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LETTER TO THE EDITOR

Dynamical maps and Cantor-like spectra for a class of one-dimensional quasiperiodic lattices

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Abstract. The Kohmoto–Kadanoff–Tang renormalisation-group method is extended to deal with the electronic properties of a class of one-dimensional quasiperiodic lattices. A unified trace map is obtained and it is shown that the energy spectra of the quasiperiodic lattices are Cantor-like, that is the spectra are self-similar and the energy gaps in the spectra are densely populated.

There is much current interest in studying the electronic properties of quasiperiodic systems and many highly sophisticated techniques have been developed [1–10]. The most influential technique is the Kohmoto–Kadanoff–Tang (KKT) renormalisation-group method [1, 7, 8], which was developed to deal with the electronic properties of a one-dimensional (1D) Fibonacci lattice. Recently, the interest in the electronic properties has been shifting towards other 1D quasiperiodic lattices [11–14]. It was shown [12, 13] that the numerically calculated wavefunctions of states with energy $E = 0$ for several two-tile quasiperiodic lattices are clearly critical, i.e. self-similar and neither extended nor localised in a standard fashion.

A 1D two-tile quasiperiodic lattice is a lattice such that the separation of successive lattice points takes a value A or B and the two tiles A and B are arranged in a quasiperiodic sequence. The most fully investigated 1D two-tile quasiperiodic lattice is the Fibonacci lattice. The sequence of A tiles and B tiles is the Fibonacci sequence S_∞, which is constructed recursively as $S_{l+1} = \{S_l, S_{l-1}\}$ for $l \geqslant 1$ with $S_0 = \{B\}$ and $S_1 = \{A\}$. A straightforward generalisation of the Fibonacci sequence is a class of quasiperiodic sequences S_∞, which are given by the recursion relation $S_{l+1} = \{S_l^n, S_{l-1}^m\}$ with $S_0 = \{B\}$ and $S_1 = \{A\}$, in which $l \geqslant 1$, and m and n are positive integers. This class of quasiperiodic sequences is here referred to as the generalised Fibonacci sequence and an alternative method for constructing them is to use the inflation symmetry $(A, B) \rightarrow (A^nB^m, A)$. Due to the construction rule for S_l, the total number F_l of tiles A and B in S_l follows the recursion relation $F_{l+1} = mF_{l-1} + nF_l$ for $l \geqslant 1$ with $F_0 = F_1 = 1$. It can easily be checked that the ratio of the total number of tiles corresponding to the lth iterate of A to the total number of tiles corresponding to the lth iterate of B is equal to $\tau_l(m, n) = F_l/F_{l-1} = m\tau_{l-1}^{-1}(m, n) + n$. Introducing $\tau(m, n) = \lim_{l\rightarrow\infty}\tau_l(m, n)$, one obtains an equation with solution $\tau(m, n) = \frac{1}{2}[(n^2 + 4m)^{1/2} + n]$. In this letter we study the electronic properties of a class of two-tile quasiperiodic lattices, namely the generalised Fibonacci lattices, in a unified way. The two types of tile A and B are arranged successively following the generalised Fibonacci sequences.

To deal with the electronic properties of 1D generalised Fibonacci lattices, we use the 1D version of an almost-periodic (discrete) Schrödinger equation

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

where V_n represents a single potential level at site n and takes two values V_A and V_B, which are arranged in a generalised Fibonacci sequence. In matrix form (1) can be written as

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

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

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

where

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

represents successive multiplications of the transfer matrices.

If N is a generalised Fibonacci number F_l, it follows from the recursion relation $S_{l+1} = \{S_l^n, S_{l-1}^m\}$ that the transfer matrix $\mathbf{M}_l \equiv \mathbf{M}^{(F_l)}$ satisfies the following recursion relation

$$\mathbf{M}_{l+1} = \mathbf{M}_{l-1}^m\mathbf{M}_l^n \qquad l \geqslant 1 \tag{6}$$

with $\mathbf{M}_0 = \mathbf{M}(\mathrm{B})$ and $\mathbf{M}_1 = \mathbf{M}(\mathrm{A})$. Since $\det \mathbf{M}_0 = \det \mathbf{M}_1 = 1$, it follows from (6) that $\mathbf{M}_l$ is unimodular, i.e. $\det \mathbf{M}_l = 1$. Thus the 2×2 real matrix $\mathbf{M}_l$ can be parametrised only by three real numbers. Since the matrix map (6) transforms $(\mathbf{M}_{l-1}, \mathbf{M}_l)$ to $(\mathbf{M}_l, \mathbf{M}_{l+1})$, it can be regarded as a 6D dynamical system. In the following we reduce this map to a trace map.

From theory of matrices the Nth power of a 2×2 unimodular matrix $\mathbf{M}_l$ is given by [15]

$$\mathbf{M}_l^N = \begin{pmatrix} a_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l) & b_l\mathcal{U}_{N-1}(x_l) \\ c_l\mathcal{U}_{N-1}(x_l) & d_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l) \end{pmatrix} \tag{7}$$

where

$$\mathbf{M}_l = \begin{pmatrix} a_l & b_l \\ c_l & d_l \end{pmatrix} \qquad x_l \equiv \tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}_l = \tfrac{1}{2}(a_l + d_l) \tag{8}$$

and $\mathcal{U}_N(x_l)$ is the Nth Chebyshev polynomial of the second kind

$$\mathcal{U}_N(x_l) = \sin[(N+1)\cos^{-1}(x_l)]/(1 - x_l^2)^{1/2}. \tag{9}$$

The Chebyshev polynomial satisfies the recursion relation

$$\mathcal{U}_N(x_l) = 2x_l\mathcal{U}_{N-1}(x_l) - \mathcal{U}_{N-2}(x_l) \qquad N \geqslant 1 \tag{10}$$

with $\mathcal{U}_{-1}(x_l) = 0$ and $\mathcal{U}_0(x_l) = 1$. Using the recursion relation (10) one can verify the result in (7) by mathematical induction.

From (6) and (7) we obtain

$$\begin{aligned} x_{l+1} &\equiv \tfrac{1}{2}\operatorname{Tr}\mathbf{M}_{l+1} = \tfrac{1}{2}\operatorname{Tr}(\mathbf{M}_{l-1}^m\mathbf{M}_l^n) \\ &= \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})g_{l+1} - \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-2}(x_{l-1})x_l \\ &\quad - \mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-1}(x_{l-1})x_{l-1} - \mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-2}(x_{l-1}) \end{aligned} \tag{11}$$

where $g_{l+1} = \tfrac{1}{2}(a_la_{l-1} + b_lc_{l-1} + c_lb_{l-1} + d_ld_{l-1})$. From (6) it follows that $(\mathbf{M}_{l-2}^{-1})^m = \mathbf{M}_{l-1}^n\mathbf{M}_l^{-1}$. By taking the trace of this equation we have

$$\mathcal{U}_{m-1}(x_{l-2})x_{l-2} - \mathcal{U}_{m-2}(x_{l-2}) = \mathcal{U}_{n-1}(x_{l-1})h_{l+1} - \mathcal{U}_{n-2}(x_{l-2})x_l \tag{12}$$

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

Since $g_{l+1} + h_{l+1} = x_lx_{l-1}$, we then obtain from (11) and (12) the trace map for the generalised Fibonacci lattices

$$\begin{aligned} x_{l+1} = \mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})\bigg[&2x_lx_{l-1} - \left(\frac{\mathcal{U}_{m-2}(x_{l-1})}{\mathcal{U}_{m-1}(x_{l-1})} + \frac{\mathcal{U}_{n-2}(x_{l-1})}{\mathcal{U}_{n-1}(x_{l-1})}\right)x_l \\ &- \frac{\mathcal{U}_{n-2}(x_l)}{\mathcal{U}_{n-1}(x_l)}x_{l-1} - \frac{\mathcal{U}_{m-1}(x_{l-2})}{\mathcal{U}_{n-1}(x_{l-1})}x_{l-2} \\ &+ \left(\frac{\mathcal{U}_{m-2}(x_{l-2})}{\mathcal{U}_{n-1}(x_{l-1})} - \frac{\mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-2}(x_{l-1})}{\mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})}\right)\bigg] \qquad l \geqslant 2 \end{aligned} \tag{13}$$

with the initial conditions

$$x_0 = \tfrac{1}{2}(E - V_{\mathrm{B}}) \qquad x_1 = \tfrac{1}{2}(E - V_{\mathrm{A}}) \tag{14a}$$

and

$$\begin{aligned} x_2 &= \mathcal{U}_{n-1}(x_1)\mathcal{U}_{m-1}(x_0)(2x_1x_0 - 1) - \mathcal{U}_{n-1}(x_1)\mathcal{U}_{m-2}(x_0)x_1 \\ &\quad - \mathcal{U}_{n-2}(x_1)\mathcal{U}_{m-1}(x_0)x_0 - \mathcal{U}_{n-2}(x_1)\mathcal{U}_{m-2}(x_0). \end{aligned} \tag{14b}$$

When $m = 1$, the map in (13) is reduced to the trace map for the previous mean lattices

$$\begin{aligned} x_{l+1} = \mathcal{U}_{n-1}(x_l)\bigg(&2x_lx_{l-1} - \frac{\mathcal{U}_{n-2}(x_{l-1})}{\mathcal{U}_{n-1}(x_{l-1})}x_l \\ &- \frac{\mathcal{U}_{n-2}(x_l)}{\mathcal{U}_{n-1}(x_l)}x_{l-1} - \frac{1}{\mathcal{U}_{n-1}(x_{l-1})}x_{l-2}\bigg) \qquad l \geqslant 2 \end{aligned} \tag{15}$$

and when $m = n = 1$ in particular, the map in (13) becomes the well known KKT trace map for the Fibonacci lattice [1, 7, 8]

$$x_{l+1} = 2x_lx_{l-1} - x_{l-2} \qquad l \geqslant 2. \tag{16}$$

The trace map in (13) is a reduced dynamical system which corresponds to a projection of the full 6D dynamical map to a 3D orbit. Merely by studying it one can determine the energy spectra of the generalised Fibonacci lattices.

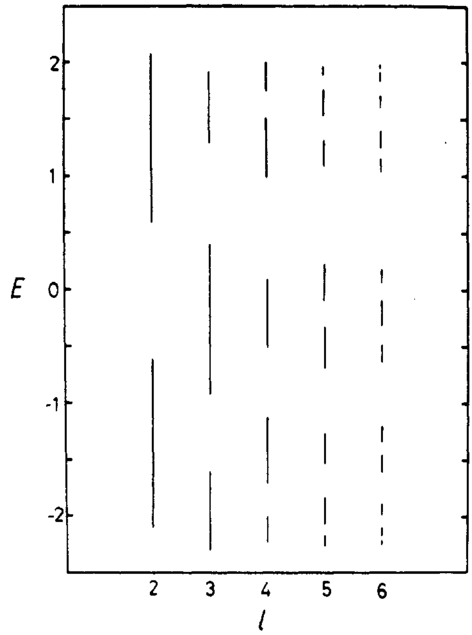

Figure 1. Band structures of the periodic systems of periods $F_l = F_{l-2} + F_{l-1}$ with $F_0 = F_l = 1$, and $l = 2, 3, 4, 5$ and 6. The two types of site potentials are chosen to be $V_A = -V_B = -0.6$. The energy spectrum of the quasiperiodic lattice is obtained by taking the limit $l \to \infty$.

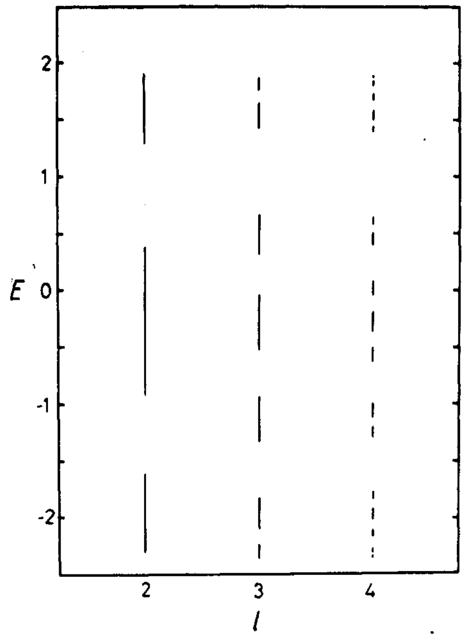

Figure 2. As figure 1, but for $F_l = F_{l-2} + 2F_{l-1}$ with $l = 2, 3$ and 4.

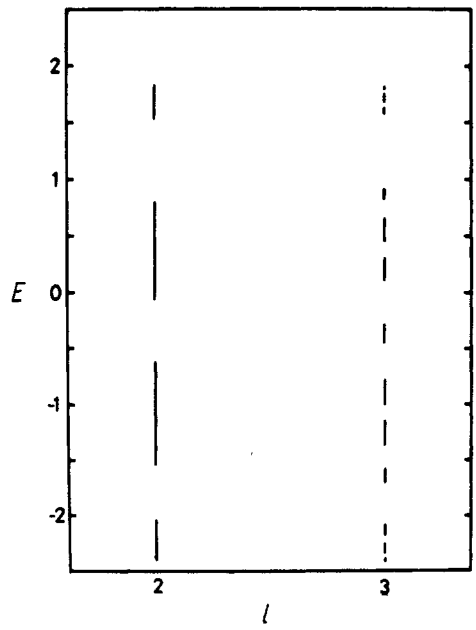

Figure 3. As figure 1, but for $F_l = F_{l-2} + 3F_{l-1}$ with $l = 2$ and 3.

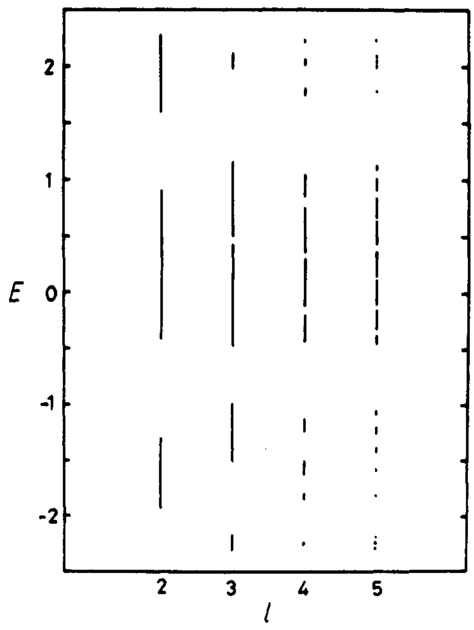

Figure 4. As figure 1, but for $F_l = 2F_{l-2} + 2F_{l-1}$ with $l = 2, 3, 4$ and 5.

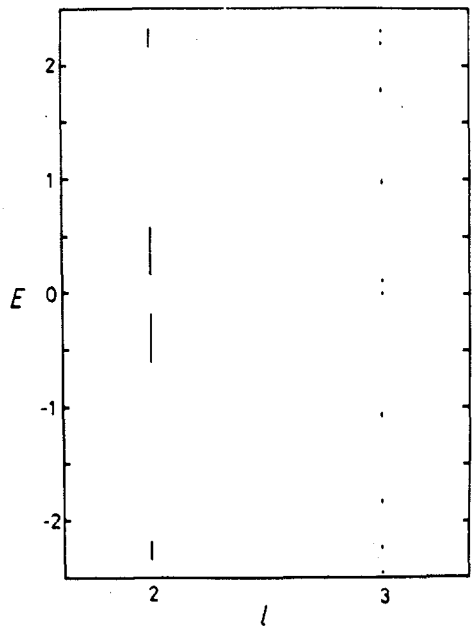

Figure 5. As figure 1, but for $F_l = 2F_{l-2} + 2F_{l-1}$ with $l = 2$ and 3.

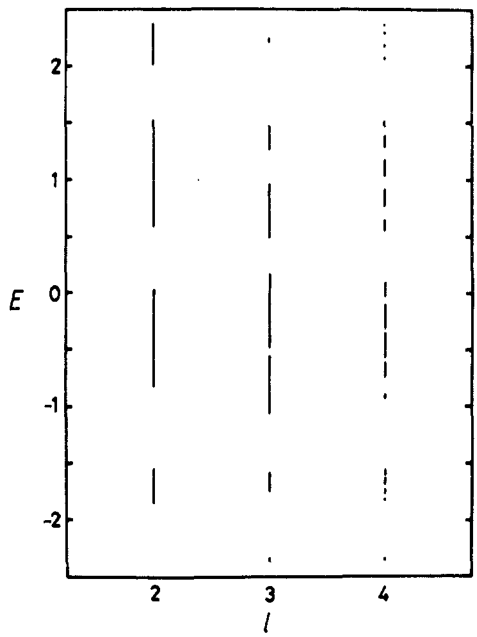

Figure 6. As figure 1, but for $F_l = 3F_{l-2} + F_{l-1}$ with $l = 2, 3$ and 4.

Assuming the eigenvalue of $\mathbf{M}^{(N)}$ is λ, i.e. $\Psi_{N+1} = \mathbf{M}^{(N)}\Psi_1 = \lambda\Psi_1$, one has

$$\lambda = \tfrac{1}{2}\{\mathrm{Tr}\,\mathbf{M}^{(N)} \pm [(\mathrm{Tr}\,\mathbf{M}^{(N)})^2 - 4\det \mathbf{M}^{(N)}]^{1/2}\}. \tag{17}$$

When the periodic (+) or antiperiodic (−) condition $\Psi_{N+1} = \pm\Psi_1$ is applied, then $\lambda = \pm 1$, and it follows from (17) that the allowed energies are determined by

$$\tfrac{1}{2}\mathrm{Tr}\,\mathbf{M}^{(N)} = \pm\tfrac{1}{2}(1 + \det \mathbf{M}^{(N)}) = \pm 1. \tag{18}$$

Let N be a generalised Fibonacci number F_l; equation (18) then becomes

$$x_l = \pm 1. \tag{19}$$

It is commonly required that the wavefunctions of a periodic system with a period of F_l should not diverge, thus the conditions for bands and gaps in the energy spectrum are respectively

$$\text{bands:} \qquad |x_l| \leqslant 1 \tag{20a}$$

$$\text{gaps:} \qquad |x_l| > 1. \tag{20b}$$

The quasiperiodic system is obtained by taking the limit $l \to \infty$, so the spectrum is obtained from the conditions in (20) in the limit of $l \to \infty$.

As typical examples, band structures obtained by the generalised KKT renormalisation-group method are shown in figures 1–6 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 $(m, n) = (1, 1), (1, 2), (1, 3), (2, 1), (2, 2)$ and $(3, 1)$, respectively. The two types of site potentials are chosen to be $V_A = -V_B = -0.6$. These figures already exhibit the exotic features of the energy spectra for the generalised Fibonacci lattices. One can see that each spectrum consists of F_l

bands and $F_l - 1$ gaps at lth iteration. As the index l gets larger, more gaps appear. In the limit of $l \rightarrow \infty$, it can be concluded that the gaps are densely populated in the energy spectra of the generalised Fibonacci lattices. Another feature is that the energy spectra of the generalised Fibonacci lattices are self-similar. The self-similarities of the energy spectra are clearly shown in figures 1, 2, 4 and 6, respectively. As more iterations corresponding to larger indices l are considered, the energy spectra corresponding to figures 3 and 5 can be also shown to be self-similar. The self-similarities and the dense distributions of the energy gaps mean that the energy spectra of the generalised Fibonacci lattices are Cantor-like.

In conclusion, electronic properties of a class of 1D quasiperiodic systems (generalised Fibonacci lattices) are studied by the generalised KKT renormalisation-group method. A unified trace map is obtained, which is a reduced dynamical system corresponding to a projection of the full 6D dynamical map to a 3D orbit. Merely by studying this trace map one can determine the energy spectra of the generalised Fibonacci lattices. It is shown that the energy spectra of the generalised Fibonacci lattices are Cantor-like, i.e. the spectra are self-similar and the energy gaps are densely distributed in the spectra.

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