Trace map, Cantor set, and the properties of a three-component Fibonacci lattice

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The electronic and phonon properties of a three-component Fibonacci lattice are studied by the dynamical map method. The trace map is obtained. The electron energy and phonon spectra, which are calculated by numerical iteration, have a structure like a Cantor set and the general dimension is calculated. The results are compared with the corresponding two-component Fibonacci lattice.

In recent decades, there has been a great deal of interest in studying the physical and geometric properties of one-dimensional (1D) deterministic nonperiodic systems. The interest stems partly from the study of the 1D Schrödinger equation with a quasiperiodic potential, the properties of electron eigenstates, and the relationship with Anderson localization.[1] The other important reason is the experimental discovery of quasicrystals in 1984 by Schechtman *et al.*[2] and the experimental work of Merlin *et al.*[3] on Fibonacci superlattices. Many highly sophisticated techniques have now been developed, and many analytical and numerical results about the electronic energy bands,[4–32] phonons,[5,6,33,34] magnetic,[6,35–39] optical[40,41] and transport[8,9,11,22,28,34,42–47] properties of these 1D nonperiodic lattices have been obtained. The lattices most frequently studied have been those defined by the two-component Fibonacci lattice[4–16,33,35,36,40–42,44] and its generalized form[11–13,17–23,37–39,43] the two-component Thue-Morse lattice[6,24–28,34,43,44,46] and hierarchical lattices.[29–32] Although these 1D nonperiodic systems lack translational invariance, they are perfectly ordered by construction. In some sense, these systems can be regarded as an intermediate case between periodic and random systems. Several authors[41,43,51,52] have discussed how different nonperiodic lattices can be arranged in a sequence from most ordered to least ordered according to their different physical and geometric properties.

On the other hand, there are several kinds of nonperiodic lattices in 1D systems, which have received little attention so far. Example are the three-component Fibonacci sequences.[12,48,50,52] Peng *et al.*[50] fabricated experimentally a three-component Fibonacci Ta/Al superlattice, using the dual-target magnetron sputtering method. They studied the structural properties of this superlattice by x-ray diffraction and by theoretical calculations. This work has stimulated the studies reported in the present paper on the electron energy bands and the phonon properties of this lattice.

The 1D three-component Fibonacci (3CF) lattice discussed by Peng *et al.*[50] is constructed out of three types of atoms A, B, and C arranged in a 3CF sequence. The 3CF sequence S_∞ is constructed recursively as

$$S_{l+1} = \{S_l, S_{l-2}\} \quad \text{for} \quad l \geq 1, \tag{1}$$

with $S_{-1} = \{B\}$, $S_0 = \{C\}$ and $S_1 = \{A\}$. Alternatively, the 3CF sequence can be generated from a seed (e.g., A) by the following substitution rule: $A \to AB$, $B \to C$, $C \to A$, which gives rise to the chain

$$ABCAABABCABCAABCAA\cdots.$$

Due to the construction rule for S_l, the total number F_l of symbols in the sequence S_l follows the recursion relation $F_{l+1} = F_l + F_{l-2}$ for $l \geq 1$, with $F_{-1} = F_0 = F_1 = 1$. In the limit as $l \to \infty$, F_{l-1}/F_l tends to the irrational value,

$$\sigma = \sqrt[3]{\tfrac{1}{2} + \tfrac{1}{6}\sqrt{\tfrac{31}{3}}} + \sqrt[3]{\tfrac{1}{2} - \tfrac{1}{6}\sqrt{\tfrac{31}{3}}} = 0.682\,32\cdots$$

where σ is the only real root of the equation, $\sigma^3 + \sigma - 1 = 0$. It is to be noted that our 3CF sequence is different from the three-component sequence introduced by Ali and Gumbs,[48] which does not appear to have been studied experimentally. They used the construction rule,

$$S_{l+1} = \{S_l, S_{l-1}, S_{l-2}\} \quad \text{for} \quad l \geq 1, \tag{2}$$

or the substitution rule: $C \to ABC$, $B \to C$, and $A \to B$. In their case, F_l satisfies the recursion relation $F_{l+1} = F_l + F_{l-1} + F_{l-2}$, and as $l \to \infty$, the ratio F_{l-1}/F_l tends to the value $\sigma^{-1} = \frac{1}{3}(1 + \frac{1}{3}\sqrt{\gamma_+} + \frac{1}{3}\sqrt{\gamma_-})$, where $\gamma_\pm = 19 \pm \sqrt{297}$. The difference between these two three-component sequences is the lack of S_{l-1} in the construction rule (1). Sequence (2) is similar to general two-component Fibonacci sequences,[12] and one can easily obtain its trace map by following the method for general two-component Fibonacci lattices. But the lattice discussed in this paper does not have this similarity.

The discrete tight-binding diagonal model is given by the equation,

$$\psi_{n+1} + \psi_{n-1} + V_n\psi_n = E\psi_n, \tag{3}$$

where V_n and ψ_n are, respectively, the site energy and the probability amplitude at the nth site, and V_n takes the three values V_a, V_b, and V_c, according to the 3CF sequence. In matrix form, Eq. (3) can be written as

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \mathbf{M}(n) \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix}, \tag{4}$$

with $\mathbf{M}(n)$ as the transfer matrix defined by

$$\mathbf{M}(n) = \begin{pmatrix} E - V_n & -1 \\ 1 & 0 \end{pmatrix}. \tag{5}$$

The wave function at an arbitrary site N is represented by

$$\begin{pmatrix} \psi_{N+1} \\ \psi_N \end{pmatrix} = \mathbf{M}^{(N)} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{6}$$

where

$$\mathbf{M}^{(N)} = \mathbf{M}(N)\mathbf{M}(N-1)\cdots\mathbf{M}(1) \quad (7)$$

represents successive multiplications of the transfer matrices.

If N is equal to F_l, it follows from the recursion relation $S_{l+1} = \{S_l, S_{l-2}\}$ that the transfer matrix $\mathbf{M}_l \equiv \mathbf{M}^{(F_l)}$ satisfies the following recursion relation:

$$\mathbf{M}_{l+1} = \mathbf{M}_{l-2}\mathbf{M}_l \quad \text{for} \quad l \geq 1, \quad (8)$$

with the initial conditions $\mathbf{M}_{-1} = \mathbf{M}(B)$, $\mathbf{M}_0 = \mathbf{M}(C)$, $\mathbf{M}_1 = \mathbf{M}(A)$, i.e.,

$$\mathbf{M}_{-1} = \begin{pmatrix} E - V_b & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{M}_0 = \begin{pmatrix} E - V_c & -1 \\ 1 & 0 \end{pmatrix},$$
$$\mathbf{M}_1 = \begin{pmatrix} E - V_a & -1 \\ 1 & 0 \end{pmatrix}.$$

Since $\det\mathbf{M}_{-1}=\det\mathbf{M}_0=\det\mathbf{M}_1=1$, it follows from Eq. (8) that $\mathbf{M}_l$ is unimodular, i.e., $\det\mathbf{M}_l = 1$ for all l. In the following, we obtain the recursion relation for $x_l = \frac{1}{2}\mathrm{Tr}(\mathbf{M}_l)$.

For the unimodular matrices $\mathbf{M}_l$ and $\mathbf{M}_{l-2}$, we have the following equation:[4]

$$\mathrm{Tr}(\mathbf{M}_l)\mathrm{Tr}(\mathbf{M}_{l-2}) = \mathrm{Tr}(\mathbf{M}_l\mathbf{M}_{l-2}) + \mathrm{Tr}(\mathbf{M}_l\mathbf{M}_{l-2}^{-1}). \quad (9)$$

Hence,

$$x_{l+1} = 2x_lx_{l-2} - \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_l\mathbf{M}_{l-2}^{-1}). \quad (10)$$

From Eq. (8), we have

$$\mathbf{M}_l = \mathbf{M}_{l-3}\mathbf{M}_{l-1} = \mathbf{M}_{l-3}\mathbf{M}_{l-4}\mathbf{M}_{l-2}$$
$$\text{or} \quad \mathbf{M}_l\mathbf{M}_{l-2}^{-1} = \mathbf{M}_{l-3}\mathbf{M}_{l-4}. \quad (11)$$

Here, we use the identities $\mathrm{Tr}(\mathbf{AB}) = \mathrm{Tr}(\mathbf{BA})$. Similarly, one can show that

$$2x_{l-3}x_{l-4} = \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_{l-3}\mathbf{M}_{l-4}) + \tfrac{1}{2}\mathrm{Tr}(\mathbf{M}_{l-4}\mathbf{M}_{l-3}^{-1}). \quad (12)$$

Also, from Eq. (8), with $l \geq 5$,

$$\mathbf{M}_{l-3} = \mathbf{M}_{l-6}\mathbf{M}_{l-4} \quad \text{or} \quad \mathbf{M}_{l-6}^{-1} = \mathbf{M}_{l-4}\mathbf{M}_{l-3}^{-1}. \quad (13)$$

From Eqs. (10–13) and the fact that for a unimodular matrix $\mathrm{Tr}(\mathbf{A}) = \mathrm{Tr}(\mathbf{A}^{-1})$, we get the recursion relation for x_l,

$$x_{l+1} = 2x_lx_{l-2} - 2x_{l-3}x_{l-4} + x_{l-6}, \qquad l \geq 5, \quad (14)$$

with initial conditions $x_{-1} = \frac{1}{2}(E - V_b)$, $x_0 = \frac{1}{2}(E - V_c)$, $x_1 = \frac{1}{2}(E - V_a)$, and $x_l = \frac{1}{2}\mathrm{Tr}(\mathbf{M}_l)$ for $l = 2, 3, 4$, and 5.

Equation (14) defines the dynamical map in a seven-dimensional space. Since the matrix map (8) transforms $(\mathbf{M}_{l-2}, \mathbf{M}_{l-1}, \mathbf{M}_l)$ to $(\mathbf{M}_{l-1}, \mathbf{M}_l, \mathbf{M}_{l+1})$ and all $\mathbf{M}_l$ are unimodular, it can be regarded as a 9D dynamical system. Our trace map (14) reduces this 9D map to a 7D dynamical system. Our trace map is different from the 6D one obtained by Ali and Gumbs for a different three-component lattice,[48] and from the 8D general three-component map discussed in Ref. 49. The Jacobian matrix of map (14) has a determinant equal to unity and is, therefore, volume preserving like the two-component Fibonacci lattice. Also, it has the trivial fixed points $x_l = 0, \pm 1$, in the same way as the map in paper.[48]

The energy spectrum is obtained by looking for energies whose corresponding wave functions ψ_{F_l} do not grow as the value of l increases. For the unimodular matrix $\mathbf{M}_l$ and periodic boundary conditions, the condition[4] that E lies in the spectrum is that $|x_l| \leq 1$. In Fig. 1, we give the electronic energy spectrum of a lattice for which the parameter values are $V_a = -V_c = 0.6$ and $V_b = 0$. One can see that the energy spectrum consists of F_l bands and $F_l - 1$ gaps at the lth iteration. As the index l gets larger, more gaps appear. In the limit of $l \to \infty$, the energy spectrum consists of an infinite number of points of measure zero, as in a Cantor set. The distribution of the energy levels is self-similar when viewed on different energy scales. This is similar to the results of the two-component Fibonacci lattice.

In order to characterize the structure of the energy spectrum, we now use the algorithm developed in Ref. 53 to calculate the global properties of the spectrum. Consider the F_l bands of the sequence S_l as a partition of S_∞, and take the measure of each band to be F_l^{-1}. Define the partition function

$$\Gamma_l(q, \tau, \{S_l\}) = \sum_{i=1}^{F_l} \frac{(F_l)^{-q}}{(w_i)^\tau},$$

where w_i is the width of the ith band and F_l^{-1} is its measure. Define

$$\Gamma(q, \tau) \equiv \lim_{l\to\infty} \Gamma_l(q, \tau, \{S_l\}). \quad (15)$$

For given q, Halsey *et al.*[53] argue that there is a unique value $\tau(q)$, such that $\Gamma(q, \tau) = \infty$ for $\tau > \tau(q)$ and $\Gamma(q, \tau) = 0$ for $\tau < \tau(q)$. These properties enable one to determine the value of $\tau(q)$. It is better, from a numerical point of view, to calculate τ from the condition that

$$\Gamma_l(q, \tau) = C\ , \quad (16)$$

where C is a nonzero constant. Evaluated for different values of q, this gives the function $\tau(q)$. Then the scaling index $\alpha(q)$ and the corresponding fractal dimension $f(\alpha)$

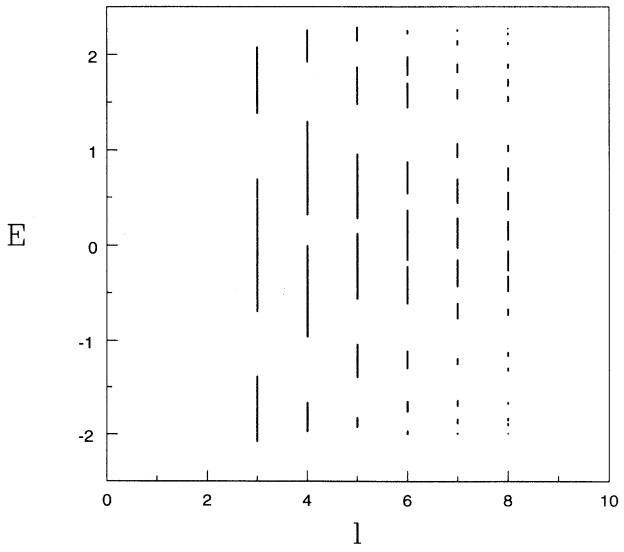

FIG. 1. Band structure of the periodic systems of periods $F_l = F_{l-3} + F_{l-1}$ and $F_{-1} = F_0 = F_1 = 1$ and $l = 3, 4, 5, 6, 7, 8$. The parameters are chosen to be $V_a = -V_c = 0.6$ and $V_b = 0$. The energy spectrum of the 3CF lattice is obtained by taking the limit $l \to \infty$.

of the subset of points with the scaling index $\alpha(q)$ are related by a Legendre transformation,

$$\alpha(q) = [d\tau(q)/dq], \quad f(\alpha) = q\alpha(q) - \tau(q). \tag{17}$$

Much information about the global properties of the spectrum is contained in the function $f(\alpha)$. The Hausdorff dimension D_H of the spectrum is just the maximum value of $f(\alpha)$. In order to speed up the convergence, we require[53] instead of Eq. (16), that $\Gamma_l/\Gamma_{l'} = 1$, where $l' > l$. The f-α curve obtained from the condition $\Gamma_{12}/\Gamma_{15} = 1$ is shown as curve 1 in Fig. 2. As one can see, it is a continuous curve and exists for a range of values $[\alpha_{\min}, \alpha_{\max}]$. This indicates that the spectrum is a multifractal set, with the most probable scaling index $\alpha_0 \approx 0.77$, and the maximum value being $f(\alpha_0) = D_H \approx 0.5$. In order to compare with the corresponding two-component systems, we plot the f-α curve for the two-component Fibonacci (2CF) lattice with parameter values $V_a = -V_b = 0.6$, as in curve 2 in Fig. 2. From Fig. 2, we can see that the most probable scaling index α_0 of the 3CF lattice is almost the same as that of the 2CF lattice. But, the Hausdorff dimension D_H and $\alpha_{\min}$ of the 3CF lattice are less than the values for the 2CF lattice, and $\alpha_{\max}$ is larger than that of the corresponding two-component lattice. This means that the allowed electronic energy regions of the 3CF lattice are smaller than those of the 2CF lattice, and the most concentrated region of the energy spectrum (corresponding to $\alpha_{\min}$) of the 3CF lattice is more concentrated, and the most rarefied region (corresponding to $\alpha_{\max}$) is more rarefied than in the case of the two-component lattice.

We now turn to the nondiagonal tight-binding model, for which the discrete Schrödinger equation is given by

$$t_{n+1}\psi_{n+1} + t_n\psi_{n-1} = E\psi_n, \tag{18}$$

where the hopping term t_l takes the values t_a, t_b, and t_c according to 3CF sequence. The phonon problem, on the other hand, is described by an equation of motion,

$$-\omega^2\psi_n = K_{n+1}\psi_{n+1} + K_n\psi_{n-1} - (K_{n+1} + K_n)\psi_n, \tag{19}$$

where ψ_n now denotes the displacement from its equilibrium position of the nth atom and the K's form a 3CF sequence with three kinds of spring constants K_a, K_b, and K_c. The matrix form of Eq. (18) is

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \mathbf{M}(t_{n+1}, t_n) \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} \tag{20}$$

and $\mathbf{M}(t_i, t_j)$ is a transfer matrix given by

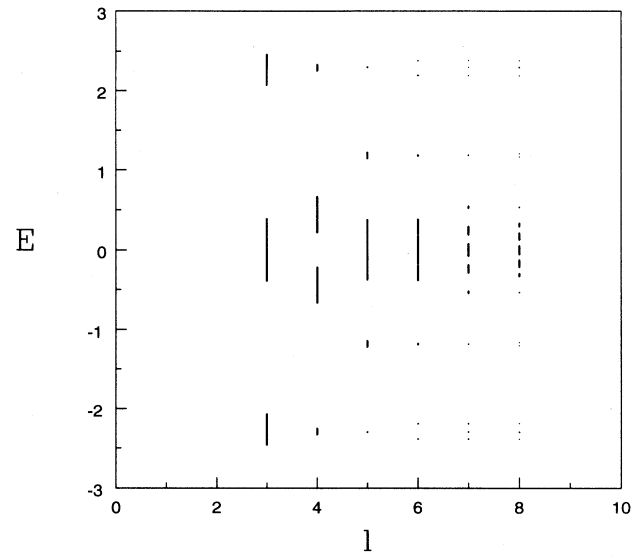

FIG. 3. Band structure of nondiagonal systems of periods F_l and $l = 3, 4, 5, 6, 7, 8$. The parameters are chosen to be $t_a = 0.5$, $t_b = 1.0$, and $t_c = 2.0$.

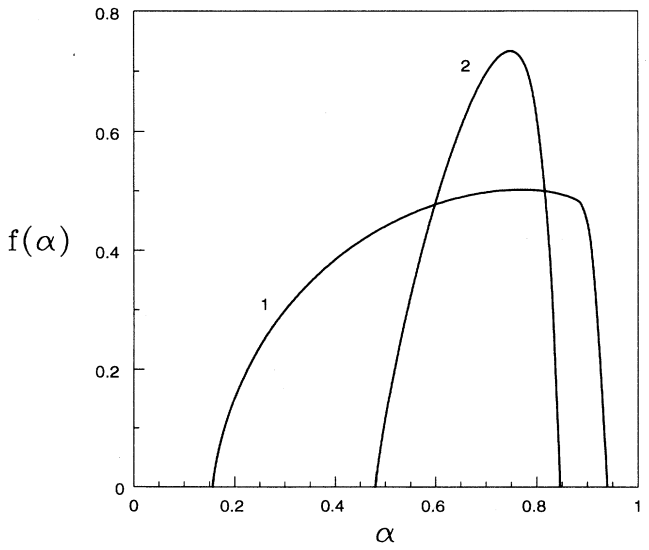

FIG. 2. The f-α curves of the spectrum of the 3CF lattice, with parameter values as in Fig. 1. (curve 1) and the corresponding 2CF lattice with parameters $V_a = -V_b = 0.6$ (curve 2). The curves are calculated from $\Gamma_{12}/\Gamma_{15} = 1$.

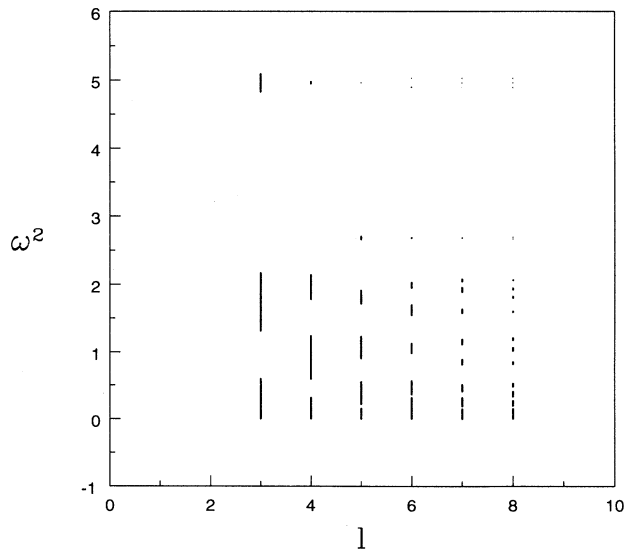

FIG. 4. The allowed ω^2 for phonon problem of system of periods F_l and $l = 3, 4, 5, 6, 7, 8$. The parameters are chosen to be $K_a = 0.5$, $K_b = 1.0$, and $K_c = 2.0$.

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

For the phonon problem, one simply makes the replacements $t_i \to K_i$ and $E \to -\omega^2 + K_i + K_j$, i.e.,

$$\mathbf{M}(K_i, K_j) = \begin{pmatrix} (-\omega^2 + K_i + K_j)/K_i - K_j/K_i & \\ 1 & 0 \end{pmatrix}.$$

The off-diagonal model is more complicated than the diagonal model in Eq. (3), since $\mathbf{M}(t_{n+1}, t_n)$ depends on two bonds and is not a unimodular matrix. However, we can obtain closed-form analytic results for the wave function at the 3CF lattice sites, by defining a transfer matrix $\mathbf{M}_l$ given recursively by Eq. (8), with initial conditions,

$$\begin{aligned} \mathbf{M}_1 &= \mathbf{M}(t_c, t_c), \\ \mathbf{M}_2 &= \mathbf{M}(t_a, t_b)\mathbf{M}(t_b, t_a), \\ \mathbf{M}_3 &= \mathbf{M}(t_a, t_c)\mathbf{M}(t_c, t_b)\mathbf{M}(t_b, t_a). \end{aligned} \tag{21}$$

$\mathbf{M}_l$ has determinant equal to unity and follows the recursion relation (8). Thus, the trace map (14) also holds for this case. The numerical results for the off-diagonal electron case and the phonon problem are shown in Figs. 3 and 4, respectively. The parameter values are taken to be $t_a = K_a = 0.5$, $t_b = K_b = 1.0$, and $t_c = K_c = 2.0$. One can see that the spectra of the off-diagonal electron and phonon models are Cantor-like sets. Furthermore, there is a qualitative difference in the energy level structures for the off-diagonal electron and phonon problems. In the electronic case, there is uniform scaling, whereas in the phonon case, at low values of ω, there are large bands and small gaps, while for higher values of ω, the bands are very narrow. This is the same as the results for the 2CF lattice.[5] The phonon problem with the spring constants uniform and the masses arranged in a 3CF sequence is dual to the phonon problem discussed above, and can be studied similarly.

In conclusion, the electron and phonon properties of a 3CF lattice is studied by the method employing a dynamical map. The trace map is obtained, which is a reduced dynamical system corresponding to a projection of the full 9D dynamical map onto a 7D space. Merely by iterating this trace map, one can determine the energy levels and the phonon spectra of the 3CF lattice. It is shown that the spectra are Cantor-like multifractal sets, and the generalized dimensions $f(\alpha)$ of the multifractial set are calculated for the diagonal electronic energy spectrum. The results are compared with those for the 2CF lattice. The electron and phonon properties of this three-component lattice have the same qualitative behavior as the 2CF lattice.

Note added in proof. After this work was completed, I learned of the paper by Wenji Deng *et al.* [Phys. Rev. B **47**, 5653 (1993)], where Eq. (14) is derived by a different method.

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