

# Splitting rules for spectra of two-dimensional Fibonacci quasilattices

Xiangbo Yang

*Physics Group, Department of Mathematics and Physics, Guangdong University of Technology, Guangzhou 510 090, China*

Youyan Liu

*CCAST (World Laboratory), P.O. Box 8730, Beijing 100 080, China  
and Department of Physics, South China University of Technology, Guangzhou 510 641, China*

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In the framework of the single-electron tight-binding on-site model, after establishing the method of constructing a class of two-dimensional Fibonacci quasilattices, we have studied the rules of energy spectra splitting for these quasilattices by means of a decomposition-decimation method based on the renormalization-group technique. Under the first approximation, the analytic results show that there exist only six kinds of clusters and the electronic energy bands split as type *Y* and consist of nine subbands. Instead of the on-site model, the transfer model should be used for the higher hierarchy of the spectra, the electronic energy spectra split as type *F*. The analytic results are confirmed by numerical simulations. [S0163-1829(97)07934-4]

## I. INTRODUCTION

In recent years, much attention has been paid to the investigation 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 one-dimensional (1D) Fibonacci quasicrystals, the band structure, which is a Cantor-like set, shows a peculiar self-similarity.<sup>1-5</sup> For 2D Penrose lattices the electronic energy spectra are much more complicated than the 1D one, even though there is also a geometric hierarchical structure.<sup>6</sup> Choy<sup>7</sup> computed the density of states for a tight-binding model numerically by the continued-fraction recursion method. Odagaki and Nguyen<sup>8</sup> studied numerically the electronic structure for three patterns of Penrose tiling with up to 426 vertices. Odagaki<sup>9</sup> gave numerical evidence that indicates the existence of a central peak with side gaps in the tight-binding electronic spectra with one type of interaction. For the 2D Fibonacci quasilattices with one kind of atom and two kinds of bond lengths, Ueda and Tsunetsugu<sup>10</sup> investigated the energy spectrum and conductance numerically. Ashraff, Luck, and Stinchcombe<sup>11</sup> studied the energy spectrum, density of states, and dynamical response function analytically and their results have been confirmed by numerical simulations. As for the decimation technique, Odagaki<sup>12</sup> applied it to 1D quasicrystals to obtain the energy bands, density, and integrated density of states. By means of a decomposition-decimation (DD) method, Fu and Lin<sup>13</sup> investigated the rules of electronic energy spectra splitting. However, the studies of the properties of electronic energy spectra of 2D Fibonacci quasilattices with three kinds of atoms and one kind of bond length, as far as we know, have not been reported yet.

For 1D Fibonacci quasilattices, by using the weak-bond approximation, Niu and Nori<sup>14</sup> applied the renormalization-group technique to investigate the electronic energy spectra, on the basis of which Liu and Sritrakool<sup>15</sup> developed a DD method to study the branching rules of energy spectra for the Fibonacci chain, which gives a clear and simple physical

picture of the electronic energy spectra. The advantage of the DD method is that it allows one to carry the calculation up to a very big cluster to obtain the spectra structure of higher hierarchies without the difficulty that usually plagues high-order perturbation calculation. By means of this method, in this paper we mainly study the law of electronic energy spectra splitting for the 2D Fibonacci quasilattices with three kinds of atoms and one kind of bond length. In Sec. II, we introduce the construction method of the quasilattices under study. In Sec. III, by means of the DD method, the electronic energy spectra structure is studied. We find that it splits into nine subbands, each of which can be studied by the transfer model. In Sec. IV, we study the influence of different atoms on the electronic energy spectra analytically. Section V is a brief summary.

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CBCBCCBCCBCCBCCBCCBCCBCC
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FIG. 1. 2D Fibonacci quasilattices with three kinds of atoms and one kind of bond length.

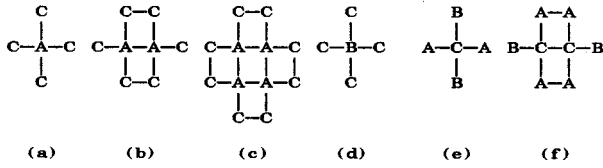


FIG. 2. Six kinds of clusters in the first renormalization procedure: (a) isolated A atom, (b) diatomic A molecules, (c) four-atom A molecules, (d) isolated B atom, (e) isolated C atom, and (f) diatomic C molecules.

## II. CONSTRUCTION OF THE SPECIAL 2D FIBONACCI QUASIPERIODIC SYSTEM

The normal 2D Fibonacci quasiperiodic system has a network form constructed by 1D Fibonacci chains in vertical and horizontal directions. The special 2D Fibonacci quasilattices under study are different from the normal one. They are not formed by one kind of atom and two kinds of bond lengths, but three kinds of atoms and one kind of bond length, for which every chain is still constructed by two kinds of atoms and forms a 1D Fibonacci chain. This kind of 2D Fibonacci quasilattice can be constructed in the following way. (i) Create two Fibonacci chains in the same way along the X and Y axes, respectively. (ii) By means of general multiplication, we obtain the following: (long) $\times$ (long)=A atoms, (short) $\times$ (short)=B atoms, and (long) $\times$ (short)=(short) $\times$ (long)=C atoms. So we can get the quasilattices

with three kinds of atoms, as shown in Fig. 1. In order to simplify the problem and enlarge the computed system, we choose the quasilattices with fourfold central rotational and mirror symmetry, by which the Fibonacci chains along the X and Y axes have the same order.<sup>13</sup>

## III. SPLITTING RULE OF SPECTRA

### A. Numerical simulations of spectra

In the framework of the single-particle tight-binding model, atomic orbitals are located at the center of the cell. The Hamiltonian reads simply

$$H = \sum_i |i\rangle E_i \langle i| + \sum'_{i,j} |i\rangle t_{ij} \langle j|, \quad (1)$$

where  $|i\rangle$  is the  $i$ th Wannier state.  $\sum'_{i,j}$  is the sum over the nearest-neighbor atoms, and  $t$  is the transfer-matrix element. In the first approximation, we assume that the transfer-matrix element  $t_{ij}$  is the same ( $-1$ ) for all pairs of atoms that are nearest neighbor with each other and zero otherwise.  $E_i$  is the site energy, which can be different for different kinds of atoms. Here we assume  $E_A = -5.0$  for A atoms,  $E_B = 5.0$  for B atoms, and  $E_C = 3.0$  for C atoms, respectively. Figure 2 shows the numerical results of electronic energy spectra.

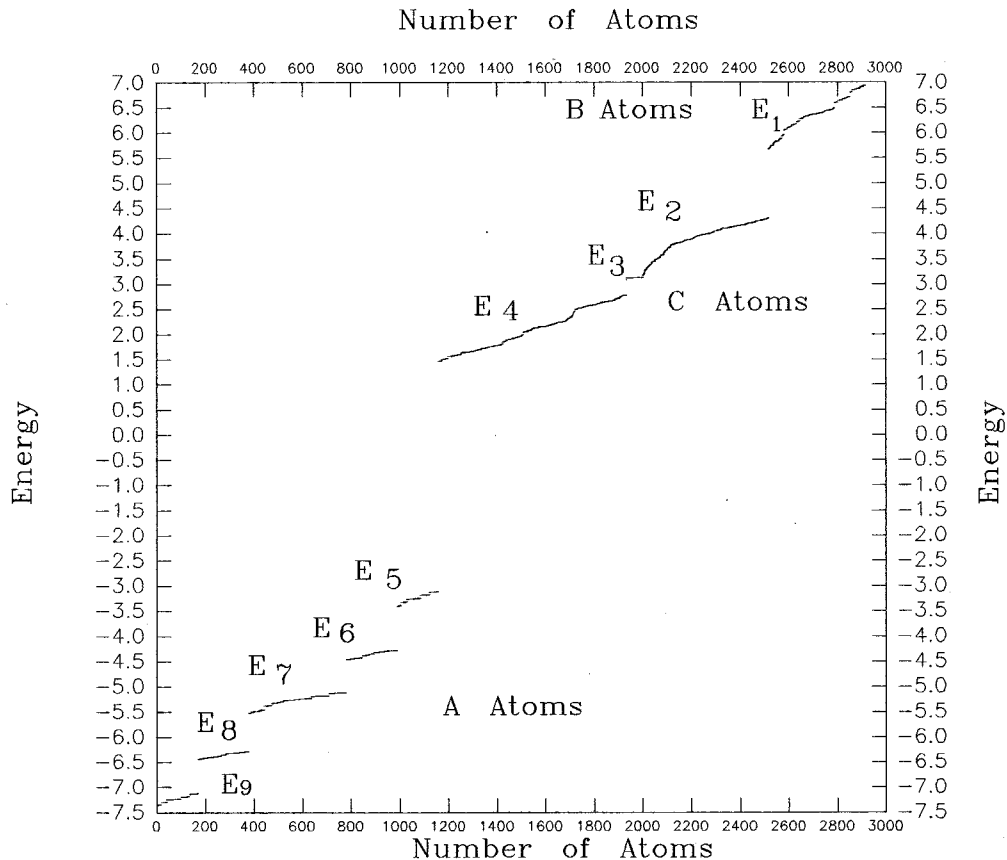


FIG. 3. Electronic energy spectra of the 2D Fibonacci quasilattices vs atom number with 2916 atoms.  $E_A = -5.0$ ,  $E_B = 5.0$ ,  $E_C = 3.0$ , and  $t = -1.0$ . There are nine subbands in the system.

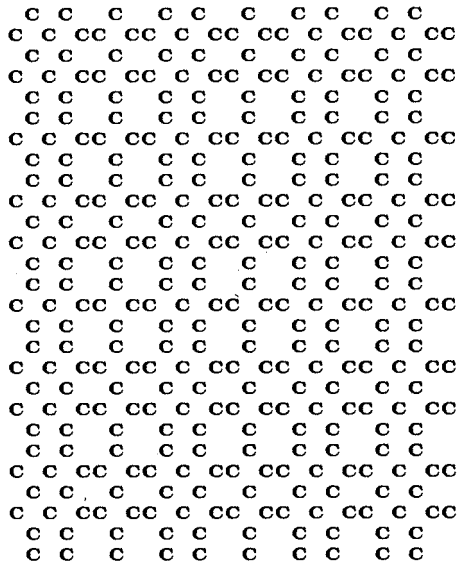


FIG. 4. 2D subquasilattice of C atoms.

### B. Analytic results of spectra

If we assume first that there is no interaction among the atoms (i.e.,  $t_{ij}=0$ ), then there are three kinds of isolated atoms in the system and three highly degenerate energies  $E_B$ ,  $E_C$ , and  $E_A$  exist. If we assume that there is an interaction only between the nearest-neighbor atoms, then the 2D Fibonacci quasilattice should contain only six kinds of isolated clusters, i.e., the isolated A atoms, diatomic A molecules, four-atom A molecules, isolated B atoms, isolated C atoms, and diatomic C molecules (see Fig. 2). Among the factors that influence the spectra splitting, the most significant effect is the resonant coupling of the same kind of atoms. For different kinds of atoms the interaction is so weak that it can be regarded as a perturbation. In this case, there are nine energy levels in the first-order approximation:  $E_1 = E_B$  for the isolated B atoms;  $E_2 = E_C - t$  and  $E_4 = E_C + t$  for the diatomic C molecules;  $E_3 = E_C$  for the isolated C atoms;  $E_5 = E_A - 2t$ ,  $E_9 = E_A + 2t$ , and the double degenerate energy level  $E_7 = E_A$  for the four-atom A molecules;  $E_6 = E_A - t$  and  $E_8 = E_A + t$  for the diatomic A molecules; and  $E_7 = E_A$  for the isolated A atoms. We denote this kind of structure as type Y. The result of numerical simulation, which confirms the above analysis, is shown in Fig. 3.

The next step is to consider the further branching of the main subbands. By the DD method, we regard an eigenstate and its corresponding ‘‘molecule’’ as a ‘‘superatom’’ with a definite energy, i.e., now there are six kinds of these superatoms, each of which forms a new 2D subquasilattice. This idea will be applied repeatedly in studying the branching rules of spectrum. Applying this idea to the present case, we could decompose the original 2D Fibonacci lattice into six Fibonacci sublattices with associated renormalized ‘‘site energy’’ and ‘‘transfer-matrix elements.’’

In fact, because of the symmetry of the energy spectrum, the second and fourth subbands, the fifth and ninth subbands, and the sixth and eighth subbands are identical. Therefore, only six kinds of main subbands exist.

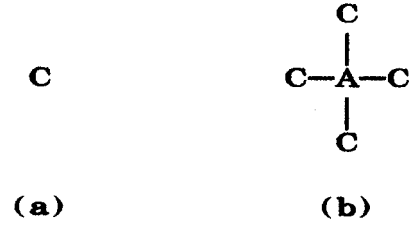


FIG. 5. Coupling interactions between isolated C atoms.

### 1. A atoms' energy spectra (the fifth to ninth subbands: $E_5-E_9$ )

Just like the isolated B atom clusters, the subquasilattices constructed by A atoms are also the normal 2D Fibonacci quasilattices with one kind of atom and two kinds of bond lengths. Therefore, the fifth to ninth subbands will further split as type F, in which the fifth and ninth sub-subbands further split as type F, the sixth and eighth as type  $F_2$ , and the seventh as type  $F_0$ .<sup>13</sup>

### 2. B atoms' energy spectra (the first subband: $E_1$ )

In second-order approximation, the interactions between atoms with the same energy is the dominant factor to affect the spectra splitting of the subband; the interactions between the different kinds of atoms or between atoms with different levels can be regarded as perturbations. The first subband structure is determined by the isolated B atom subquasilattice, which is just the normal 2D Fibonacci quasilattice with one kind of atom and two kinds of bond lengths, the energy spectrum properties of which have been studied by Fu and Liu.<sup>13</sup> It is found that the spectra split into five as type F.

### 3. C atoms' energy spectra (the second to fourth subbands: $E_2-E_4$ )

The subquasilattice of C atoms, as shown in Fig. 4, is different from the normal 2D Fibonacci one. Its spectra do not split as type F, but as follows.

(a) *Isolated C atoms' energy spectra (the third subband:  $F_3$ ).* This subband is formed by the degenerate energy level  $E = E_C$  of the isolated C atoms. Only two kinds of clusters shown in Fig. 5 exist in the subquasilattice: (a) isolated C atoms and (b) isolated C clusters, with an A atom intervening between every two such clusters. The subband spectra of (a) clusters do not split, but remain to be the highly degenerate level  $E = E_C$ . This kind of atom amounts to one-fifth of the total. For the (b) cluster, because of the equivalence of the four C atoms, we have  $E_1 = E_2 = E_3 = E_4$ . Perturbed weakly by the central C atoms, the energy level decreases to  $E_i = E_C + t_A$  ( $i=1,2,3,4$ ;  $t_A < 0$ ). The atoms in this kind of cluster amount to four-fifths of the total. The subband of isolated C atoms splits in the way of one into two as type  $Y_C$ .

For the isolated C atoms shown in Fig. 5(a), its subquasilattice is the same as the second subquasilattice of the di-

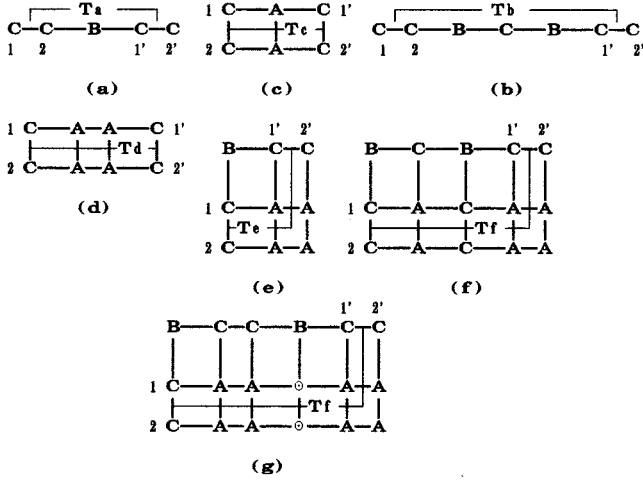


FIG. 6. Coupling interactions between diatomic  $C$  molecules.

atomic  $C$  molecules. So its subbands split as type  $Y_{CC}$  (one into seven). The subquasilattice of the next-nearest-neighbor  $C$  clusters is the normal 2D Fibonacci quasilattice again. Its subbands split as type  $F$  (one into five).

(b) *Diatomic  $C$  molecules' energy spectra (the second and fourth subbands:  $E_2$  and  $E_4$ ).* This subband is formed by the degenerate level  $E = E_C \pm t$  of diatomic  $C$  molecules. In performing the decomposition-decimation procedure for the diatomic molecule degenerate states, we have to investigate seven types of coupling interactions, which are shown in Figs. 6(a)–6(g). For the strong interaction between the superatoms with the same state (i.e., diatomic  $C$  molecules, diatomic  $A$  molecules, etc.) we choose matrix element  $t_s = -1.0$ . We choose  $t_w = -0.1$  for the weak interaction between superatoms with different states. By means of the decomposition-decimation procedure we have calculated the seven renormalized transfer-matrix elements corresponding to the seven types of coupling interactions studied. By the order shown in the Fig. 6, they are, respectively,

$$T_a = t_w^2/2, \quad T_b = 0, \quad T_c = T_a/2t_s, \quad T_d = -2T_a/2t_s, \\ T_e = 0, \quad T_f = 0, \quad T_g = 0. \quad (2)$$

Therefore, the second and fourth subbands split as type  $Y_{CC}$  (one into seven),

$$E_1 = E_C \pm 1, \quad E_{2,3} = E_C \pm t \pm T_a, \quad E_{4,5} = E_C \pm t \pm T_C, \\ E_{6,7} = E_C \pm t \pm T_d. \quad (3)$$

Figure 3 shows the energy spectra of isolated  $C$  atoms and diatomic  $C$  molecules.

For the supermolecules of  $C$  shown in Figs. 6(a), 6(c), and 6(d), all of their subquasilattices form Fibonacci quasilattices again. The first and seventh, second and sixth, and third and fifth subbands of the  $Y_{CC}$  spectra split as type  $F$ . We do not know yet how the fourth subband splits because of its complicated structure. Summing up all of the results obtained, we finally obtain the whole spectrum structure for the 2D Fibonacci quasilattices with three kinds of atoms and one kind of bond length, which is schematically shown in Fig. 7.

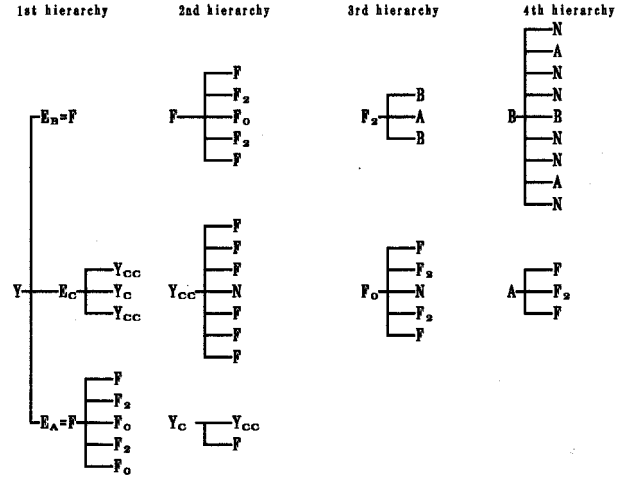


FIG. 7. Electronic energy structure of the total electronic spectra.

#### IV. INFLUENCE ON THE ENERGY SPECTRA

The number and the polarity of each kind of atom in the quasilattice studied are quite different. The number of  $B$  atoms is small and the polarity is very weak, so its interaction with other kinds of atoms can be treated as a perturbation. On the other hand, the number of  $A$  and  $C$  atoms is quite large and the polarity is very strong, especially for the diatomic  $C$  molecules, the interaction of which is dominant.

##### A. Change of the position of energy spectra

###### 1. Downward shift of energy spectra of $A$ atoms

The ‘bare energy’ of  $A$  atoms  $E_A = -5.0$ , but numerical calculation shows that the center of the corresponding subband is located at  $E_A = -5.25$ , i.e., the energy level shifts downward. Now we present the details of the calculation. The Hamiltonian of the isolated  $A$  atoms shown in Fig. 2(a) can be written as

$$H = \begin{pmatrix} E_C & 0 & -1 & 0 & 0 \\ 0 & E_C & -1 & 0 & 0 \\ -1 & -1 & E_A & -1 & -1 \\ 0 & 0 & -1 & E_C & 0 \\ 0 & 0 & -1 & 0 & E_C \end{pmatrix}. \quad (4)$$

The secular equation is

$$\lambda I - H = 0, \quad (5)$$

where  $I$  is a unit matrix. When we choose  $E_A = -5.0$  and  $E_C = 3.0$ , by formula (5) we get the energy eigenvalues

$$\lambda = -5.472\ 136, 3.0, 3.0, 3.0, 3.472\ 136. \quad (6)$$

The Hamiltonian of the  $A$  four-atom molecule shown in Fig. 2(c) is

$$H = \begin{pmatrix} E_C & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ -1 & E_C & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & E_A & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & E_C & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & E_C & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & -1 & E_A & -1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & E_C & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & E_C & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & E_A & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & E_C & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & E_C & 1 \\ 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & E_A \end{pmatrix}, \quad (7)$$

where  $E_A = -5.0$  and  $E_C = 3.0$ . We obtain the eigenenergies

$$\lambda = -7.216\ 990\ 8, -5.246\ 157\ 5, -5.246\ 157\ 3, \\ -3.274\ 917\ 4, 2.0, 2.130\ 457\ 2, 2.130\ 457\ 4, 2.216\ 990\ 6, 4.0, 4.115\ 700\ 2, 4.115\ 700\ 2, 4.274\ 917\ 4. \quad (8)$$

From formulas (6) and (8), we see that the center of the energy spectra of  $A$  atoms shifts downward from  $E_A = -5.0$  because of the interaction with  $C$  atoms. Although the number of  $C$  atoms is a little more than that of  $A$  atoms, the proportion of diatomic  $C$  molecules with strong polarity in the total  $C$  atoms is much larger than that of  $A$  atoms. This is the reason why the  $A$  atoms' energy spectra shift downward.

### 2. Upward shift of energy spectra of $B$ atoms

The bare energy of  $B$  atoms  $E = 5.0$ , but by calculation the center of the corresponding subband is  $E_B = 6.35$ . The shift comes from the repelling interactions between  $C$  and  $A$  atoms, especially from  $C$  atoms. The Hamiltonian of the isolated  $B$  atoms shown in Fig. 2(d) is

$$H = \begin{pmatrix} E_C & 0 & -1 & 0 & 0 \\ 0 & E_C & -1 & 0 & 0 \\ -1 & -1 & E_B & -1 & -1 \\ 0 & 0 & -1 & E_C & 0 \\ 0 & 0 & -1 & 0 & E_C \end{pmatrix}, \quad (9)$$

where  $E_C = 3.0$  and  $E_B = 5.0$ . We obtain eigenenergies

$$\lambda = 1.763\ 932\ 1, 3.0, 3.0, 3.0, 3.0, 6.236\ 068\ 0. \quad (10)$$

The number of  $C$  atoms is much larger than that of  $B$  atoms and two-thirds of the  $C$  atoms are in the form of diatomic  $C$  molecules and only one-third of the  $C$  atoms are isolated, but all of  $B$  atoms are isolated. Repelled by the large number of  $C$  atoms with strong polarity, the spectra of  $B$  atoms shift upward obviously.

### B. Change of the shape of energy spectra

The interactions between atoms change not only the position of electronic energy subbands, but also the symmetry of the energy spectra structure.

### 1. Energy spectra of $B$ atoms (five subbands)

In the second hierarchy energy spectra of  $B$  atoms split as type  $F$ :  $B_{21} = F$ ,  $B_{22} = F_2$ ,  $B_{23} = F_0$ ,  $B_{24} = F_2$ , and  $B_{25} = F$ . Repelled by the large number of strongly polarized diatomic  $C$  molecules, the shape of the third hierarchy energy spectra of  $B$  atoms is changed. The lower the energy spectra, the narrower the gaps of the energy spectra and the smaller the number of atoms.

Some of the superatoms with lower energy in the third or higher hierarchies are excited to higher-energy levels. This breaks the symmetry of the energy spectra in the third, fourth, and higher hierarchies. The top part of the energy spectra of  $B$  atoms splitting is wider than those of the bottom one.

### 2. Energy spectra of $A$ atoms (five subbands)

This is just like the case of  $B$  atoms. Because of the number of  $A$  atoms being smaller than that of  $C$  atoms and its polarity much stronger, the symmetry of the energy spectrum structure is not broken seriously.

### 3. Energy spectra of $C$ atoms

The number of diatomic  $C$  clusters is two times that of the isolated  $C$  atoms, so the energy spectra of isolated  $C$  atoms are condensed about the center and its energy spectra are slightly split. On the other hand, the self-interactions between diatomic  $C$  molecules are stronger; they are very close to those between the isolated  $C$  atoms. This phenomenon is like the formation of hybridized orbit, so the energy spectrum picture is quite different from the standard one.

## V. SUMMARY

We have presented the construction method of the 2D Fibonacci quasilattices with three kinds of atoms and one kind of bond length. Even though three different kinds of

atoms exist in the quasilattice, every chain is composed of only two kinds of atoms.

By means of the DD method based on the renormalization-group technique, we analyzed the splitting rules of every subband. The way of splitting of the energy spectra is mainly determined by the resonant coupling among the states with the same energy. The quasilattice is composed of six kinds of clusters (i.e., ‘‘superatoms’’). In the first hierarchy, the electronic energy spectra split into nine subbands. For the second hierarchy, all of the subbands split as type  $F$  (one into five). Those of isolated  $C$  atoms and

diatomic  $C$  molecules split as type  $Y_C$  and  $Y_{CC}$ , respectively. For the whole system, the interaction among the three kinds of atoms changes the position of the electronic energy spectra. The repelling effect of  $C$  atoms is important because atom  $C$  has the highest population among the three kinds of atoms and two-thirds of them form diatomic  $C$  molecules. It causes the energy spectra of  $B$  atoms to move upward significantly and the energy spectra of the isolated  $C$  atoms are condensed closely about the center with very small gaps, while the energy spectra of  $A$  atoms shift downward as a whole.

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