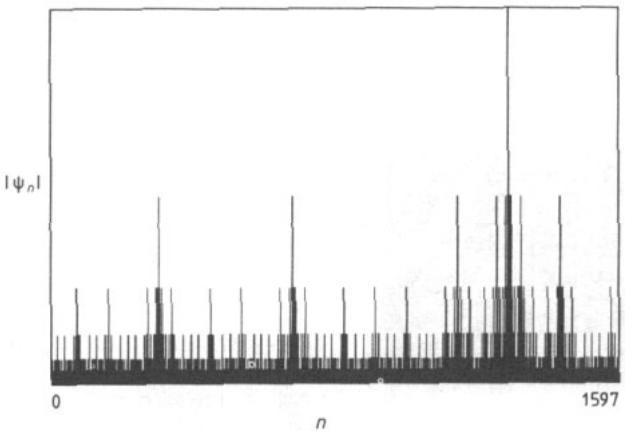

Figure 4. Wavefunction of the system with $(m, n) = (1, 1)$, which is calculated at $E = 0$ and exhibits typical critical characteristic. The two kinds of hopping matrix elements are chosen to be $t_A = 1$ and $t_B = 2$ in this figure and the following ones.

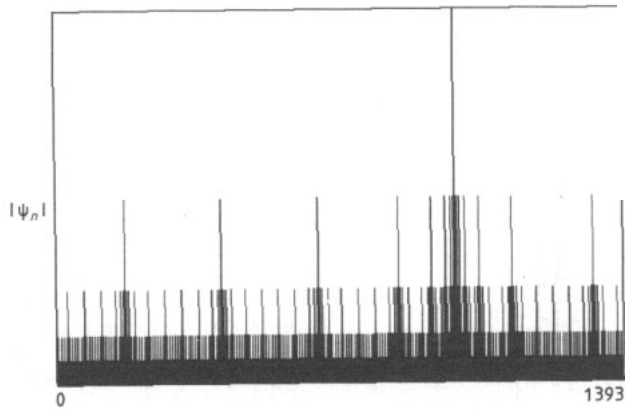

Figure 5. Wavefunction of the system with $(m, n) = (1, 2)$, which is calculated at $E = 0$ and shows critical characteristic.

critical, i.e. self-similar and neither extended nor localized in a standard fashion [23, 28, 29]. We have also calculated the wavefunctions at $E = 0$ of some systems embodied in those with $m = 1$ and $n \geqslant 3$ and found that they are critical as well. However, the situation differs as $m \neq 1$. For instance, the wavefunctions shown in figures 6 and 7 are quite different from each other; one is extended with two kinds of amplitudes and the other has a strong degree of spatial localization in each of the two peaks. It can be seen that the extended behaviour of the wavefunction plotted in figure 6 is consistent with the character of the energy spectrum of the system with $(m, n) = (2, 1)$ that there are larger bands and smaller gaps in the central region $E \sim 0$ of the energy spectrum (see figure 1(*c*)), and the spectrum tends to be continuous in this region as $l \rightarrow \infty$. Contrary to our numerical result, Gumbs and Ali [3, 8] claimed that they found a new type of localized wavefunction at $E = 0$ for the system with $(m, n) = (2, 1)$. In our judgment, their results for the system with $(m, n) = (2, 1)$ as well as those with $(m, n) = (1, 2)$ and $(1, 3)$ were calculated in error, since they chose by mistake the initial conditions only suitable to the Fibonacci lattice with $(m, n) = (1, 1)$ as those of the matrix map (2.5) for all the generalized Fibonacci lattices.

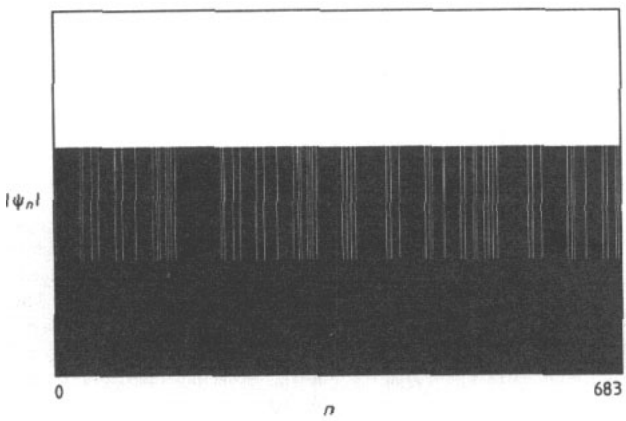

Figure 6. Wavefunction at $E = 0$ of the system with $(m, n) = (2, 1)$, which is extended with strong degree of spatial extension.

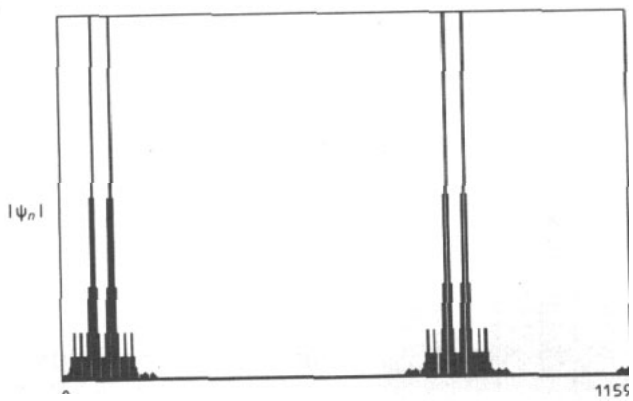

Figure 7. Wavefunction at $E = 0$ of the system with $(m, n) = (3, 1)$, in which each of the two peaks has strong degree of spatial localization.

4.2. Wavefunctions at $E \neq 0$

It was found for the Fibonacci lattice [23, 28, 29] that there are also many energies except $E = 0$, at which the wavefunctions are still critical. As to the generalized Fibonacci lattice with $(m, n) = (1, 2)$, the situation is similar. However, for the generalized Fibonacci lattices with $(m, n) = (2, 1)$ and $(3, 1)$, the situation is more complicated.

Figures 8 and 9 are the wavefunctions of the system with $(m, n) = (2, 1)$, which are numerically calculated at $E = 1.0972226$ and 2.62525247, respectively. One sees that the wavefunction at $E = 1.0972226$ has the tendency to be localized, while that at $E = 2.62525247$ is critical. However, the degree of spatial localization is not strong for the wavefunction at $E = 1.0972226$. The wavefunctions shown in figures 10–12 are those of the system with $(m, n) = (3, 1)$, which are calculated at $E = 1.000685$, 1.4997 and 1.552472566785, respectively. It is clear that the wavefunction at $E = 1.000685$ is extended, while that at $E = 1.552472566785$ is localized with strong degree of spatial localization. As for that at $E = 1.4997$, although the wavefunction is still critical, it has some degree of spatial extension. In addition to the above energies, it is found in our numerical calculations that there are many other energies at which the wavefunctions are critical. It is also found that when the wavefunction is extended at a certain energy,

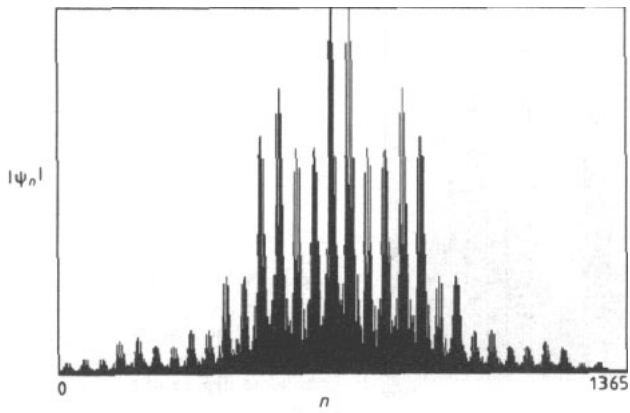

Figure 8. Wavefunction of the system with $(m, n) = (2, 1)$, which is calculated at $E = 1.0972226$ and has the tendency to be localized.

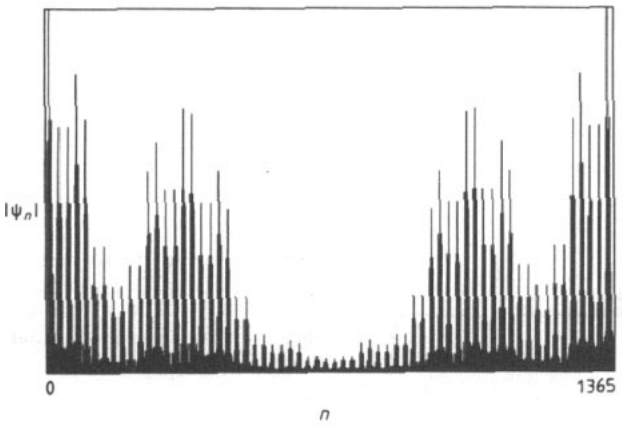

Figure 9. Wavefunction of the system $(m, n) = (2, 1)$, which is calculated at $E = 2.62525247$ and shows critical characteristic.

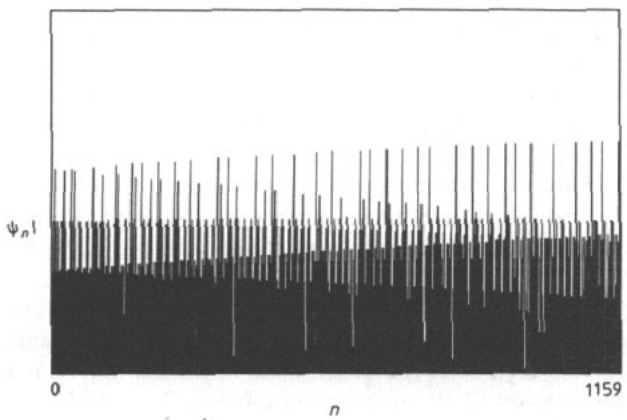

Figure 10. Wavefunction of the system with $(m, n) = (3, 1)$, which is calculated at $E = 1.000685$ and has strong degree of spatial extension.

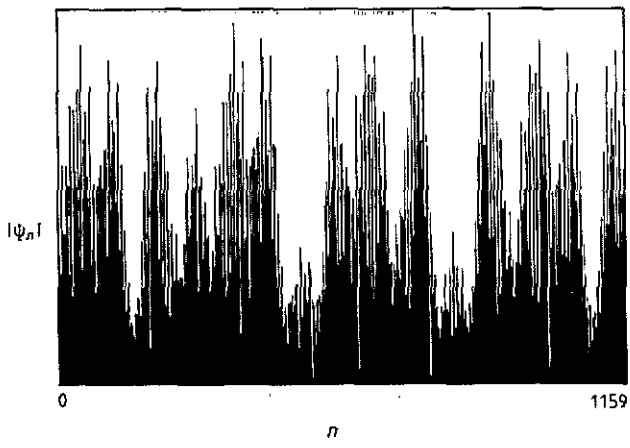

Figure 11. Wavefunction of the system with $(m, n) = (3, 1)$, which is calculated at $E = 1.4997$. Though the wavefunction is still critical, it has some degree of spatial extension.

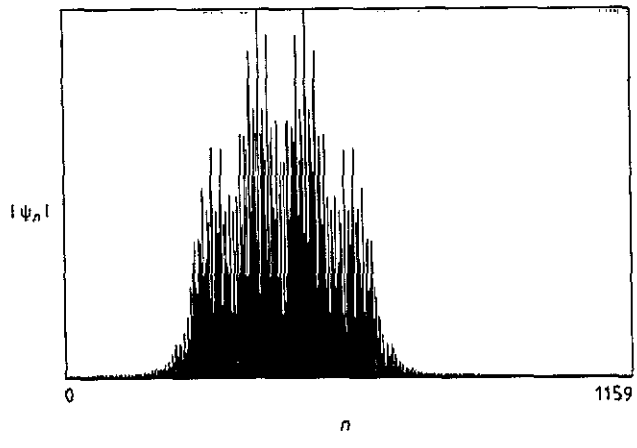

Figure 12. Wavefunction of the system with $(m, n) = (3, 1)$, which is calculated at $E = 1.552472566785$ and has strong degree of spatial localization.

a wider energy region in the vicinity of this energy always exists, in which the wavefunctions are extended or tend to be extended. As for the localized wavefunctions found in our calculations, they only seem to exist in extremely narrow energy regions.

For the hopping matrix elements chosen as $t_A = 1$ and $t_B = 2$, it is found in our calculations that the energy spectra are symmetric about the line $E = 0$. For the systems with $(m, n) = (1, 2)$ and $(2, 1)$, the energy $E = 0$ is allowed for all finite systems of size F_l, $l \geqslant 1$, implying that $E = 0$ is the allowed energy of the infinite systems as well. This conclusion can be easily derived by studying the trace map (2.19) with $(m, n) = (1, 2)$ and $(2, 1)$, respectively, since $x_l = 0$ for $E = 0$ and all positive integers l, yielding the condition $|x_l| \leqslant 1$ always satisfied. However, the energy $E = 0$ is allowed only for some finite systems with $(m, n) = (1, 1)$ and $(3, 1)$ (see figures 1(*a*) and (*d*)). As for other energies ($E \neq 0$) employed in our numerical calculations, they are allowed for the chosen finite systems.

From (2.22) and (2.23) it can be seen that there is a well-defined constant of motion I for the system with $m = 1$ and $n \geqslant 1$, while there is not such an invariant for the systems with $m \neq 1$. The quantity I has a similar form to that of the Fibonacci lattice [21], which remains invariant under the transformation (2.19) and does not flow to $I = 0$ or $I = \infty$.

Since $I = 0$ and $I = \infty$ correspond to the extended and localized states, respectively, therefore the invariant behaviour of I under the transformation (2.19) indicates that the wavefunctions are neither extended nor localized in a standard way [28]. This is why the appearances of the wavefunctions of the systems with $m = 1$ and $n \geqslant 1$ are analogous to one another and the situation differs for the systems with $m \neq 1$.

As those of the Fibonacci lattice [29, 33–35], the energy spectra and the wavefunctions of the generalized Fibonacci lattices are generally multifractal, which can be studied using the calculational method developed by Halsey *et al* [36]. For several generalized Fibonacci lattices with $m = 1$, Holzer [4] calculated the multifractal indices $f(\alpha)$ and α and found that the curves $f(\alpha)$ vs α are continuous and analogous to that for the Fibonacci lattice with slight differences in numerical values. For the critical states of the generalized Fibonacci lattices with $m \neq 1$, the situation should be similar since continuous multifractal indices are the generic feature of the critical states [34]. However, there are also extended and localized states in the generalized Fibonacci lattices with $m \neq 1$, of which the indices $f(\alpha)$ and α are completely different from those of the critical states. For the extended states, $f(\alpha)$ consists of two points and the indices $f(\alpha)$ and α are determined at a single point by $(\alpha, f(\alpha)) = (1, 1)$, while $f(\alpha)$ and α are $(\alpha, f(\alpha)) = (0, 0)$ and $(\alpha, f(\alpha)) = (\infty, 1)$ for the localized states [34, 35]. In addition, there are wavefunctions with the tendency to be extended or localized in the generalized Fibonacci lattices. These two kinds of wavefunctions also exist in the Fibonacci lattice [33], of which the multifractal indices are different in numerical values from those of the typical critical wavefunctions as shown in figures 4 and 5. Since these wavefunctions look similar to those of disordered systems at the mobility edges, it becomes necessary and important to study in detail the nature of these exotic states in the generalized Fibonacci lattices and explore the possibilities of the presence of mobility edges.

5. Summary

The electronic properties of the generalized Fibonacci lattices are studied. The model used is the off-diagonal tight-binding model. The dynamical maps are obtained, which determine the spectral behaviour of the electron states of the generalized Fibonacci lattices. It is found that the energy spectra are Cantor-like, i.e. they are self-similar and exhibit dense distributions of energy gaps. For some systems, it is clear that in the energy spectra there are certain energy regions in which the bands are larger, with vanishing gaps.

Associated with the exotic features of the energy spectra of the generalized Fibonacci lattices, the wavefunctions are critical at many energies. It is found for some systems that there are wavefunctions which are extended or localized in certain energy regions. However, for the localized electron states, the corresponding energy regions are extremely narrow. In these systems, wavefunctions with the tendency to be extended or localized are also found, which look similar to those of the disordered systems at the mobility edges.

Acknowledgments

We would like to thank Professor Youyan Liu and Wenji Deng for stimulating discussions, and the referees for helpful suggestions. The Laboratory of Atomic Imaging of

Solids, Chinese Academy of Sciences is also thanked for hospitality to J Q You. This work has been supported by the National Natural Science Foundation of China.

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