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Phonon properties of a class of one-dimensional quasiperiodic systems

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The Kohmoto-Kadanoff-Tang renormalization-group method is extended to study the phonon properties of a class of one-dimensional quasiperiodic systems. Two models are employed, which correspond to the equation of motion for phonon problems with spring constants equal and two types of masses arranged successively in generalized Fibonacci sequences, and that for phonon problems with masses equal and two types of spring constants in generalized Fibonacci sequences. It is shown that the phonon spectra of the quasiperiodic systems are Cantor-like and do not have uniform scalings. Particularly the low-lying phonon excitations tend to be extended in the low-frequency limit.

I. INTRODUCTION

Since the experimental discovery by Shechtman *et al.*[1] of the icosahedral quasicrystal in a rapidly quenched Al-Mn alloy, quasiperiodic systems have received much theoretical attention, mainly in their electronic and phonon properties.[2–17] The studies showed interesting exotic properties associated with the lack of translational invariance and with the existence of long-range orientational order in the systems. Particularly, the extensively- and well-investigated quasiperiodic system is the one-dimensional (1D) Fibonacci lattice, of which the electronic properties were studied[18–20] before the discovery of the icosahedral quasicrystal, and for which a dynamical map approach now known as the KKT renormalization-group method was developed by Kohmoto, Kadanoff, and Tang.[18] Recently the interest has been shifting towards other 1D quasiperiodic systems.[21–23] For the electronic problems of several 1D quasiperiodic systems, it was shown[21,22] that the numerically calculated wave functions of the states with energy $E=0$ are clearly critical, i.e., self-similar and neither extended nor localized in a standard way, as in the case of the Fibonacci lattice.

The Fibonacci lattice is a canonical 1D version of quasicrystals. A straightforward generalization of this quasiperiodic system is a class of 1D two-tile quasiperiodic lattices, namely the generalized Fibonacci lattices, in which the separation of successive lattice points takes value A or B. The sequences of tiles A and B in the generalized Fibonacci lattices are the generalized Fibonacci sequences S_∞, which are constructed recursively as $S_{l+1}=\{S_l^n|S_{l-1}^m\}$ with $S_0=\{B\}$ and $S_1=\{A\}$, in which $l\geq 1$, m and n are positive integers. An alternative way of constructing them is to use the inflation symmetries $(A,B)\rightarrow(A^nB^m,A)$. Due to the construction rule of S_l, the total number F_l of tiles A and B in S_l satisfies the recursion relation $F_{l+1}=mF_{l-1}+nF_l$ for $l\geq 1$ with $F_0=F_1=1$. It can be easily 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 $\tau_l(m,n)=F_l/F_{l-1}=m\tau_{l-1}^{-1}(m,n)+n$, which tends to $\tau(m,n)=\frac{1}{2}[(n^2+4m)^{1/2}+n]$ in the limit $l\rightarrow\infty$.

In present paper we study the phonon properties of a class of two-tile quasiperiodic systems, namely the generalized Fibonacci lattices, in a unified way. Although the KKT renormalization-group method is at first developed to study the electronic problem of the Fibonacci lattice, it can be also applied to deal with the phonon problem.[2,5] In Sec. II we extend the KKT renormalization-group method to study the phonon properties of the generalized Fibonacci lattices. In Sec. III the Cantor-like phonon spectra are discussed and some numerical results are presented. Section IV is a summary.

II. EXTENDED KKT RENORMALIZATION-GROUP METHOD

Consider a 1D chain of atoms of masses $\{m_n\}$ connected by spring constants $\{K_n\}$. The equation of motion for low-lying phonon excitations is

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

where ψ_n denotes the displacement of the nth atom from its equilibrium position. For mathematical simplicity and the applicability of the KKT scheme to phonon problems of the generalized Fibonacci lattices, the following two models, corresponding to $K_n=1$ and $m_n=1$, respectively, are employed:

$$-m_n\omega^2\psi_n=\psi_{n+1}+\psi_{n-1}-2\psi_n \ , \tag{2}$$

$$-\omega^2\psi_n=K_{n+1}\psi_{n+1}+K_n\psi_{n-1}-(K_{n+1}+K_n)\psi_n \ , \tag{3}$$

where the masses $\{m_n\}$ take two values m_A and m_B arranged successively in a generalized Fibonacci sequence, and $\{K_n\}$ is a generalized Fibonacci sequence with two kinds of spring constants K_A and K_B.

In matrix form, (2) and (3) can be written as

$$\underline{\Psi}_{n+1}=\underline{M}(n)\underline{\Psi}_n \tag{4}$$

and

$$\underline{\Psi}_{n+1}=\underline{M}(n+1,n)\underline{\Psi}_n \ , \tag{5}$$

where the displacement $\underline{\Psi}_n$ is a column vector $(\psi_n,\psi_{n-1})^t$ and the transfer matrices $\underline{M}(n)$ and $\underline{M}(n+1,n)$ are 2×2 unimodular matrices

$$\underline{M}(n)=\begin{bmatrix} 2-m_n\omega^2 & -1 \\ 1 & 0 \end{bmatrix} \tag{6}$$

and

$$\underline{M}(n+1,n)=\begin{bmatrix} (K_{n+1}+K_n-\omega^2)/K_{n+1} & -K_n/K_{n+1} \\ 1 & 0 \end{bmatrix} . \tag{7}$$

The displacement at an arbitrary site N is given by

$$\underline{\Psi}_{N+1}=\underline{M}^{(N)}\underline{\Psi}_1 \ , \tag{8}$$

where

$$\underline{M}^{(N)}=\underline{M}(N)\underline{M}(N-1)\cdots\underline{M}(2)\underline{M}(1) \tag{9}$$

or

$$\underline{M}^{(N)}=\underline{M}(N+1,N)\underline{M}(N,N-1)\cdots\underline{M}(2,1) \tag{10}$$

is successive multiplications of the transfer matrices.

If N is a generalized Fibonacci number F_1, it follows from the recursion relation $S_{l+1}=\{S_l^n|S_{l-1}^m\}$ that the transfer matrix $\underline{M}_l\equiv\underline{M}^{(F_l)}$ satisfies the recursion relation

$$\underline{M}_{l+1}=\underline{M}_{l-1}^m\underline{M}_l^n \ , \tag{11}$$

with initial conditions

$$\underline{M}_0=\underline{M}(B)=\begin{bmatrix} 2-m_B\omega^2 & -1 \\ 1 & 0 \end{bmatrix} \tag{12a}$$

and

$$\underline{M}_1=\underline{M}(A)=\begin{bmatrix} 2-m_A\omega^2 & -1 \\ 1 & 0 \end{bmatrix} \tag{12b}$$

for model (2), and the following initial conditions for model (3):

$$\underline{M}_1=\underline{M}(A,A) \tag{13a}$$

and

$$\underline{M}_2=\underline{M}(A,B)[\underline{M}(B,B)]^{m-1}\underline{M}(B,A)[\underline{M}(A,A)]^{n-1} \ , \tag{13b}$$

in which the four types of transfer matrices are

$$\underline{M}(A,A)=\begin{bmatrix} (2K_A-\omega^2)/K_A & -1 \\ 1 & 0 \end{bmatrix} , \tag{14a}$$

$$\underline{M}(B,B)=\begin{bmatrix} (2K_B-\omega^2)/K_B & -1 \\ 1 & 0 \end{bmatrix} , \tag{14b}$$

$$\underline{M}(A,B)=\begin{bmatrix} (K_A+K_B-\omega^2)/K_A & -K_B/K_A \\ 1 & 0 \end{bmatrix} , \tag{14c}$$

and

$$\underline{M}(B,A)=\begin{bmatrix} (K_B+K_A-\omega^2)/K_B & -K_A/K_B \\ 1 & 0 \end{bmatrix} . \tag{14d}$$

Since $\det\underline{M}_0=\det\underline{M}_1=1$, it follows from (11) that $\underline{M}_l$ is unimodular, i.e., $\det\underline{M}_l=1$. Thus the 2×2 real matrix $\underline{M}_l$ can be parametrized only by three real numbers, and the matrix map (11) can be regarded as a 6D dynamical system. By taking the trace of (11) and $(\underline{M}_{l-2}^{-1})^m=\underline{M}_{l-1}^n\underline{M}_l^{-1}$, respectively, we obtain a unified trace map for the generalized Fibonacci lattices[24]

$$\begin{aligned} x_{l+1}=&\,\mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1}) \\ &\times\left[2x_lx_{l-1}-\left[\frac{\mathcal{U}_{m-2}(x_{l-1})}{\mathcal{U}_{m-1}(x_{l-1})}+\frac{\mathcal{U}_{n-2}(x_{l-1})}{\mathcal{U}_{n-1}(x_{l-1})}\right]x_l\right. \\ &\left.-\frac{\mathcal{U}_{n-2}(x_l)}{\mathcal{U}_{n-1}(x_l)}x_{l-1}-\frac{\mathcal{U}_{m-1}(x_{l-2})}{\mathcal{U}_{n-1}(x_{l-1})}x_{l-2}+\left[\frac{\mathcal{U}_{m-2}(x_{l-2})}{\mathcal{U}_{n-1}(x_{l-1})}-\frac{\mathcal{U}_{n-2}(x_l)\mathcal{U}_{m-2}(x_{l-1})}{\mathcal{U}_{n-1}(x_l)\mathcal{U}_{m-1}(x_{l-1})}\right]\right] , \end{aligned} \tag{15}$$

with initial conditions

$$x_0=1-\tfrac{1}{2}m_B\omega^2, \quad x_1=1-\tfrac{1}{2}m_A\omega^2 \tag{16a}$$

and

$$x_2=\mathcal{U}_{n-1}(x_1)\mathcal{U}_{m-1}(x_0)(2x_1x_0-1)-\mathcal{U}_{n-1}(x_1)\mathcal{U}_{m-2}(x_0)x_1-\mathcal{U}_{n-2}(x_1)\mathcal{U}_{m-1}(x_0)x_0-\mathcal{U}_{n-2}(x_1)\mathcal{U}_{m-2}(x_0) \tag{16b}$$

for model (2), and the following initial conditions for model (3):

$$x_1 \equiv \tfrac{1}{2}\mathrm{Tr}\underline{M}_1 = 1 - \tfrac{1}{2}(\omega^2/K_A), \quad x_2 \equiv \tfrac{1}{2}\mathrm{Tr}\underline{M}_2 \tag{17a}$$

and

$$x_3 = \mathcal{U}_{n-1}(x_2)\mathcal{U}_{m-1}(x_1)[\tfrac{1}{2}\mathrm{Tr}(\underline{M}_1\underline{M}_2)] - \mathcal{U}_{n-1}(x_2)\mathcal{U}_{m-2}(x_1)x_2 - \mathcal{U}_{n-2}(x_2)\mathcal{U}_{m-1}(x_1)x_1 - \mathcal{U}_{n-2}(x_2)\mathcal{U}_{m-2}(x_1) , \tag{17b}$$

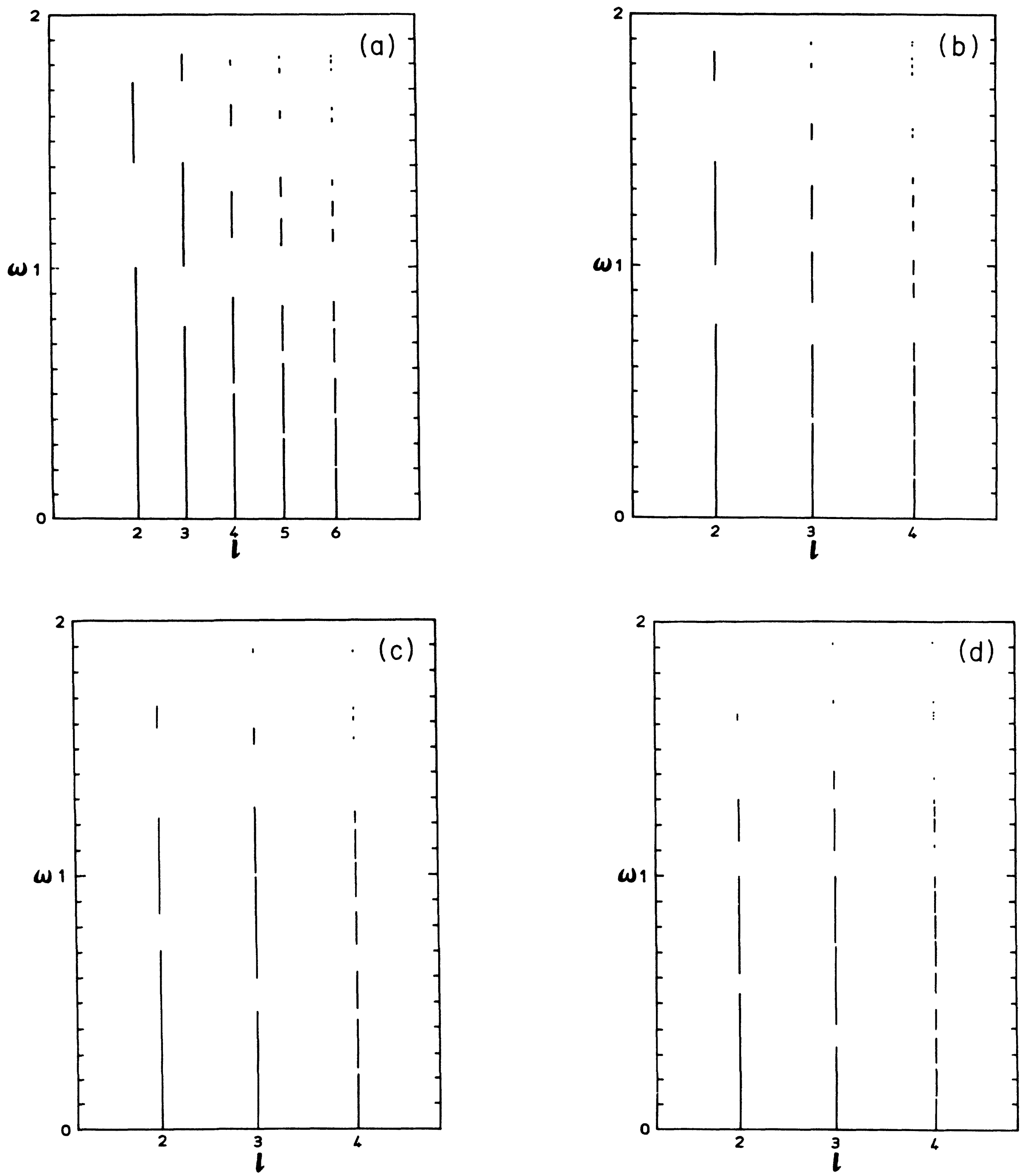

FIG. 1. Band structures of the periodic systems of periods $F_l = mF_{l-2} + nF_{l-1}$ for $l \geq 2$ with $F_0 = F_1 = 1$. (a) $m=1$, $n=1$, $l=2$, 3, 4, 5, and 6; (b) $m=1$, $n=2$, $l=2$, 3, and 4; (c) $m=2$, $n=1$ $l=2$, 3, and 4; (d) $m=3$, $n=1$, $l=2$, 3, and 4. The two types of masses are chosen to be $m_A=1$ and $m_B=2$. The phonon spectra of the quasiperiodic systems are given by the limit $l \to \infty$.

where $x_l \equiv \frac{1}{2}\mathrm{Tr}\underline{M}_l$, and $\mathcal{U}_N(x_l)$ is the Nth Chebyshev polynomial of the second kind,

$$\mathcal{U}_N(x_l)=\frac{\sin[(N+1)\cos^{-1}(x_l)]}{\sin[\cos^{-1}(x_l)]}\ , \tag{18}$$

which obeys the recursion relation

$$\mathcal{U}_N(x_l)=2x_l\mathcal{U}_{N-1}(x_l)-\mathcal{U}_{N-2}(x_l)\ . \tag{19}$$

When $m=n=1$, in particular, the map (15) is reduced to the well-known KKT trace map for the Fibonacci lattice[18]

$$x_{l+1}=2x_l x_{l-1}-x_{l-2}\ . \tag{20}$$

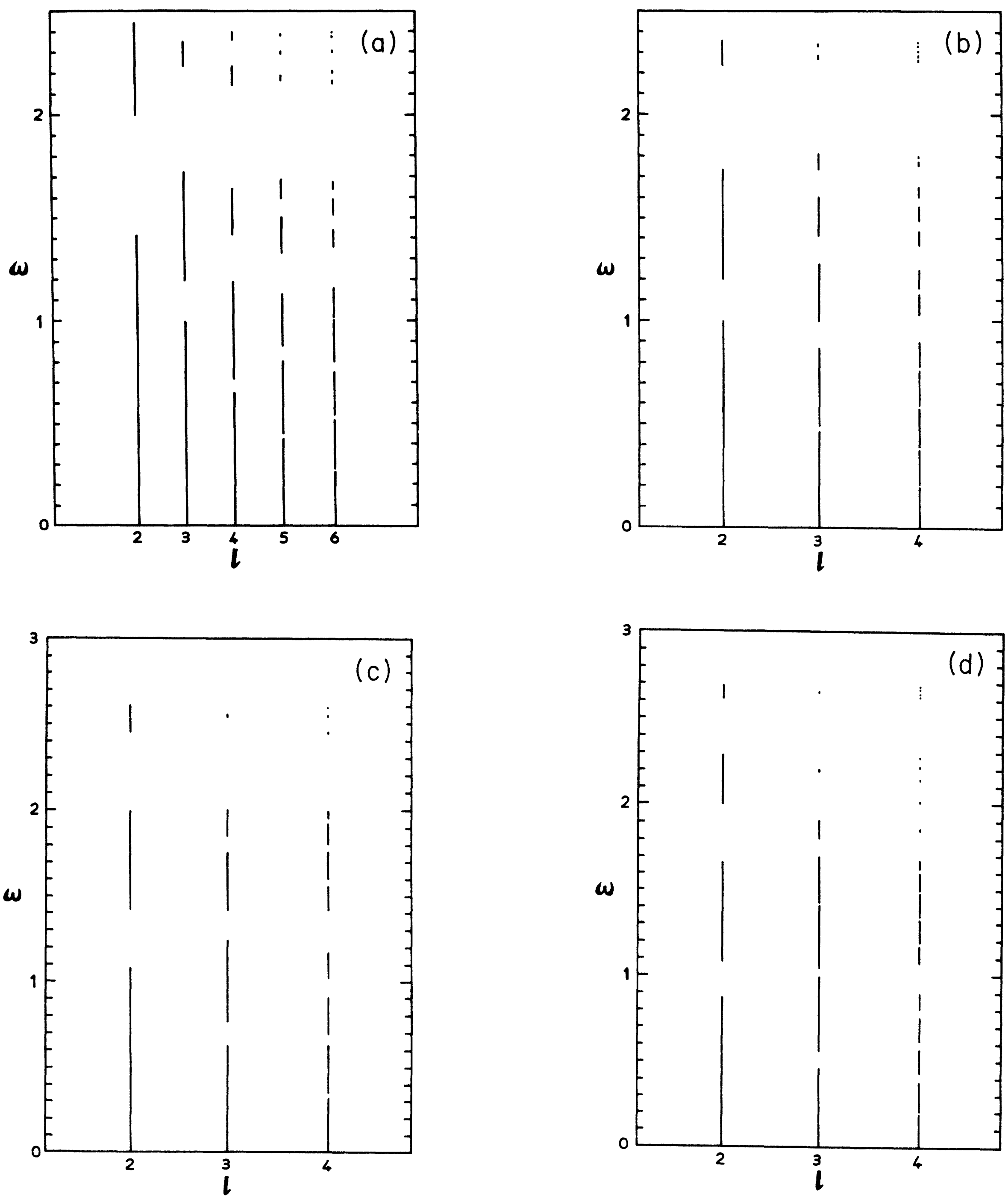

FIG. 2. Band structures of the periodic systems of periods $F_l=mF_{l-2}+nF_{l-1}$ for $l\geq 2$ with $F_0=F_1=1$. (a) $m=1$, $n=1$, $l=2$, 3, 4, 5, and 6; (b) $m=1$, $n=2$, $l=2$, 3, and 4; (c) $m=2$, $n=1$, $l=2$, 3, and 4; (d) $m=3$, $n=1$, $l=2$, 3, and 4. The two types of spring constants are chosen to be $K_A=1$ and $K_B=2$. The phonon spectra of the quasiperiodic systems are obtained in the limit $l\rightarrow\infty$.

The trace map (15) is a reduced dynamical system, which corresponds to a projection of the full 6D dynamical map (11) onto a 3D orbit. By merely studying it one can determine the phonon spectra of the generalized Fibonacci lattices.

III. CANTOR-LIKE PHONON SPECTRA

Assuming the eigenvalue of the unimodular transfer matrix $\underline{M}_l$ is λ, i.e., $\underline{\Psi}_{F_l+1}=\underline{M}_l\underline{\Psi}_1=\lambda\underline{\Psi}_1$, one has

$$\lambda=\tfrac{1}{2}\{\mathrm{Tr}\underline{M}_l\pm[(\mathrm{Tr}\underline{M}_l)^2-4]^{1/2}\} \ . \tag{21}$$

When the periodic (+) or antiperiodic (−) condition $\underline{\Psi}_{F_l+1}=\pm\underline{\Psi}_1$ is applied, then $\lambda=\pm1$, and it follows from (21) that the allowed frequencies are determined by

$$x_l=\pm1 \ . \tag{22}$$

Commonly, it is required that the displacements $\{\underline{\Psi}_n\}$ of atoms in a periodic system with a period of F_l should not diverge, thus the conditions for bands and gaps in the phonon spectrum are, respectively,

$$\text{bands:} \ |x_l|\le 1 \ , \tag{23a}$$

$$\text{gaps:} \ |x_l|>1 \ . \tag{23b}$$

The quasiperiodic system is obtained by the limit $l\to\infty$, so the phonon spectrum is obtained from the conditions in (23) in the limit $l\to\infty$.

As typical examples, band structures are presented in Figs. 1 (a)–(d) and Figs. 2(a)—2(d) for the phonon problems of periodic systems with periods $F_l=mF_{l-2}+nF_{l-1}$ for $l\ge2$ with $F_0=F_1=1$, in which $(m,n)=(1,1)$, (1,2), (2,1), and (3.1), respectively. The two types of masses in model (2) are chosen to be $m_A=1$ and $m_B=2$, and the two types of spring constants in model (3) are chosen to be $K_A=1$ and $K_B=2$. Comparing Figs. 1(a)–1(d) one by one with Figs. 2(a)—2(d), one sees that they look similar with each other, especially in the lower parts of the phonon spectra. These figures already show the exotic features of the phonon spectra for the generalized Fibonacci lattices. One can see that each phonon 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 $1\to\infty$, it can be concluded that the gaps are densely populated in the phonon spectra of the generalized Fibonacci lattices. Another feature concerning the phonon spectra is that they are self-similar. The self-similarities and the dense distributions of the gaps mean that the phonon spectra of the generalized Fibonacci lattices are Cantor-like. However, the phonon spectra do not have uniform scalings, analogous to what occurs in the phonon spectrum of the Fibonacci lattice. At low values of ω, there are large bands and small gaps, while the bands are very narrow for higher values of ω. The characteristic of larger bands and smaller gaps at lower values of ω indicates that as $\omega\to0$, the low-lying phonon excitations tend to be extended, as in the case of phonon problem of the Fibonacci lattice.[2–4] The dispersion relation then asympototically becomes $\omega=Ck$, and the low-frequency integrated density of states of phonon is linear in ω for a given generalized Fibonacci lattice.

IV. SUMMARY

We extend the KKT renormalization-group method to deal with the phonon properties of a class of 1D quasiperiodic systems (the generalized Fibonacci lattices). Two models are employed, which correspond to the equation of motion for phonon problems with spring constants equal and two types of masses arranged successively in generalized Fibonacci sequences, and that for phonon problems with masses equal and two types of spring constants in generalized Fibonacci sequences. A unified trace map with only different initial conditions is obtained, which is a reduced dynamical system corresponding to a projection of the full 6D dynamical map onto a 3D orbit. By merely studying it one can determine the phonon spectra for the phonon problems of the generalized Fibonacci lattices. For a given generalized Fibonacci lattice, the phonon spectra obtained using different models are similar to each other, especially in the lower parts of the spectra. It is showed that the phonon spectra of the generalized Fibonacci lattices are Cantor-like, i.e., the spectra are self-similar and the gaps are densely populated in the spectra. In addition, the phonon spectra do not have uniform scalings; at low values of ω, there are large bands and small gaps, while the bands are very narrow for high values of ω. In particular, the low-lying phonon excitations tend to be extended as $\omega\to0$, as in the case of crystalline structures.

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[1]D. Shechtman, I. Blech, D. Gratias, and J. W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984).
[2]M. Kohmoto and J. R. Banavar, Phys. Rev. B **34**, 563 (1986).
[3]J. P. Lu, T. Odagaki, and J. L. Birman, Phys. Rev. B **33**, 4809 (1986).
[4]F. Nori and J. P. Rodriguez, Phys. Rev. B **34**, 2207 (1986).
[5]J. M. Luck and D. Petritis, J. Stat. Phys. **42**, 289 (1986).
[6]M. Fujita and K. Machida, Solid State Commun. **59**, 61 (1986).
[7]H. De Raedt and T. Schneider, Z. Phys. B **71**, 287 (1988).
[8]T. Odagaki and D. Nguyen, Phys. Rev. B **33**, 2184 (1986).
[9]T. C. Choy, Phys. Rev. Lett. **55**, 2915 (1985).
[10]M. Kohmoto and B. Sutherland, Phys. Rev. B **34**, 3849 (1986).
[11]B. Sutherland, Phys. Rev. B **34**, 3904 (1986).
[12]M. Kohmoto, B. Sutherland, and C. Tang, Phys. Rev. B **35**, 1020 (1987).
[13]J. P. Lu and J. L. Birman, Phys. Rev. B **36**, 4471 (1987).

[14]J. Q. You, J. Phys. C **21**, L1015 (1988).
[15]J. Q. You and J. R. Yan, Z. Phys. B **77**, 275 (1989).
[16]M. Arai, T. Tokihiro, T. Fujiwara, and M. Kohmoto, Phys. Rev. B **38**, 1621 (1988).
[17]N. Nishiguchi and T. Sakuma, Phys. Rev. B **38**, 7370 (1988).
[18]M. Kohmoto, L. P. Kadanoff, and C. Tang, Phys. Rev. Lett. **50**, 1870 (1983).
[19]S. Ostlund, R. Pandit, D. Rand, H. J. Schellnhuber, and E. Siggia, Phys. Rev. Lett. **50**, 1873 (1983).
[20]M. Kohmoto and Y. Oono, Phys. Lett. **102A**, 145 (1984).
[21]G. Gumbs and M. K. Ali, Phys. Rev. Lett. **60**, 1081 (1988); J. Phys. A **21**, L517 (1988).
[22]M. Holzer, Phys. Rev. B **38**, 1709 (1988); **38**, 5756 (1988).
[23]J. M. Luck, Phys. Rev. B **39**, 5834 (1989).
[24]J. Q. You and Q. B. Yang, J. Phys. Condens. Matter (to be published).