Splitting rules for the electronic spectra of two-dimensional Fibonacci-class quasicrystals with one kind of atom and two bond lengths

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On the basis of the substitution rules for a one-dimensional Fibonacci-class chain, we construct twodimensional Fibonacci-class quasicrystals with one kind of atom and two bond lengths. In the framework of the single-electron tight-binding nearest-interaction transfer model, we study the splitting rules of the electronic energy spectra for two-dimensional Fibonacci-class quasicrystals by means of a decomposition-decimation method based on a renormalization-group technique, and we also calculate the electronic energy spectra numerically. It is found that there exist only three kinds of clusters— $n \times n$, $n \times (n+1)$, and $(n+1) \times (n$ +1)—for all classes of two-dimensional quasilattices, and that the electronic energy bands split as Y_{m-n-l} . The general formula of the number for energy levels is obtained. We discover that there is a kind of so-called Fibonacci-class-number set for the parameters used to describe the energy-level number, and we obtain the set formulas. The experienced formula are sought out. The analytical results are confirmed by numerical simulations.

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I. INTRODUCTION

There has been a large number of studies on the properties of quasicrystals and quasiperiodic systems since the experimental discovery of fivefold symmetry in the diffraction pattern of metallic alloys, found by Shechtman *et al.*¹ in 1984. In general, to study an aperiodic system one will face two problems: self-similarity and quasiperiodicity.² A self-similar structure is produced by the substitution rule, and a quasiperiodic lattice is constructed by the projection method.³ The former reflects the inflation symmetry, while the latter characterizes that its Fourier spectrum consists of Bragg peaks. Several groups studied the relationship between these two sides.⁴⁻¹⁰ Before 1992, the one-dimensional (1D) quasiperiodic Fibonacci chain [FC(1)] was a unique perfect quasiperiodic model with the above two properties. Since then, 1D FC(1) quasilattices, or the superlatice systems constructed following the FC(1) sequence, attracted much attention from both physicists and mathematicians for many years,¹¹⁻²⁴ because its structure is not only relatively very simple but also possesses the main characteristics of quasicrystals. In 1985, Merlin et al.²⁰ reported a realization of a quasiperiodic superlattice grown by molecular-beam epitaxy, and presented the x-ray and Raman-scattering measurements of the sample, consisting of alternating layers of GaAs and AlAs, to form a FC(1) sequence in which the ratio of incommensurate periods is equal to the golden mean τ . To exhibit the localization of classical waves, the authors of Ref. 18 suggested an ideal experiment. They studied the transmission of light through dielectric multilayers consisting of two kinds of layers, which are arranged following a 1D FC(1) sequence; their theoretical results were confirmed by a dielectric multilayer experiment.²¹ Afterwards, Tamura and Wolfe²² studied acoustic-phonon transmission through a realistic FC(1) supperlattice theoretically, and obtained some results for the transmission spectra. Zhu and Ming²³ analyzed a FC(1) optical superlattice made from a single crystal with quasiperiodic laminar ferroelectric domain structures, and studied the second-harmonic-generation (SHG) light in this system. Zhu *et al.*²⁴ fabricated a nonlinear optical superlattice of LiTaO₃ in which two building blocks *A* and *B* were arranged as a FC(1) sequence, and measured the quasi-phase-matched SHG spectrum of it.

Trying to find a consummate quasiperiodic superlattices like FC(1), Huang and co-workers^{25–30} proposed a so-called intergrowth quasiperiodic model [FC(2)] in 1992, and investigated the main characteristics of it in detail. Based on researches concerning FC(1) and FC(2), Fu et al.² designed a class of flawless quasiperiodic models which contain FC(1)and FC(2) in 1997, and called them "Fibonacci-class quasilattices" [FC(n)]. They studied the energy spectra splitting rules and gap-labeling properties of a 1D FC(n). Recently we³¹⁻³³ obtained results for the transmission properties of light through multilayers constructed following a 1D FC(n)sequence, and found the laws for the output power of SHG light derived from ferroelectric multidomains arranged by 1D FC(n) orders. Being the theoretical basis for researches into the optical properties of materials, naturally it is a very interesting problem to investigate the splitting rules for electronic energy spectra of the two-dimensional FC(n) quasicrystals, which comprise a general quasilattice model.

During the past 17 years, much attention has been paid to studies of the electronic properties of quasilattices, especially the energy spectrum structure, which is an important aspect in the physical properties of quasicrystals. It is generally known that for the 1D FC(1) quasicrystals, the band structure, which is a Cantor-like set, shows a peculiar self-similarity because of its hierarchical geometric structure. But for 2D Penrose lattices, its topological structure is much more complicated than its 1D counterparts; there was no unusual self-similarity to be found for its energy spectra.^{34–36} As for a 2D FC(1) quasicrystal with one kind of atoms and two bond lengths, this is quite different from the case of 2D Penrose tiling. The energy spectrum of this was



FIG. 1. The 2D FC(2) with one kind of atom and two kinds of bond lengths.

researched,^{37–40} and Fu *et al.*⁴⁰ found that its spectrum has a variety of multifurcating structures. By means of the decomposition-decimation (DD) method, based on the renormalization-group technique, we⁴¹ studied the rules of energy spectra splitting for 2D FC(1) quasilattices with three kinds of atoms and one kind of bond lengths. There also exists a perfect self-similarity for this spectra. The electronic properties of 1D quasiperiodic materials constructed following another general model were studied by Iguchi.^{42,43}

The DD method was created by Liu and Sritrakool¹⁵ on the basis of the result obtained in Ref. 12, and it allows one only to calculate the influence between resonant couplings of the same kind of atoms in the same state in each hierarchy. Thus it is possible to compute very large clusters to obtain the electronic energy spectra structure of higher hierarchies without the difficulty that plagues high-order perturbation calculations. In this paper, using this method, we mainly study the splitting rules for a 2D FC(*n*) with one kind of atoms and two bond lengths, and obtain interesting so-called *Fibonacci-class-number sets*. In Sec. II, the construction of this class of 2D quasicrystals is introduced. By means of the DD method, the splitting rules for spectra of 2D FC(*n*) are studied in Sec. III, and Sec. IV is a brief summary.

II. 2D FC(n) WITH ONE KIND OF ATOM AND TWO BOND LENGTHS

A 2D FC(n) with one kind of atoms and two bond lengths under study has network forms constructed by a corresponding 1D FC(n) chain in two directions, and can be composed in the following way.

(i) Create one FC(n) chain in a horizontal direction by the substitution rules

$$S_0 = B,$$

$$B \to B^{n-1}A,$$
(1)

$$A \to B^{n-1}AB$$

which shows the following sequence:

$$\underbrace{B.\dots.B}_{n-1}A.\dots,\underbrace{B.\dots.B}_{n-1}AB\dots,\underbrace{B.\dots.B}_{n-1}AA\dots$$
(2)



FIG. 2. The 2D FC(3) with one kind of atom and two kinds of bond lengths.

(ii) Make "*B*" units in Eq. (2) decide "short" bond lengths between atoms for the horizontal lattices, and order "*A*" unite to define "long" bond lengths, respectively.

(iii) By the same step as that for horizontal chains, we can obtain a vertical sequence with the same order of bond lengths; then the 2D FC(n) can be obtained. Figures 1 and 2 show a 2D FC(2) with one kind of atoms and two bond lengths, and a 2D FC(3), respectively.

III. SPLITTING RULES FOR SPECTRA OF 2D FC(n)

A. Numerical simulations of spectra

In the framework of the single-particle tight-binding transfer model, atomic orbitals are all located at the center of the cell, and the single-site energy ϵ_i is a constant for all of the atoms; then the Hamiltonian can be simply written as

$$H = \sum_{i} |i\rangle \epsilon_{i} \langle i| + \sum_{i,j} ' |i\rangle t_{ij} \langle j|, \qquad (3)$$

where $|i\rangle$ is the *i*th Wannier state, $\Sigma'_{i,j}$ is the sum over the nearest-neighbor atoms, and t_{ij} is the transfer-matrix element



FIG. 3. The electronic energy spectra of the 2D FC(2) vs atom numbers with 10 000 atoms, where the single-site energy $\epsilon_i = 0.0$, and the transfer-matrix elements contain two kinds of values $t_s = -1.0$ (strong) and $t_w = -0.1$ (weak), corresponding to short and long bonds, respectively.



FIG. 4. The electronic energy spectra of the 2D FC(3) vs atom numbers with 10 000 atoms, where the single-site energy $\epsilon_i = 0.0$, and the transfer-matrix elements contain two kinds of values t_s = -1.0 (strong) and $t_w = -0.1$ (weak), corresponding to short and long bonds, respectively.

which contains two kinds of elements t_s (strong) and t_w (weak) corresponding to short and long bonds. In order to solve the problem simply, we assume $t_s = -1.0$, $t_w = -0.1$, and $\epsilon_i = 0.0$ for all *i*. Figures 3 and 4 show the numerical results of electronic spectra of a 2D FC(2) and 2D FC(3), respectively. From Fig. 3 one can see that the spectra of a 2D FC(2) split as 13 subbands, and we denote this kind of structure as type Y_{2-2-1} , where the parameters of the symbol Y_{n-m-1} are defined as follows: *n* is the class number of FC(*n*), *m* denotes the dimension number for the quasicrystal, and *l* indicates the sorting number of the atoms, respectively. Similarly, the spectra for a 2D FC(3) divide into 25 branches. This type was called type Y_{3-2-1} by us.

B. Analysis of the spectra by means of the DD method

(i) Making use of the DD method,¹⁵ one can presume that there exists no interaction among the atoms (i.e., $t_{ij}=0$) in the first approximation; then the 2D FC(*n*)'s are broken into isolated atoms, and there is only one highly degenerate energy 0.0 in the systems.

(ii) In the second approximation only the interactions between the nearest-neighbor atoms are calculated and weak bonds are absent (i.e., $t_{ij}=t_{\text{nearest-neighbor}}=-1.0$ and t_{ij} $=t_{\text{others}}=0.0$); then the 2D FC(*n*) contains only three kinds of isolated clusters: $n \times n$, $n \times (n+1)$, and $(n+1) \times (n+1)$ molecules. At present, for example, there only exist 2×2, 2×3, and 3×3 kinds of clusters in the 2D FC(2), as illustrated in Fig. 1. In this case, the spectra of the $n \times (n+1)$ clusters are nondegenerate, and will split into $n \times (n+1)$ subbands. The spectra for the $n \times n$ and $(n+1) \times (n+1)$ clusters all have degenerate energy levels; the splitting rules for their spectra are very complicated and there exists a kind of interesting phenomenon in these systems called the Fibonacci-class-number set Y_{n-m-1} , which is discussed in detail in the next section.

C. Fibonacci-class-number sets $\{Y_{n-m-l}\}$

In the second approximation the number of total energy levels for the $n \times n$ clusters (including degenerate ones) can be obtained by formulas (4) and (5):

$$N_{n \times n} = n \times n, \tag{4}$$

$$N_{n \times n} = n + 2 \sum_{i=1}^{\lfloor n/2 \rfloor} (1 + 2a_{n \times n,i}).$$
(5)

In Eq. (5) the brackets represent the greatest integer function, the first number *n* at the right side means that the middle electronic energy level with the value of 0.0 is *n* degenerate, the first digit 2 from left to right denotes that the upper and lower levels are *symmetries* and that the point of symmetry is 0.0, the signal 1 after the sum signal Σ means returns to a nondegenerate level, and the parameter 2 of item $a_{n \times n,i}$ shows that there exist $a_{n \times n,i}$ doubly degenerate lines between every nondegenerate one; all of the numbers $a_{n \times n,i}$ tend toward a set of certain values with the cluster number *n*'s increasing, forming the so-called Fibonacci-class number set Y_{n-m-l} , where $a_{n \times n,i}$ can be given as

$$a_{n \times n,0} = 0, \quad a_{n \times n,5i+1} = 8i+1 \quad (i \ge 0),$$

$$a_{n \times n,5i+2} = 8i+3 \quad (i \ge 0),$$

$$a_{n \times n,5i+3} = 8i+4 \quad (i \ge 0), \quad a_{n \times n,5i+4} = 8i+6 \quad (i \ge 0),$$

$$a_{n \times n,5i} = 8i+7 \quad (i \ge 0).$$

The splitting for the $n \times n$ cluster is shown as Fig. 5, where numbers in the parentheses are the degenerate degrees of the energy levels.

On the other hand, we calculate a 2D square cluster with 101 atoms on every side, and obtain the first order splitting

$$10\ 201 = 101 \times 101 = 101 + 2\sum_{i=1}^{50} (1 + 2a_{101 \times 101,i}), \quad (7)$$

where $a_{101\times101,i}$ (*i*=1,...,50) takes the values as 1, 3, 4, 6, 7, 9, 11, 12, 14, 15, 17, 20, 18, 24, 22, 26, 27, 29, 30, 32, 34, 37, 35, 40, 42, 44, 44, 47, 51, 48, 56, 55, 57, 60, 64, 65, 68, 73, 74, 77, 80, 88, 87, 96, 97, 107, 115, 125, 143, and 164, respectively. Figure 6 shows the fitting curve which was designed by the experimental formulas

$$a_{n \times n,i} = c_1 i + c_2 i^{c_3},$$

$$c_1 = 1.686\,93 \pm 0.020\,06,$$

$$c_2 = (3.4566 \times 10^{-16}) \pm (6.6024 \times 10^{-16}),$$

$$c_3 = 10.200\,91 \pm 0.442\,48,$$
(8)

where the points shown by up triangles are those of the realistic 10 201 cluster, and the circle-shaped dots are limit values which are decided by formula (6). It was shown that many of the realistic $a_{101\times101,i}$ spots are coincident with the

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FIG. 5. Electronic energy structure of the electronic spectra for an $n \times n$ cluster.

stable limit specks. The curve constructed by practical points will tend to become the straight line defined by limit dots with increasing n's.

Now, by means of Eq. (5), we obtain formula (9) for the number of lines with different energy values for the first-order splitting spectra of an $n \times n$ cluster:

$$N'_{n \times n} = 1 + 2 \sum_{i=1}^{\lfloor n/2 \rfloor} (1 + a_{n \times n, i}).$$
(9)

Deducting the degenerate energy levels of the $n \times n$ cluster and the $(n+1) \times (n+1)$ molecules from the system, one obtains the general formulas (10) and (11) for numbers of levels with different energies of the first-order splitting spectra of the 2D FC(*n*) (*n*>1), because the splitting rules of the 2D FC(1) was studied in detail by Fu *et al.*²



FIG. 6. The fitting curve figure of Fibonacci-class-number sets for a cluster with $101 \times 101 = 10201$ atoms.

(i) When n=2k+1 ($k \ge 1$), the number of the levels is

$$N'_{FC(2k+1)} = 1 + 2(k+2)(2k+1) + 2a_{(2k+2)\times(2k+2),(k+1)} + 2\sum_{i=1}^{k} [a_{(2k+1)\times(2k+1),i} + a_{(2k+2)\times(2k+2),i}].$$
(10)

(ii) When n=2k ($k \ge 1$), the amount of the lines is

$$N'_{FC(2k)} = 1 + 2k(2k+3) + 2\sum_{i=1}^{k} [a_{2k\times 2k,i} + a_{(2k+1)\times(2k+1),i}].$$
 (11)

D. Comparison with numerical results

In order to compare the analytical results with the numerical calculations shown in Figs. 3 and 4 for the 2D FC(2) and 2D FC(3), we assume that the transfer-matrix element t_{ij} is the same (-1) for all pairs of atoms that are nearest neighbors to each other, and is zero otherwise. Then the Hamiltonians of 2×2, 2×3, and 3×3 clusters exist in the 2D FC(2) can be written as

$$H_{2\times2} = \begin{pmatrix} E & t & t & 0 \\ t & E & 0 & t \\ t & 0 & E & t \\ 0 & t & t & E \end{pmatrix}, \qquad (12)$$
$$H_{2\times3} = \begin{pmatrix} E & t & 0 & t & 0 & 0 \\ t & E & t & 0 & t & 0 \\ 0 & t & E & 0 & 0 & t \\ t & 0 & 0 & E & t & 0 \\ 0 & t & 0 & t & E & t \\ 0 & 0 & t & 0 & t & E \end{pmatrix}, \qquad (13)$$

$$H_{3\times3} = \begin{pmatrix} E & t & 0 & t & 0 & 0 & 0 & 0 & 0 \\ t & E & t & 0 & t & 0 & 0 & 0 & 0 \\ 0 & t & E & 0 & 0 & t & 0 & 0 & 0 \\ t & 0 & 0 & E & t & 0 & t & 0 & 0 \\ 0 & t & 0 & t & E & t & 0 & t & 0 \\ 0 & 0 & t & 0 & t & E & 0 & 0 & t \\ 0 & 0 & 0 & t & 0 & 0 & E & t & 0 \\ 0 & 0 & 0 & 0 & t & 0 & t & E & t \\ 0 & 0 & 0 & 0 & 0 & t & 0 & t & E \\ \end{pmatrix} .$$
(14)

Solving the secular equation $\lambda I - H = 0$ for Eqs. (12), (13), and (14), where *I* is a unit matrix, we obtain the following eigenvalues of the above three kinds of clusters, respectively:

$$E_4 = 2t$$
, 0 (double degenerate), $-2t$, (15)

$$E_{6} = (\sqrt{2}+1)t, \quad t, \ (\sqrt{2}-1)t, \quad -(\sqrt{2}-1)t,$$

$$-t, \ -(\sqrt{2}+1)t, \qquad (16)$$

 $E_9 = 2\sqrt{2}t$, $\sqrt{2}t$ (double degenerate),

0 (three degenerate),

$$-\sqrt{2}t$$
 (double degenerate), $-2\sqrt{2}t$. (17)

Then 13 levels with different energies for the 2D FC(2) are obtained as follows, where only was the nearest interaction calculated:

FC(2):
$$e_1 = 2\sqrt{2}t$$
, $e_2 = (\sqrt{2} + 1)t$, $e_3 = 2t$,
 $e_4 = \sqrt{2}t$ (double degenerate),
 $e_5 = t$, $e_6 = (\sqrt{2} - 1)t$,
 $e_7 = 0$ (five degenerate), $e_8 = -e_6$, (18)

 $e_9 = -e_5$, $e_{10} = -e_4$ (double degenerate),

$$e_{11} = -e_3, \quad e_{12} = -e_2, \quad e_{13} = -e_1.$$

We denote this kind of structure as type Y_{2-2-1} . Although the realistic fine spectra is much more complicated than that of the calculations, the values of all of the centers for the 13 main subbands nearly fit the above computing results. That is to say, the analytical results are confirmed by numerical simulations.

Similarly, making use of the above method, one can obtain a conclusion for the 2D FC(3), and the data for the splitting type Y_{3-2-1} are

FC(3):
$$e_1 = 2ut$$
, $e_2 = (u + \sqrt{2})t$, $e_3 = 2\sqrt{2}t$,
 $e_4 = \sqrt{5}t$ (double degenerate),
 $e_5 = (v + \sqrt{2})t$, $e_6 = ut$,

$$e_9 = t$$
 (double degenerate), $e_{10} = (\sqrt{2} - v)t$,

$$e_{11} = vt, \quad e_{12} = (u - \sqrt{2})t,$$

 $e_{13} = 0$ (seven degenerate), $e_{14} = -e_{12};$
 $e_{15} = -e_{11}, \quad e_{16} = -e_{10},$
(19)

$$e_{17} = -e_9$$
 (double degenerate), $e_{18} = -e_8$,
 $e_{19} = -e_7$ (double degenerate), $e_{20} = -e_6$,
 $e_{21} = -e_5$, $e_{22} = -e_4$ (double degenerate),
 $e_{23} = -e_3$, $e_{24} = -e_2$, $e_{25} = -e_1$,

where

$$u = \frac{\sqrt{5}+1}{2}, \quad v = \frac{\sqrt{5}-1}{2}.$$
 (20)

In fact, the practical spectra structures are influenced by the quantity of the clusters and the percentage of the molecules. For the 2D FC(3), as an example, the center of the subband with the largest energy values for 16 atom clusters is located at $E_{4\times4,1} = -(\sqrt{5}+1)t\approx 3.236$, but the realistic range for $E_{4\times4,1}$ values is from 3.245 57 to 3.242 09. The shift comes from the repelling actions given by a large number of polar 3×4 clusters and nonpolar 3×3 clusters. For the same reason, the shape of the spectra will also be changed by the interaction. The widths of the three subbands for a 16-atom cluster over the symmetry point E=0.0 are all less than 0.01, but the ones for 12-atoms molecules are all larger than 0.07. The latter is usually nine times larger than the former.

IV. SUMMARY

On the basis of the substitution rules for the 1D FC(n), we constructed a 2D FC(n) with one kind of atoms and two bond lengths. In the framework of the single-particle tightbinding nearest interaction transfer model, we have studied the splitting rules of electronic energy spectra for the 2D FC(n) analytically by means of the DD method, based on the renormalization-group technique, and we also calculated the electronic energy spectra for the 2D FC(2) and 2D FC(3)numerically. It was found that there only exist three kinds of clusters— $n \times n$, $n \times (n+1)$, and $(n+1) \times (n+1)$ —for the entire class of 2D quasilattices, and that the electronic energy bands split as Y_{m-n-1} . The general formula for the number of energy levels was obtained. We discovered that there is a kind of so-called Fibonacci-class number set for the parameters used to describe the energy level number; we also obtain the set's formula. The formula was explored. The analytical results were compared with numerical calculations by taking the influences between clusters with different quantities and different polarities into account. The former was confirmed by the latter.

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