

Perfect self-similarity of energy spectra and gap-labeling properties in one-dimensional Fibonacci-class quasilattices

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One-dimensional Fibonacci-class quasilattices are proposed and studied, which are constructed by the substitution rules $B \rightarrow B^{n-1}A$, $A \rightarrow B^{n-1}AB$. We have proved that this class of binary lattices is self-similar and also quasiperiodic. By the use of the renormalization-group technique, it has been proved that for all Fibonacci-class lattices the electronic energy spectra are perfect self-similar, and the branching rules of spectra are obtained. We analytically prove that each energy gap can be simply labeled by a characteristic integer, i.e., for the Fibonacci-class lattices there is a universal gap-labeling theorem [Phys. Rev. B **46**, 9216 (1992)]. [S0163-1829(97)10705-6]

I. INTRODUCTION

Quasiperiodic systems have received extensive interest since the experimental discovery of fivefold symmetry in the diffraction pattern of metallic alloys.¹ In particular, much attention has been devoted to the electronic properties of the Fibonacci lattice, which provides a prototype model for studying the quasiperiodic systems.²⁻⁹ The distinguished feature lies in the fact that the energy spectrum is neither absolutely continuous nor purely pointed, but singular continuous, and the eigenstates are critical between the extended and localized ones. On the other hand, many non-Fibonacci models have been studied, mainly by generalizing the Fibonacci substitution rules $B \rightarrow A$, $A \rightarrow AB$. Among them, so-called generalized Fibonacci sequences, which are given by the substitutions $A \rightarrow A^m B^n$, $B \rightarrow A$, have been extensively studied.¹⁰⁻¹⁷ Investigations have revealed their many similar properties as those of the Fibonacci lattice. However, whether these models can be called "quasiperiodic" or only "aperiodic" is an interesting question. In an earlier work, Bombieri and Taylor¹⁸ pointed out that any infinite chain obtained by a substitution rule possessing the Pisot property can be constructed with a projection method, so the quasiperiodicity is preserved. According to this criterion, a family of generalized Fibonacci sequences generated by $A \rightarrow A^n B$, $B \rightarrow A$ are quasiperiodic,¹² for which the same properties as in the Fibonacci case can be expected to exist. This conclusion has been confirmed by a lot of work.

To study an aperiodic system, one will face two problems: self-similarity and quasiperiodicity. In general, a self-similar structure is produced by the substitution rule, and a quasiperiodic lattice is constructed by the projection method.¹⁹ The

former reflects the inflation symmetry, while the latter characterizes that its Fourier spectrum consists of Bragg peaks. The relationship between these two sides has been studied recently.²⁰⁻²⁵

In this paper, we restrict ourselves to the binary sequences. A binary substitution τ is formally defined by its simultaneous action on two letters A and B , which replaces each letter with a finite word, of the form

$$\tau: \begin{cases} A \rightarrow \tau(A) = a_1 a_2 \cdots a_{\alpha+\beta} \\ B \rightarrow \tau(B) = b_1 b_2 \cdots b_{\gamma+\delta} \end{cases} \quad (1)$$

In this expression, each a_i or b_i stands for a letter, α and β denote the number of letters of A and B in $\tau(A)$, and γ and δ are the number of A and B in $\tau(B)$. The substitution matrix associated with τ is defined as follows:

$$M_\tau = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix}. \quad (2)$$

Here M_τ only describes the contents of $\tau(A)$ and $\tau(B)$ in letters of each type, irrespective of the order in which these letters occur.

Repeatedly using the substitution (1), a finite word is developed to an infinite sequence Σ , and we have $\Sigma = \tau(\Sigma)$. Thus an infinite abstract sequence is obtained, which is self-similar. A physical structure corresponding to Σ can be produced by regarding the two letters A and B as two kinds of atomic spacing l_A and l_B in a one-dimensional chain.

Luck *et al.*²⁰ have shown that a chain generated by the substitution (1) is quasiperiodic if and only if the associated substitution matrix (2) fulfills two conditions: Pisot property and unit determinant. The structure thus obtained can be alternatively built as sections of periodic patterns in a two-dimensional space. Along the same line, Wen *et al.*²⁴ have proposed following a class of substitution rules to generate quasiperiodic chains which share some typical properties with the Fibonacci chain. The substitution matrix is

$$M_\tau = \begin{pmatrix} f_{k-1} + n f_{k-2} & f_{k-2} \\ f_{k-2} + n f_{k-3} & f_{k-3} \end{pmatrix}, \quad (3)$$

where f_k is the Fibonacci number with the initial condition $f_{-1} = f_0 = 1$ and $f_k = 0$ for all $k \leq -2$, defined by the recursion relation $f_{k+2} = f_{k+1} + f_k$, and n is a non-negative integer. They have also argued that the condition under which a quasiperiodic chain can be obtained with the standard projection method is that the substitution rule is invertible.

On the other hand, Odagaki and Kaneko²³ have studied the self-similarity of a quasiperiodic sequence given by

$$F_k(\alpha) = [(k+1)\alpha] - [k\alpha] \quad (k = 1, 2, 3, \dots), \quad (4)$$

where $[x]$ denotes the integer part of x , and α is an irrational parameter in $(0, 1)$. The sequence thus obtained consists of two elements 1 and 0, which can be replaced with two length units l_A and l_B to construct a one-dimensional chain. They have proven that the structure given by Eq. (4) is self-similar if and only if α is a quadratic irrational number. Lin *et al.*²⁵ have also confirmed this result. By establishing the correspondence between a substitution rule and a transformation on the value of α , they have concluded that the necessary condition for a self-similar sequence that is generated by the substitution rule and can be obtained by the projection method is that the substitution rule is a simple composition of the general transformations $A \rightarrow A^n B$, $B \rightarrow A$.

Although the above sequences are quasiperiodic and geometrically self-similar, the electronic spectral structure may vary a lot. Unlike the Fibonacci chain, their regular self-similarity does not show up definitely in the energy spectra.¹¹⁻¹⁷ An appealing question is thus raised: does the regular or *perfect* self-similarity of the energy spectrum also exist in other structures as in the Fibonacci lattice? As an answer, Huang, Liu, and Mo²⁶ have by chance found a quasilattice, called the intergrowth sequence (IS) model by them, and proved that it has a perfect self-similar spectrum. Especially, further investigation displays that in other aspects of electronic properties this model is also same as the Fibonacci lattice, such as the gap-labeling properties, localization of the electronic states, multifractal properties of electronic wave function, even the transmission of light.²⁷ We consider that the intergrowth sequence should not be a unique model which possesses the same electronic properties as the Fibonacci lattice, but should there be a class of them. In other words, in the set of general transformation stated by Lin *et al.* there should be a class of special transformation, the electronic properties of which have perfect self-similarity. The rest of the set do not have the same properties. Motivated by this idea we have successively found a class of one-dimensional binary lattices, which are both self-similar and quasiperiodic. The Fibonacci and intergrowth sequences

become two special cases of the class. By analyzing the splitting patterns of the energy spectra, we find that the spectra are perfectly self-similar with a regular hierarchical structure. The integrated density of states exhibits a ‘‘devil’s stair case’’ structure and each energy gap can be simply labeled by a unique characteristic integer. All these are the typical properties of the Fibonacci lattice. Therefore, we can consider this class of quasilattices a most intrinsic generalization of the Fibonacci lattice, and call it Fibonacci-class (FC) quasilattices. We organize this paper as follows.

In Sec. II, we introduce this class of sequences and their mathematical characters. These Fibonacci-class lattices can be obtained by the substitution rules as well as by the projection method. Section III is devoted to study the electronic energy spectra of FC lattices. By the use of the renormalization-group technique we have obtained their self-similar spectra and branching rules. In Sec. IV the gap-labeling rules are obtained by calculating the occupation probabilities of energy levels in every subband. We have analytically proved that for FC lattices there exists a universal gap-labeling theorem, i.e., every energy gap of the spectrum can be labeled by a unique characteristic integer. Finally, a brief summary is given in Sec. V.

II. THE FIBONACCI-CLASS SEQUENCES

A Fibonacci chain is described by the substitutions $B \rightarrow A$, $A \rightarrow AB$, while the IS sequence is generated by $B \rightarrow BA$, $A \rightarrow BAB$. By extrapolation, we study the following substitution rules:

$$B \rightarrow B^{n-1}A, \quad A \rightarrow B^{n-1}AB, \quad (5)$$

where n is a positive integer and B^n denotes a string of n B 's. For a specific number of n , a sequence is obtained by repeatedly using the substitution rules. If we set $n = 1$, the substitution rules turn back to the Fibonacci case $B \rightarrow A$, $A \rightarrow AB$, and if the $n = 2$ it is exactly the intergrowth sequence. Because this class of lattices shares many common features with the Fibonacci lattice, which will be discussed below, we suggest calling this class of sequences the Fibonacci-class (FC) sequences, and an individual member with certain n is denoted as $FC(n)$. Let S_l denote the l th finite chain beginning with $S_1 = B$, $S_2 = B^{n-1}A$, then we have the following recursion relations for the $FC(n)$ sequence:

$$S_l = S_{l-1}^n S_{l-2} \quad (l \geq 3), \quad (6)$$

and F_l , the number of elements contained in the l th sequence, satisfy the corresponding relations

$$F_1 = 1, \quad F_2 = n, \quad F_l = n F_{l-1} + F_{l-2} \quad (l \geq 3). \quad (7)$$

There exists an irrational limitation on F_{l-1}/F_l ,

$$\sigma_n = \lim_{l \rightarrow \infty} \frac{F_{l-1}}{F_l} = \frac{1}{2} (\sqrt{n^2 + 4} - n). \quad (8)$$

The associated substitution matrix of Eq. (5) is

$$M_n = \begin{pmatrix} 1 & 1 \\ n & n-1 \end{pmatrix}. \quad (9)$$

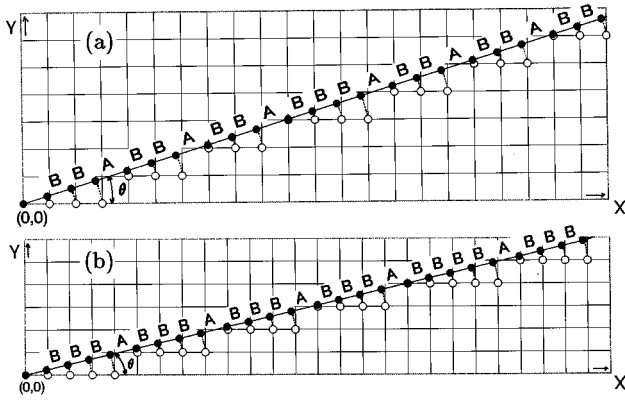


FIG. 1. Illustration for obtaining the FC(n) sequences with the projection method. (a) FC(3) sequence with $\tan\theta=(\sqrt{13}-3)/2$. (b) FC(4) sequence with $\tan\theta=\sqrt{5}-2$.

Its characteristic equation $x^2+nx-1=0$ has two real roots, one greater than 1 in absolute value and another less than 1, and it is obvious that $\det M_n = -1$. Therefore, both the Pisot condition and the unit determinant requirement are satisfied; thus the sequence is quasiperiodic.^{18,19} The positive eigenvalue of M_n is exactly

$$\sigma_n = \frac{1}{2} (\sqrt{n^2+4} - n), \tag{10}$$

which is an irrational quadratic number between (0,1), and can also be expressed in the form of continued fraction

$$\sigma_n = \frac{1}{n + \frac{1}{n + \frac{1}{n + \frac{1}{n + \dots}}}} \tag{11}$$

This means the FC sequences can be obtained with the projection method.^{24,25}

To obtain a FC(n) sequence by the projection method, we consider a two-dimensional periodic lattice with square unit cells of dimension 1×1 whose edges are aligned with the X and Y axes, respectively. Then, construct a projection line oriented at angle θ with respect to the X axis and let $\tan\theta = \sigma_n$. For only a small subset of unit cells does the projection line pass through the right-hand vertical edge of the unit. In Fig. 1 the projection method to obtain the FC(3) and FC(4) sequences is shown. The hollow circles are the set of points corresponding to the lower right-hand corner of each unit cell; their coordinates are $(N, \lfloor N \tan\theta \rfloor)$, where $\tan\theta = (\sqrt{13}-3)/2$ for FC(3), $\tan\theta = (\sqrt{5}-2)$ for FC(4), and $\lfloor \cdot \rfloor$ denotes the greatest integer function. The projection of these points onto the projection line are indicated by the solid circles, their coordinates along the projection line are

$$L_N = N \cos\theta + \sin\theta \lfloor N \tan\theta \rfloor. \tag{12}$$

The distances between two neighboring sites on the projection line take two values $l_A = (\cos\theta + \sin\theta)$ and $l_B = \cos\theta$ which are denoted respectively by A and B in Fig. 1. If we replace l_A and l_B with 1 and 0, the expression form (4) is available here with $\alpha = \sigma_n$.

From their algebraic and geometric features stated above, we know that the FC sequences are both self-similar and quasiperiodic.

Furthermore it is convenient to introduce another class of sequences which will occur in the renormalization-group procedure to analyze the energy spectrum below. Their substitution rules are

$$B \rightarrow B^{n-2}A, \quad A \rightarrow B^{n-2}AB^{n-2}AB. \tag{13}$$

and it is easy to see that for this class of sequences, we have

$$S_1 = B, \quad S_2 = B^{n-2}A, \quad S_l = S_{l-1}^n S_{l-2} \quad (l \geq 3). \tag{14}$$

For the convenience of description, we call these sequences the *relative* sequences of FC(n), and denote them as $R(n)$. We should note that the recursion relations of $R(n)$ are the same as those of FC(n) given in Eq. (2) but with different initial conditions, while the substitution rules of $R(n)$ are different from those of FC(n).

III. SELF-SIMILAR SPECTRAL STRUCTURES

To deal with the electronic properties of a one-dimensional FC(n) quasilattice, we consider the tight-binding Hamiltonian

$$H = \sum_i |i\rangle \varepsilon_i \langle i| + \sum_{i,j} ' |i\rangle t_{ij} \langle j|, \tag{15}$$

where ε_i is the site energy at site i , and t_{ij} is the nearest-neighbor hopping integral. In general, two kinds of models are studied. One is the transfer version, for which ε_i is constant for all i , and t_{ij} take two values t_A and t_B arranged according to the FC(n) sequence. The other is the on-site version, for which t_{ij} is constant while ε_i take two values ε_A and ε_B constructing a FC(n) sequence. In the following, we will concentrate on the transfer version; the on-site version can easily be treated in the same way.⁶ For the transfer version, we choose $\varepsilon_i = 0$ for all i , and the corresponding Schrödinger equation for site i is

$$t_{i-1,i} \psi_{i-1} + t_{i,i+1} \psi_{i+1} = E \psi_i. \tag{16}$$

Before going on, let us recall some results given in the previous literature on the spectral structure of the Fibonacci quasilattice. It is well known that the spectrum of a Fibonacci chain constructs a Cantor set, indicating the spectrum has a hierarchical structure.²⁻⁶ In the first hierarchy, there are three bands, and each band will split into three subbands in the second hierarchy. This splitting pattern holds for any hierarchy; thus it turns out to be a perfect self-similar spectrum. Here, we would like to emphasize again that there is not any kind of generalized Fibonacci lattices which possesses this perfect self-similar spectrum.

Now we turn to analyze the spectral properties of the FC(n) lattices with n greater than 2. For this purpose we can use the decomposition-decimation method,⁷ of which the main idea is the weak-bond approximation and the resonant coupling based on the perturbation theory, that allows us to obtain the splitting rules of the spectrum in an intuitive way.

As the first example we consider the FC(3), i.e., the $n=3$ case. The bond sequence of the FC(3) is as follows:

the Fibonacci lattice every subband of any hierarchy will split into three sub-subbands to form the Cantor spectrum. On the other hand, the intergrowth model studied by Huang, Liu, and Mo is exactly the FC(2) case, its spectral properties coincident with the conclusion stated above.²⁶

IV. GAP-LABELING RULES

It is a well-known fact that the energy spectrum of the Fibonacci lattice exhibits a trifurcating structure with infinite number of gaps.²⁻⁹ Each gap corresponds to a step in the integrated density of states (IDOS) picture defined as $I(E) = \int_{-\infty}^E \rho(E') dE'$ with $\rho(E)$ being the density of states.⁹ The infinite number of steps construct a ‘‘devil’s stair case’’ pattern. The step heights of the IDOS can be labeled by characteristic integers; this fact has been proven by the number theory⁸ and also by the renormalization approach.⁹ In Sec. III, we have shown that the spectra of the FC(n) lattice have self-similar and hierarchical structure. In this section, we will analytically demonstrate that the FC(n) lattices have a universal gap-labeling rule.

To obtain the number of energy levels in every subband, we first notice that the FC(n) and $R(n)$ sequences have the same recursion relations

$$S_l = S_{l-1}^n S_{l-2} \quad (l > 2), \quad (19)$$

where S_l denotes the l th finite sequence with the initial conditions $S_1 = B$, $S_2 = B^{n-1}A$ for FC(n) and $S_1 = B$, $S_2 = B^{n-2}A$ for $R(n)$. If we denote by F_l the number of elements A and B contained in the l th sequence, then we have the corresponding relation

$$F_l = nF_{l-1} + F_{l-2} \quad (l > 2), \quad (20)$$

with the initial conditions $F_1 = 1$, $F_2 = n$ for FC(n) and $F_1 = 1$, $F_2 = n - 1$ for $R(n)$. From Eq. (20) it is easily proven that the ‘‘golden mean’’

$$\sigma_n = \lim_{l \rightarrow \infty} \frac{F_{l-1}}{F_l}. \quad (21)$$

We now calculate the number of energy levels in a subband and its ratio to the total number of levels, which is called the occupation probability (OP).⁹ The global structure of the energy spectrum of a FC(n) quasilattice is of type X . For a FC(n) chain of the l th generation, there are F_l eigenenergies totally. In the first hierarchy of the spectrum, there are $(n+1)$ X bands and n Y bands; the number of levels in each X and Y bands are, respectively,

$$N_X = F_{l-2}, \quad (22)$$

$$N_Y = F_{l-1} - F_{l-2},$$

which can be proved by the equality $(n+1)N_X + nN_Y = F_l$. So the OP of the X and Y bands in the whole spectrum are, respectively,

$$\rho_X = \lim_{l \rightarrow \infty} \frac{F_{l-2}}{F_l} = \sigma^2, \quad (23)$$

$$\rho_Y = \lim_{l \rightarrow \infty} \frac{F_{l-1} - F_{l-2}}{F_l} = \sigma - \sigma^2.$$

In Eq. (23) and hereafter, σ_n is written as σ for the sake of simplicity.

In the second hierarchy of the spectrum, an X band splits into $(n+1)$ X subbands and n Y subbands; their number of levels and OP are

$$N_{XX} = F_{l-4},$$

$$N_{XY} = F_{l-3} - F_{l-4}, \quad (24)$$

$$\rho_{XX} = \lim_{l \rightarrow \infty} \frac{F_{l-4}}{F_l} = \sigma^4,$$

$$\rho_{XY} = \lim_{l \rightarrow \infty} \frac{F_{l-3} - F_{l-4}}{F_l} = \sigma^3 - \sigma^4.$$

A Y band splits into n X subbands and $(n-1)$ Y subbands; their number and OP are

$$N_{YX} = F_{l-3},$$

$$N_{YY} = F_{l-2} - F_{l-3}, \quad (25)$$

$$\rho_{YX} = \lim_{l \rightarrow \infty} \frac{F_{l-3}}{F_l} = \sigma^3,$$

$$\rho_{YY} = \lim_{l \rightarrow \infty} \frac{F_{l-2} - F_{l-3}}{F_l} = \sigma^2 - \sigma^3.$$

Equations (22)–(25) give an approach to calculate the OP of any hierarchy of the spectrum. Consequently, we can see that the OP for a type X subband in any hierarchy preserves the form of σ^i , and the OP for a type Y subband in any hierarchy always has the form of $\sigma^i - \sigma^{i+1}$, where i is a positive integer.

In addition, we have

$$\sigma^2 = 1 - n\sigma. \quad (26)$$

From this equation together with the recursion relation (20), using the deductive method, we obtain the following important expression:

$$\sigma^i = (-1)^i (F_{i-1} - F_i \sigma) \quad (i > 1). \quad (27)$$

It is easy to prove that the step heights of IDOS can be written as⁹

$$I(E_n) = \sum_{i=1}^n \rho(i), \quad (28)$$

where $\rho(i)$ is the occupation probability of the i th subband in the studied hierarchy, and E_n is the highest energy of the n th sub-subband. $I(E_n)$ is therefore the IDOS up to the energy E_n , and corresponds to a step of the IDOS ‘‘stair.’’

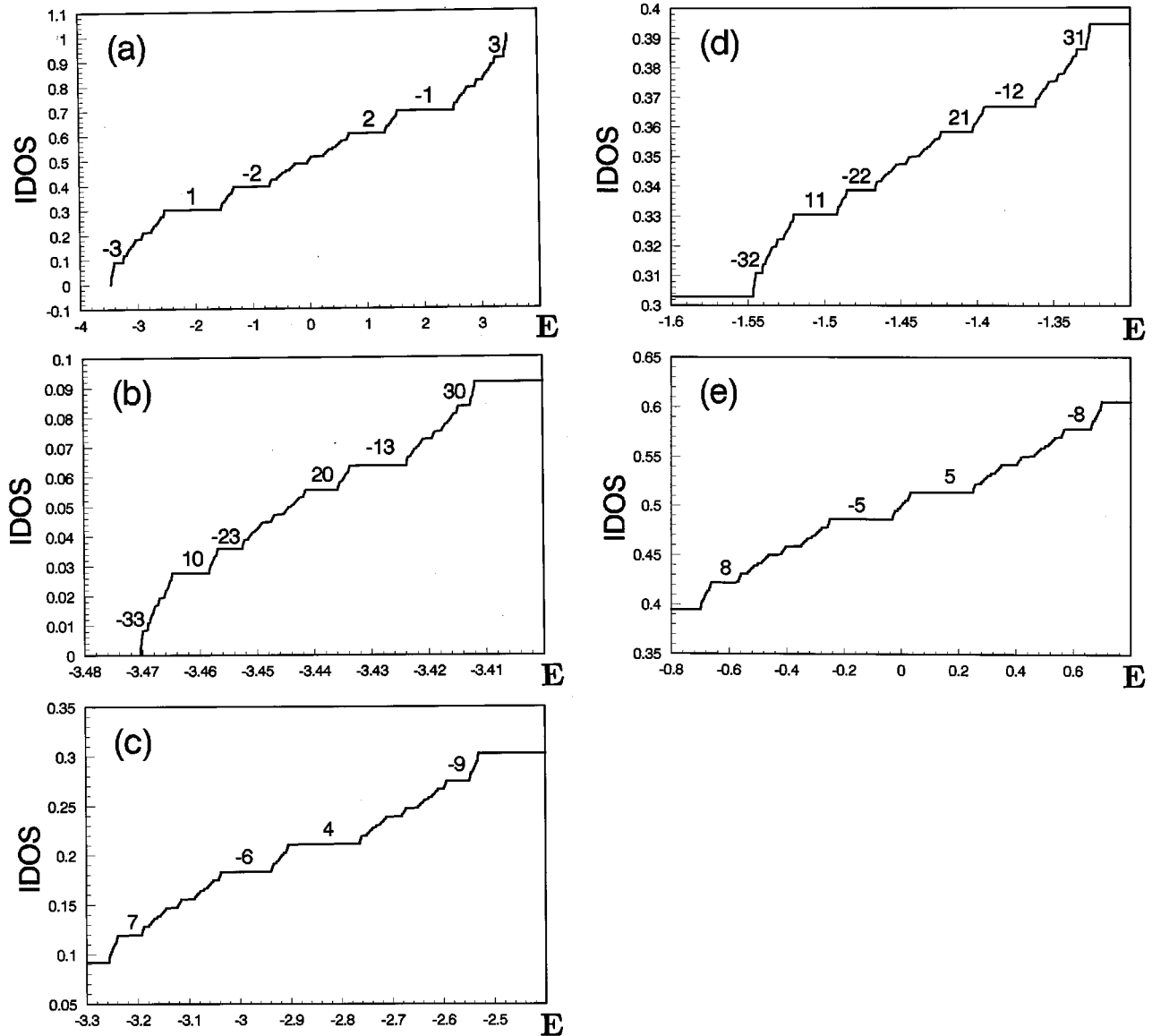


FIG. 3. Numerical calculations for the integrated density of states of the FC(3) sequence with $\varepsilon_i=0$, $t_A=1$, and $t_B=2$. The splitting pattern shown in Fig. 2(a) is confirmed. The gap-labeling number m 's corresponding to the main gaps in the first and second hierarchies are presented. (a) is the whole spectrum and (b)–(e) are the enlarged plots of the four main bands.

From the above equations (22)–(28), we can see that the step height of IDOS can be expressed as

$$I = \sum_i K_i \sigma^i = m' + m\sigma, \quad (29)$$

where K_i , m' , and m are integers.⁹ Because of the irrationality of σ_n (here the subscript n is restored) and $I < 1$, Eq. (31) can be finally expressed as

$$I = \{m\sigma_n\}, \quad (30)$$

where $\{x\}$ represents the fractional part of x , and σ_n is the “Golden mean” for the FC(n) lattice. This is a universal gap-labeling theorem for FC lattices. Because σ_n is an irrational number, we can see that the $\{m\sigma_n\}$ for different gaps

are absolutely different. Consequently, every gap of any hierarchy of the spectrum, which corresponds to a step of IDOS, is uniquely characterized by a definite integer m . It means that m is the characteristic number of a gap, so we can use m to label the gaps. The gap-labeling index m can be easily calculated from the formulas (24)–(30).

Figures 3 and 4 are the numerical results of the IDOS for the FC(3) and FC(4) quasilattices, by which the branching rules analytically obtained in Sec. III and schematically shown in Fig. 2 are very well confirmed. In the figures the characteristic number m 's are presented for the first and second hierarchies of the spectrum, which are in very good agreement with the above analysis. Because the spectrum is symmetric about $E=0$, the characteristic numbers are anti-symmetric, so it is proper to show only a half of the second hierarchy of the spectrum in the figures.

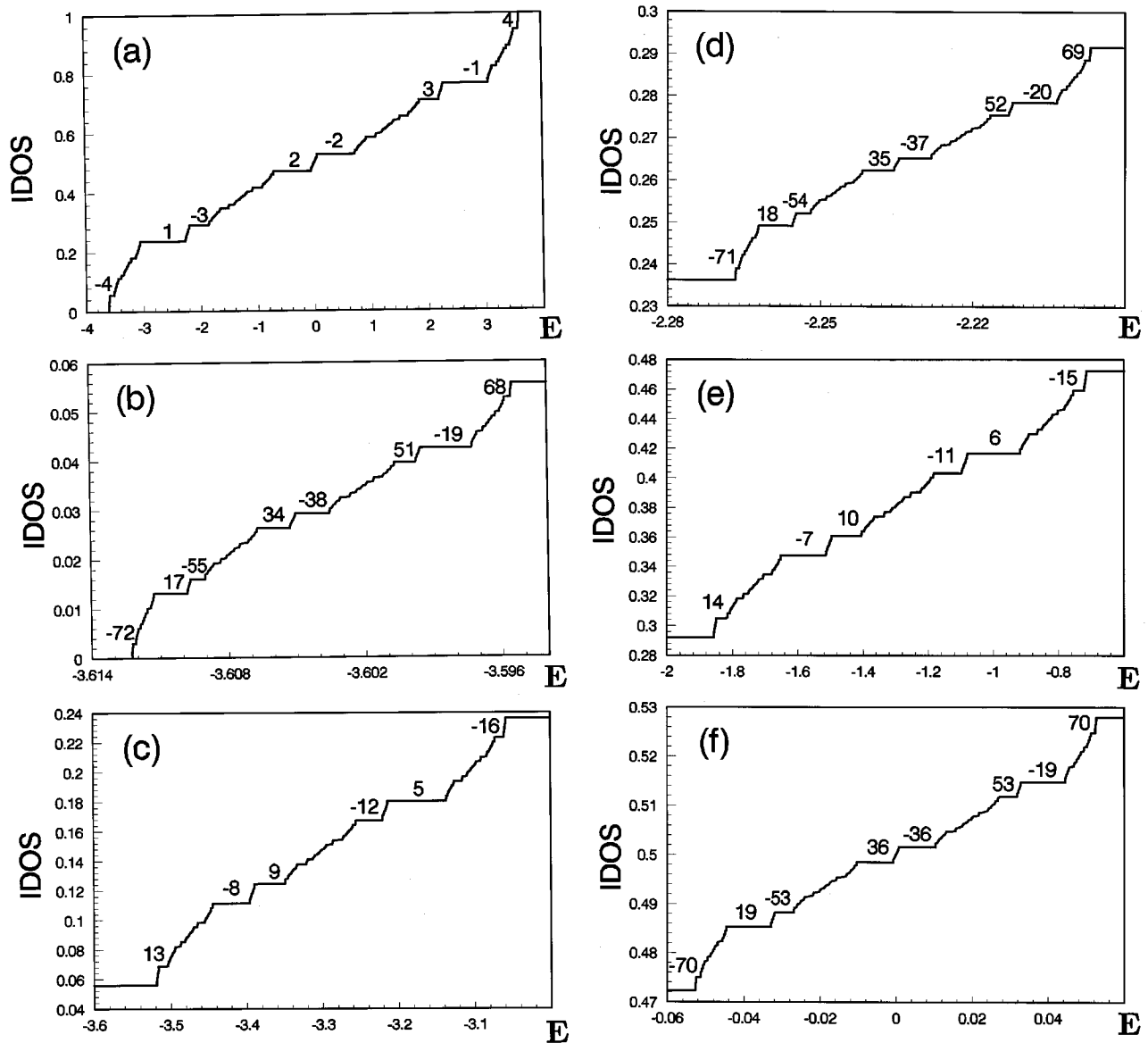


FIG. 4. Numerical calculations for the FC(4) quasilattice with the same parameters as in Fig. 3. The splitting pattern shown in Fig. 2(b) is confirmed and the main gap-labeling numbers are given. (a) is the whole spectrum and (b)–(f) are the enlarged plots of the five main bands.

V. BRIEF SUMMARY

A quasiperiodic lattice always has a singular continuous spectrum, but the perfect self-similarity of the sequence is not definitely reflected in the energy spectrum because in the framework of a tight-binding model the spectral properties are determined by the detailed structure of the quasilattice, not only by the quasiperiodicity. In this article we have proposed a Fibonacci class of one-dimensional structures and studied their spectral properties. First we proved that the FC sequences are both self-similar and quasiperiodic. By the use of the real-space renormalization-group technique, we analytically show that the energy spectrum of a FC(n) lattice is perfectly self-similar and obtain its branching rules for all the hierarchies. This distinguished feature allows us to label the energy gaps in a uniform way and an universal gap-labeling

rule is established. The analytical results are very well confirmed by the numerical calculations. The spectral properties commonly possessed by the present FC(n) models are typical in the well studied Fibonacci lattice. We can thus conclude that the FC lattices are the most intrinsic generalization of the original Fibonacci lattice. Other electronic features discovered in the Fibonacci lattice, such as the self-similar critical wave functions and their multifractal spectra, are also expected to universally exist in the FC quasilattices. This work is undertaken.

The perfect self-similarity of electronic properties presented in this article, in principle, only exists in the self-similar quasiperiodic chains, since in the framework of a tight-binding model there is a corresponding relationship between the constructions of quasiperiodic chains and their

electronic properties. Therefore, the non-self-similar quasi-periodic chains would not possess a same kind of perfect similarity of electronic properties. But to what degree their electronic properties would show self-similarity is an interesting problem. It seems to us there are very few papers devoted to this topic yet.

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