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Electronic properties of the generalized Thue–Morse lattices: a dynamical-map approach

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Abstract. As an extension of the Thue–Morse lattice, we consider the generalized Thue–Morse lattices associated with the sequences S_∞ given by the recursion relation $S_{l+1} = \{S_l^n, \bar{S}_l^m\}$ for $l \geqslant 0$ with $S_0 = \{AB\}$, in which m and n are positive integers and $\bar{S}_l$ is the complement of S_l obtained by interchanging A and B in S_l. A unified trace map is derived to study the electronic energy spectra for the diagonal tight-binding model. The results show that the spectra exhibit a new kind of self-similarity.

1. Introduction

In recent years, the electronic properties of the one-dimensional (1D) quasiperiodic systems have been extensively studied [1–7]. The Fibonacci lattice associated with the Fibonacci sequence S_∞ which is given by the recursion relation $S_{l+1} = \{S_l, S_{l-1}\}$ for $l \geqslant 1$ with $S_0 = \{B\}$ and $S_1 = \{A\}$, where A and B represent two different tiles, has been well investigated. In order to explain the energy spectrum and the scaling properties of the Fibonacci lattice, Kohmoto, Kadanoff and Tang (KKT) [1] introduced a dynamical-map method. More recently much attention has been paid to other 1D quasiperiodic and aperiodic systems [8–25], and in particular the generalized Fibonacci lattices [12–21] and the Thue–Morse lattice [22–25], for which the underlying sequences are the generalized Fibonacci sequences and the Thue–Morse sequence, respectively. As a straightforward generalization of the Fibonacci sequence, the generalized Fibonacci sequences are constructed recursively by $S_{l+1} = \{S_l^n, S_{l-1}^m\}$ with $S_0 = \{B\}$ and $S_1 = \{A\}$, where m and n are positive integers. The KKT method was extended to study the excitation problems of the generalized Fibonacci lattices [12–21] and a unified trace map was obtained [14, 18]. Results showed that these lattices exhibit richer physical properties than the Fibonacci lattice does. The construction rule of the Thue–Morse sequence is $S_{l+1} = \{S_l, \bar{S}_l\}$ for $l \geqslant 0$ with $S_0 = \{AB\}$, in which $\bar{S}_l$ is the complement of S_l obtained by interchanging A and B in S_l. The roots of the characteristic equation of the Thue–Morse sequence are 2 and 0, which satisfy the Pisot–Vijayaraghavan (PV) property. However, it is interesting that, in spite of the PV property of the associated substitution matrix, the

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Thue–Morse sequence is not quasiperiodic, and that its Fourier transform does not contain any Bragg peak, since it is purely singular continuous [8–11]. This result indicates that the Thue–Morse lattice deserves further investigations. On the other hand, stimulated by the generalization of the Fibonacci sequence, we introduce the generalized Thue–Morse sequences.

The generalized Thue–Morse sequences introduced here can be regarded as a straightforward generalization of the Thue–Morse sequence and are constructed by the recursion relation $S_{l+1} = \{S_l^n, \bar{S}_l^m\}$ with $S_0 = \{AB\}$, in which m and n are positive integers and the meaning of $\bar{S}_l$ is the same as that in the Thue–Morse case. From the construction rule of S_l, the total number F_l of tiles A and B in S_l follows the recursion relation $F_{l+1} = (m+n)F_l$ with $F_0 = 2$. Obviously, the total number of the letters in S_l is $F_l = 2(m+n)^l$. In this paper, we derive a unified trace map to study the spectra properties of the generalized Thue–Morse lattices in the framework of the KKT method and expect more interesting results emerging.

2. Dynamical maps

To study the electronic properties of the generalized Thue–Morse lattices, we employ the diagonal tight-binding model

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

where ψ_n is the wavefunction at site n, E the energy and V_n the site energy that takes two values V_A and V_B arranged in a generalized Thue–Morse sequence.

Equation (1) can be written as

$$\boldsymbol{\Psi}_{n+1} = \mathbf{M}(n)\boldsymbol{\Psi}_n \tag{2}$$

where $\boldsymbol{\Psi}_n$ is a column vector $(\psi_n, \psi_{n-1})^t$ and $\mathbf{M}(n)$ is a 2×2 unimodular matrix

$$\mathbf{M}(n) = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}. \tag{3}$$

The wavefunction at an arbitrary site N is given by

$$\boldsymbol{\Psi}_{N+1} = \mathbf{M}^{(N)}\boldsymbol{\Psi}_1 \tag{4}$$

where

$$\mathbf{M}^{(N)} = \mathbf{M}(N)\mathbf{M}(N-1)\ldots\mathbf{M}(2)\mathbf{M}(1) \tag{5}$$

is successive multiplications of the transfer matrices. If N is a generalized Thue–Morse number F_l, the matrix $\mathbf{M}_l \equiv \mathbf{M}^{(F_l)}$ satisfies the following recursion relation:

$$\begin{aligned} \mathbf{M}_{l+1} &= \bar{\mathbf{M}}_l^m \mathbf{M}_l^n \\ \bar{\mathbf{M}}_{l+1} &= \mathbf{M}_l^m \bar{\mathbf{M}}_l^n \end{aligned} \tag{6}$$

with initial conditions $\mathbf{M}_0 = \mathbf{M}(B)\mathbf{M}(A)$ and $\bar{\mathbf{M}}_0 = \mathbf{M}(A)\mathbf{M}(B)$, in which $\mathbf{M}_l$ and $\bar{\mathbf{M}}_l$ correspond to the sequences S_l and $\bar{S}_l$, respectively. Since $x_0 = \bar{x}_0$, it follows from equation (6) that

$$x_l = \bar{x}_l \qquad l \geq 0 \tag{7}$$

where $x_l \equiv \frac{1}{2}\operatorname{Tr}\mathbf{M}_l$ and $\bar{x}_l \equiv \frac{1}{2}\operatorname{Tr}\bar{\mathbf{M}}_l$, in which Tr denotes the trace of a matrix. The

recursion relation (6) can be considered as a non-linear dynamical mapping problem. The matrices $\mathbf{M}_l$ and $\bar{\mathbf{M}}_l$ are unimodular; so each of these can be parametrized by three real numbers. From the basic relation (7), we think that the map which transforms $(\mathbf{M}_l, \bar{\mathbf{M}}_l) \to (\mathbf{M}_{l+1}, \bar{\mathbf{M}}_{l+1})$ is five dimensional.

By taking the trace of equation (6), we have

$$x_{l+1} = g_l \mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-1}(x_l) - x_l[\mathcal{U}_{m-2}(x_l)\mathcal{U}_{n-1}(x_l) + \mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-2}(x_l)] + \mathcal{U}_{m-2}(x_l)\mathcal{U}_{n-2}(x_l) \tag{8}$$

where $g_l = \frac{1}{2}(a_l\bar{a}_l + b_l\bar{c}_l + c_l\bar{b}_l + d_l\bar{d}_l)$,

$$\mathbf{M}_l = \begin{pmatrix} a_l & b_l \\ c_l & d_l \end{pmatrix} \qquad \bar{\mathbf{M}}_l = \begin{pmatrix} \bar{a}_l & \bar{b}_l \\ \bar{c}_l & \bar{d}_l \end{pmatrix}$$

and $\mathcal{U}_n(x_l) = \sin[(n+1)\cos^{-1}(x_l)]/\sin[\cos^{-1}(x_l)]$ is the nth Chebyshev polynomial of the second kind which obeys the recursion relation

$$\mathcal{U}_n(x_l) = 2x_l\mathcal{U}_{n-1}(x_l) - \mathcal{U}_{n-2}(x_l) \qquad n \geq 1 \tag{9}$$

with the initial conditions $\mathcal{U}_{-1} = 0$ and $\mathcal{U}_0 = 1$.

From equation (6), we obtain two relations as follows:

$$\mathbf{M}_{l-1}^m = \bar{\mathbf{M}}_l(\bar{\mathbf{M}}_{l-1}^{-1})^n \qquad \bar{\mathbf{M}}_{l-1}^n = (\mathbf{M}_{l-1}^{-1})^m\bar{\mathbf{M}}_l. \tag{10}$$

According to equations (8) and (10), we derive a unified trace map for the generalized Thue–Morse lattices

$$x_{l+1} = \mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-1}(x_l)[g_l - Y_{mn}(x_l)x_l + Z_{mn}(x_l)] \tag{11}$$

$$g_l = \mathcal{U}_{m-1}(x_{l-1})\mathcal{U}_{n-1}(x_{l-1})\{4x_lx_{l-1}^2 - 2x_{l-1}^2W_{mn}(x_{l-1}) - 4x_lx_{l-1}Y_{mn}(x_{l-1}) + x_lY_{mn}^2(x_{l-1}) + [P_{mn}(x_{l-1}) + 3Y_{mn}(x_{l-1})]x_{l-1} - Q_{mn}(x_{l-1}) - Z_{mn}(x_{l-1})W_{mn}(x_{l-1})\} + 1 \tag{12}$$

with initial conditions

$$x_0 = \tfrac{1}{2}(E - V_A)(E - V_B) - 1 \tag{13}$$

$$x_1 = \mathcal{U}_{m-1}(x_0)\mathcal{U}_{n-1}(x_0)[g_0 - x_0Y_{mn}(x_0) + Z_{mn}(x_0)] \tag{14}$$

where

$$P_{mn}(x_l) = \mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-2}(x_l)/\mathcal{U}_{n-1}^2(x_l) + \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-2}(x_l)/\mathcal{U}_{m-1}^2(x_l) \tag{15}$$

$$Q_{mn}(x_l) = [\mathcal{U}_{m-2}^2(x_l) + \mathcal{U}_{n-2}^2(x_l)]/\mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-1}(x_l) \tag{16}$$

$$W_{mn}(x_l) = \mathcal{U}_{m-1}(x_l)/\mathcal{U}_{n-1}(x_l) + \mathcal{U}_{n-1}(x_l)/\mathcal{U}_{m-1}(x_l) \tag{17}$$

$$Y_{mn}(x_l) = \mathcal{U}_{m-2}(x_l)/\mathcal{U}_{m-1}(x_l) + \mathcal{U}_{n-2}(x_l)/\mathcal{U}_{n-1}(x_l) \tag{18}$$

$$Z_{mn}(x_l) = \mathcal{U}_{m-2}(x_l)\mathcal{U}_{n-2}(x_l)/\mathcal{U}_{m-1}(x_l)\mathcal{U}_{n-1}(x_l) \tag{19}$$

$$g_0 = \tfrac{1}{2}(E - V_A)^2(E - V_B)^2 - 2[E - \tfrac{1}{2}(V_A + V_B)]^2 + 1. \tag{20}$$

The trace map (11) which transforms $(x_l, x_{l-1}) \to (x_{l+1}, x_l)$ is two dimensional (2D). By merely studying the 2D trace map, one can determine the energy spectra of the gen-

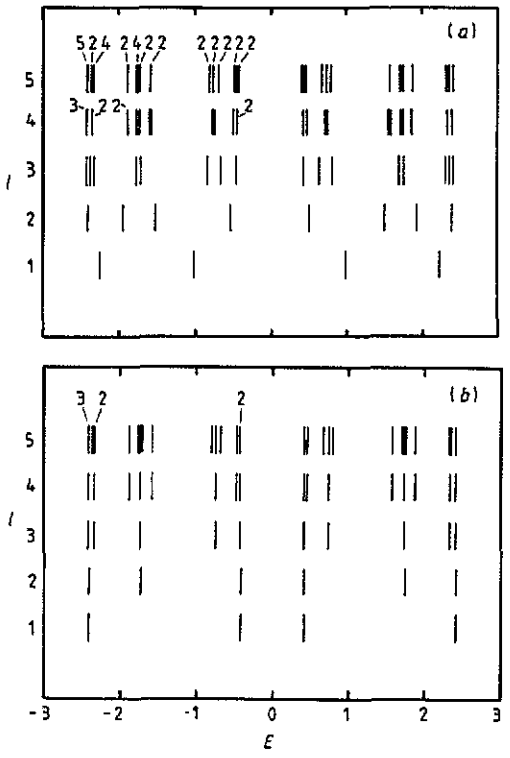

Figure 1. Energy spectra of periodic systems of periods $F_l = (m+n)F_{l-1}$ for $l \geq 1$ with $F_0 = 2$, $m = n = 1$ and $l = 1, 2, 3, 4$ and 5; (*a*) antiperiodic condition employed; (*b*) periodic condition employed. The site energies V_A and V_B are chosen to be $V_A = -V_B = 1$. Each number inside the figure labels the corresponding actual energy levels.

eralized Thue–Morse lattices. When $m = n = 1$ in particular, the map (11) is reduced to the trace map for the Thue–Morse lattice [22], i.e.

$$x_{l+1} = 4x_l x_{l-1}^2 - 4x_{l-1}^2 + 1. \tag{21}$$

3. Energy spectra

When a periodic or an antiperiodic condition is applied, the energy spectrum of the periodic system with unit cell S_l is determined by

$$x_l = \pm 1. \tag{22}$$

The energy spectrum of a generalized Thue–Morse lattice is obtained in the limit $l \to \infty$.

The energy spectra of the periodic systems with periods $F_l = (m+n)F_{l-1}$ for $l \geq 1$ with $F_0 = 2$ are presented in figures 1, 2 and 3, in which $(m, n) = (1, 1), (1, 2)$ and $(2, 2)$, respectively. The two types of site energy are chosen to be $V_A = -V_B = 1$ and the eigenvalues of the energy are represented by vertical line segments. We need to mention that, owing to the geometrical properties of the construction rule of the generalized Thue–Morse sequences, the energy spectrum of the system with $(m, n) = (2, 1)$ is the same as that of the system with $(m, n) = (1, 2)$. We can see from figures 1, 2 and 3 that the energy spectra are symmetric around the energy $E = 0$ and composed of six main clusters for the Thue–Morse lattice, and ten main clusters for $(m, n) = (1, 2)$ and $(2, 2)$. In particular, the energy spectra exhibit an exotic kind of self-similarity. For

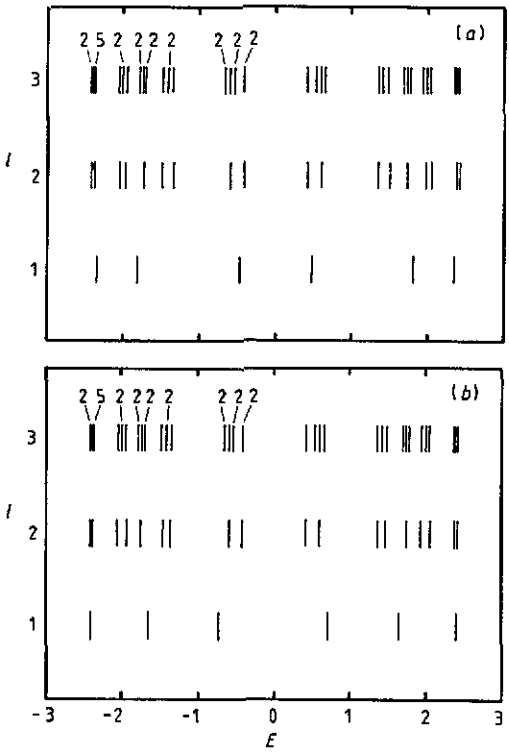

Figure 2. As for figure 1, but for $m = 1, n = 2$ with $l = 1, 2$ and 3.

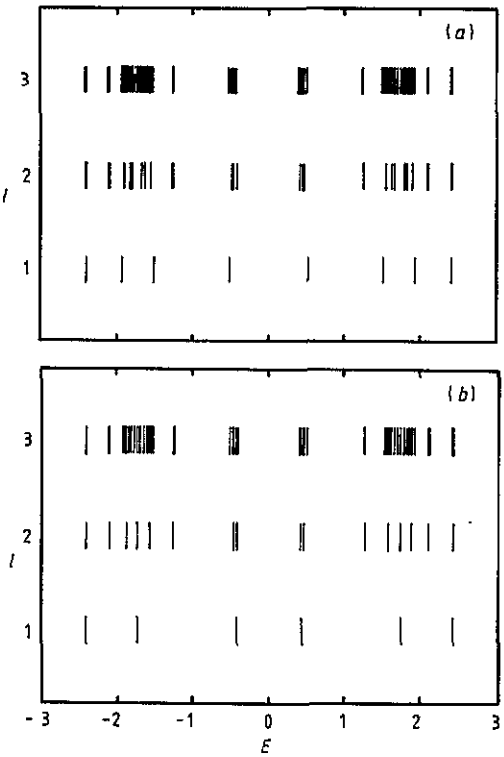

Figure 3. As for figure 1, but for $m = n = 2$ with $l = 1, 2$ and 3.

convenience of description, we order the clusters of energy levels in figures 1 and 2 from left to right. From figure 1(*a*), one sees that, when *flipped*, the third main cluster of energy levels at the lth ($l \geqslant 3$) generation is similar to the supercluster composed of the first two main clusters at the $(l-1)$th generation. Analogously in figures 2(*a*) and (*b*), when the fifth main cluster of energy levels at the lth generation is flipped, it is similar to the supercluster consisting of the first four main clusters at the $(l-1)$th generation. This new kind of self-similar behaviour in the energy spectra is here referred to as the flipped self-similarity. The flipped self-similarity cannot be clearly seen in figure 3(*a*) because the eigenstates are distributed so densely. However, it is clear that the feature of the lattice for $(m, n) = (2, 2)$ is the presence of dense 'Bloch-like' clusters (the third main cluster and the eighth main cluster from left to right in figure 3) similar to the results of Kolář and Ali [21] for the magnetic excitation spectra of the generalized Fibonacci systems associated with the sequences $S_{l+1} = \{S_l, S_{l-1}^2\}$ and $S_{l+1} = \{S_l, S_{l-1}^3\}$. In the energy spectrum shown in figure 1(*b*), because of the periodic condition employed, there is degeneration for some energy levels, making the flipped self-similarity not preserved. However, when the condition $|x_l| = 1 - \delta$ is chosen, in which δ is an arbitrary small positive number, it is found that the degeneration disappears and the energy spectrum recovers the flipped self-similarity. There is also degeneration for some energy levels in the spectrum shown in figure 3(*b*). The degenerations of the energy levels can be understood by analysis of the corresponding trace maps. As an example, we examine

the trace map given by equation (21) for the Thue–Morse lattice. From equation (21), when the periodic condition is employed, i.e. $x_l = 1$, the eigenvalues are determined by $x_{l-1} = 1$ and $x_{l-2}^2 = 0$. The latter condition is actually equivalent to $x_{l-2} = 0$. It is for this reason that the number of the eigenvalues for periodic system with unit cell S_l in the periodic condition is less than the Thue–Morse number F_l; this is different from the case when the antiperiodic condition is applied, implying that there is degeneration for some energy levels.

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