Splitting rules for the electronic energy spectra of 2D FC(n) with three kinds of atoms and one bond length

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Abstract. In this paper we study the splitting rules of energy spectra for two-dimensional Fibonacci-class quasilattices (FC(n)) with three kinds of atoms (A, B, and C) and one bond length by means of a decomposition-decimation method, and find that the sublattices of B atoms and C atoms are different from those of normal two-dimensional FC(n) and the corresponding splitting manners are new and interesting. B atom forms a kind of two-dimensional so-called FC(n)′, which structure is some different from that of normal FC($n-1$) ($n \geq 2$), but the spectra lines are as the same as that of the latter. C atom forms two kinds of interesting one-dimensional periodic chains: n-atom chain and ($n-1$)-atom chain, which spectra will both tend to become continuous, respectively. The analytical results are confirmed by numerical simulations.

PACS. 71.23.Ft Quasicrystals – 63.90.+t Other topics in lattice dynamics – 33.70.Jg Line and band widths, shapes, and shifts

1 Introduction

There have been a large number of studies on the properties of the quasiperiodic systems since the experimental discovery of fivefold symmetry in the diffraction pattern of metallic alloys by Shechtman et al. [1]. Particularly, from this on, much attention has been paid to one-dimensional (1D) Fibonacci chain [FC(1)] or the superlattice systems constructed following the FC(1) sequence because of its structure's not only having the main characteristics of the quasicrystals but also being relatively very simple. Merlin et al. [2] presented the X-ray and Raman scattering measurements to the sample, consists of alternating layers of GaAs and AlAs to form FC(1) sequence in which the ratio of incommensurate periods is equal to the golden mean τ. Kohmoto et al. [3] 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 [4]. Afterwards, Tamura and Wolfe [5] studied acoustic-phonon transmission through a realistic FC(1) superlattice theoretically, and obtained some results for the transmission spectra. Zhu and Ming [6] analyzed a FC(1) optical superlattice made from a single crystal with quasiperiodic laminar ferroelectric domain structures, and studied the second-harmonic-generation light (SHGL) in this system. Zhu et al. [7] fabricated a nonlinear optical superlattice

of LiTaO$_3$ in which two building blocks A and B were arranged as a FC(1) sequence, and measured the quasi-phase-matched SHGL spectrum of it.

Trying to find a consummate quasiperiodic superlattices like FC(1), Huang et al. [8] proposed a so-called inter-growth quasiperiodic model [FC(2)], and investigated the main characteristics of it in detail. Based on researches concerning FC(1) and FC(2), Fu et al. [9] designed a class of flawless quasiperiodic models which contain FC(1) and FC(2), and called them "Fibonacci-class quasilattices" [FC(n)]. They studied the splitting rules of energy spectra and gap-labeling properties of 1D FC(n). Yang et al. [10–12] 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 SHGL derived from ferroelectric multidomains arranged by 1D FC(n) orders. For the electronic energy spectra of two-dimensional (2D) FC(n) with one kind of atom and two bond lengths, based on the decomposition-decimation (DD) method, Fu et al. [13] researched the splitting rules of FC(1), i.e., the normal square Fibonacci quasilattices, and the splitting laws for FC(n) ($n \geq 2$) have been studied by Yang et al. [14] and Li et al. [15]. As for the 2D FC(n) with three kinds of atoms and one bond length, Yang et al. [16] investigated the spectra splitting rules of FC(1). However, as we know, the researches for the case of $n \geq 2$ have not been reported yet.

The DD method was created by Liu and Sritrakool [17] on the basis of Niu and Nori's studies [18], and it allows one only to calculate the influence between resonant
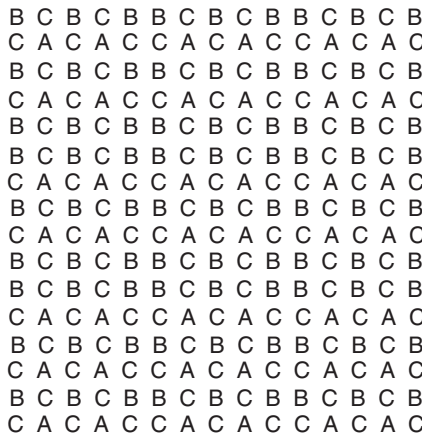
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Fig. 1. 2D FC(2) with three kinds of atoms and one bond length.

Fig. 2. Electronic energy spectra of the 2D FC(2) vs. atom number with 3025 atoms, where $E_A = -5.0$, $E_B = 5.0$, and $E_C = 3.0$.

couplings of the same kinds 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 2D FC(n) ($n \geq 2$) with three kinds of atoms and one bond length, and find that either the structures of the sub-lattices or splitting manners of electronic energy spectra are quite different from that of normal 2D FC(n). For the structures, there exist interesting periodic sub-chains and so-called FC(n)′ sub-quasilattice. For the spectra, except those normal cantor-like branches, there exist some continuous ones yet. In Section 2, we introduce the construction method of the quasilattices. In Section 3, the splitting rules for electronic energy spectra are studied. We also research the influence of different atoms on the electronic energy spectra analytically in Section 4, and Section 5 is a brief summary.

2 2D FC(n) with three kinds of atoms and one bond length

The normal 2D FC(n) has a network form constructed by 1D FC(n) in vertical and horizontal directions. The 2D FC(n) under study are different from the normal one. They are not formed by one kind of atom and two 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 FC(n). This kind of 2D FC(n) can be constructed in the following way: (1) Create two 1D FC(n) in the same way along the X and Y axes, respectively. (2) By means of general multiplication, we obtain the following: (long) × (long) = A atoms, (short) × (short) = B atoms, and (long) × (short) = (short) × (long) = C atoms. So we can get the quasilattices with three kinds of atoms and one bond length. The structure of FC(2) is demonstrated in Figure 1.
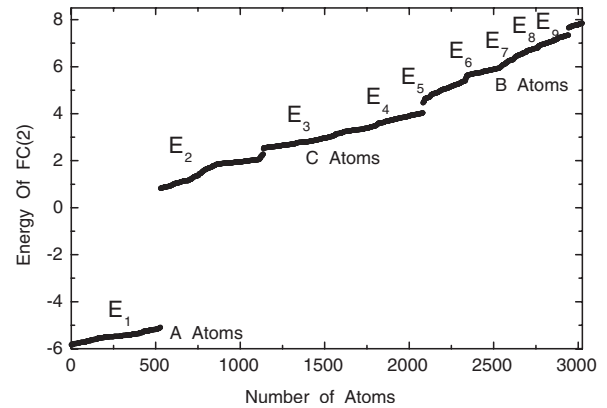
3 Splitting rules of 2D FC(n)

3.1 Numerical simulations of spectra

In the framework of the single-particle tight-binding model, atomic orbits are located at the center of the cell. The Hamiltonian can be simply written as

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

where $|i\rangle$ is the ith 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 (i.e., a unit bond value for simplicity) 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. If the values for site energies are too small, the spectra for each kind of atoms will split crossover each other and then it is difficult to distinguish the splitting types for the spectra of atoms. In order to show the structures of sub-spectra for each kind of atoms clearly, 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 for FC(2).
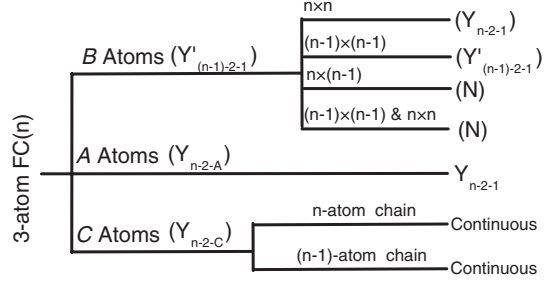
3.2 Analytical results of spectra

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 exist three highly degenerate energies E_A, E_B, and E_C. If we assume that there is an interaction only between the nearest-neighbor atoms, then the 2D FC(n) should contain only six kinds of isolated clusters, i.e., the isolated A atoms, $n \times n$ B clusters, $(n-1) \times (n-1)$ B clusters, $(n-1) \times n$ B clusters, $(n-1)$-atom C chains, and n-atom C chains. Among the

Table 1. Spectral rules for normal FC(n) and FC(n)$'$ ($n \geq 2$).

	item	spectra number (*type*)
normal FC(n)	first hierarchy	$N'_{FC(n)}$ (*type* Y_{n-2-1})
	second hierarchy	$L_{FC(n)}$
	$(n+1) \times (n+1)$	$N'_{FC(n)}$ (*type* Y_{n-2-1})
	$n \times (n+1)$	3 ($n=2$); 5 ($n \geq 3$)
	$n \times n$	$N'_{FC(n-1)}$ (*type* $Y'_{(n-1)-2-1}$)
	$(n+1) \times (n+1)$ and $n \times n$	$N'_{FC(n-1)}$ (*type unknown*)
FC(n)$'$	first hierarchy	$N'_{FC(n-1)}$ (*type* $Y'_{(n-1)-2-1}$)
	second hierarchy	L'_B
	$n \times n$	
	$n \times (n-1)$	same as that of FC(n)
	$(n-1) \times (n-1)$	see context
	$n \times n$ and $(n-1) \times (n-1)$	

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 and under the first approximation, there are $N'_{FC(n)-3atoms}=2n + N'_{FC(n-1)}$ energy levels: 1 for isolated A atoms, $N'_{FC(n-1)}$ for B molecules, $(n-1)$ for $(n-1)$-atom C chains, and n for n-atom C chains.

The next step is to consider the further branching of the main sub-bands. By the DD method, we regard an eigenstate and its corresponding "molecule" as a "super-atom" with definite energy, i.e., there are six kinds of super-atoms, each of which forms a subquasilattice. This idea will be applied repeatedly in this paper.

3.2.1 A atoms' energy spectra

Under the second-order approximation, the sub-quasilattices constructed by isolated A atoms are the normal 2D FC(n) with one kind of atom and two bond lengths, and the spectrum splits into $N'_{FC(n)}$ subbands as type Y_{n-2-1} [14].

3.2.2 B atoms' energy spectra

For B atoms, under the first approximation there exist three kinds of clusters: $n \times n$, $(n-1) \times (n-1)$, and $n \times (n-1)$, which construct so-called FC(n)$'$ and the structure is some different from that of the normal 2D FC(n). In Table 1, we compare their spectra with each other in detail, where the total number of the spectra lines $L_{FC(n)}$ was obtained in our latest work [15]. The total number of the sub-spectra for the second hierarchy of B atoms is

$$L'_B = \begin{cases} 37, & n = 2 \\ 2n^4 - 2n^2 + 8n + 1, & n \geq 3 \end{cases}. \quad (2)$$

Fig. 3. Electronic energy structure of the electronic spectra.

3.2.2.1 Spectra for n × n B clusters

The sub-quasilattices of $n \times n$ B clusters are normal 2D FC(n), and the corresponding spectra split as type $Y_{n-2-1}(1 : N'_{FC(n)})$ (see Tab. 1 and Fig. 3). For its main subband, there are $(n^2 - 3n + 4)$ lines for the first hierarchy, therefore the total number of the spectral lines for the second hierarchy is

$$L'_{B\{n \times n\}} = (n^2 - 3n + 4) \times N'_{FC(n)}. \quad (3)$$

3.2.2.2 Spectra for (n − 1) × (n − 1) B clusters

The sub-quasilattices of $(n-1) \times (n-1)$ B clusters are 2D FC(n)$'$, and the spectra split as type $Y'_{(n-1)-2-1}$ ($1 : N'_{FC(n-1)}$) (see Tab. 1 and Fig. 3). The sum of the spectral lines is

$$L'_{B\{(n-1) \times (n-1)\}} = \begin{cases} 5, & n = 2 \\ (2n - 4) \times N'_{FC(n-1)}, & n \geq 3 \end{cases}. \quad (4)$$

Table 2. The coupling interactions of B and C clusters for FC(2) and FC(3), where t_A is the coupling interaction between A atom and isolated C atom, t_B is that between B atom and isolated C atom, and $t_A < 0$, $t_B < 0$.

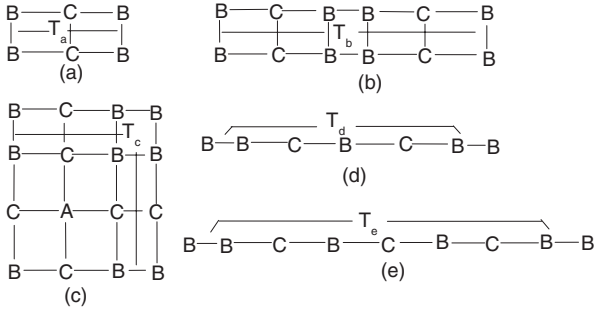|		T_a	T_b	T_c	T_d	T_e	T_f
FC(2)	diatomic B clusters	$t_w{}^2/2t_s$	0	0	0	0	–
	isolated C atoms	$+t_B$	$+t_B, +t_B + t_A$ and $+2t_B + 2t_A$	$+t_B, +t_B + t_A, +2t_B + t_A$ and $+2t_B + 2t_A$	–	–	–
	diatomic C molecules	$t_w{}^2/2t_s$	$-t_w{}^2/t_s$	$-T_a/\sqrt{2}$	0	0	0
FC(3)	six-atom B molecules	$t_w{}^2/2t_s$	$T_a/\sqrt{2}$	0	0	–	–

Fig. 4. Coupling interactions between diatomic B clusters of 2D FC(2).

3.2.2.3 Spectra for n × (n − 1) B clusters

Figure 4 is the coupling interactions between diatomic B clusters of 2D FC(2). We calculate all of the five kinds of renormalized transfer-matrix elements and find that there exist only one non-zero interaction, shown as Table 2. The sub-spectra for diatomic B molecules split in the way of one into three. Figure 5 is the coupling interactions between six-atom B clusters of 2D FC(3). The result is that there exist two non-zero renormalized transfer-matrix elements, and every subband for six-atom B clusters of FC(3) splits into five. Then the formula of the total subbands for $n \times (n-1)$ B clusters of FC(n) can be written as follows:

$$L'_{B\{n \times (n-1)\}} = \begin{cases} 6, & n = 2 \\ 5(n^2 - n), & n \geq 3 \end{cases}. \tag{5}$$

3.2.2.4 Middle spectrum for B clusters

The middle spectrum for B clusters is formed by two kinds of sub-clusters: $(n-1) \times (n-1)$ and $n \times n$ B molecules. The interaction for the former is much stronger than that of the latter, thus the splitting rule for the middle spectrum is mainly decided by the former, i.e., the middle spectrum splits in the way of one into $N'_{FC(n-1)}$ (see Tab. 1 and Fig. 3), and the total number of its subband lines is

$$L'_{B\{[(n-1) \times (n-1)]\ \&\ [n \times n]\}} = 1 \times N'_{FC(n-1)}. \tag{6}$$

3.2.3 C atoms' energy spectra

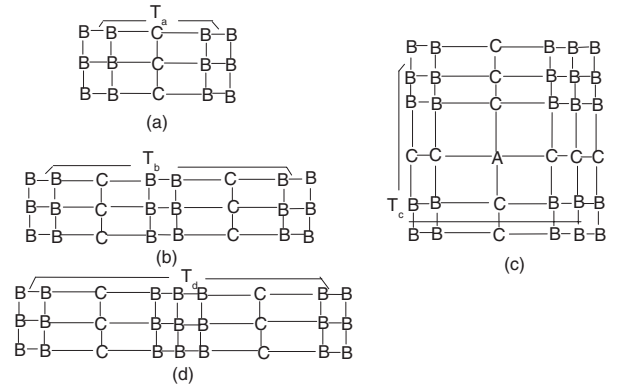C atoms construct two kinds of interesting 1D chains: one is $(n-1)$-atom chain, the other is n-atom chain. With

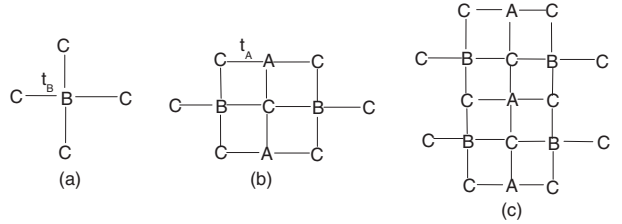**Fig. 5.** Coupling interactions between six-atom B clusters of 2D FC(3).

Fig. 6. Coupling interactions between isolated C atoms of 2D FC(2).

the increment of n, they become more and more perfect 1D periodic lattices and their sub-spectra all tend to be continuous and smooth.

On the other hand, when n is not very large, these two kinds of super-atoms are not 1D chains but simple clusters, and their sub-spectra are all discrete lines but not continuous bands. For example, in FC(2) model, they are isolated C atoms and diatomic C molecules, respectively; we calculate the renormalized transfer-matrix elements of C atoms for FC(2) (see Figs. 6 and 7) analytically (see Tab. 2) and obtain four and seven discrete lines for their sub-spectra, respectively. The numerical simulations for C atoms of FC(2), FC(3) and FC(5) are obtained and are shown in Figure 8, where Figure 8a1 ∼ Figure 8c1 are the sub-spectra of 1D $(n-1)$-atom C chain for FC(2), FC(3) and FC(5), respectively; and Figure 8a2 ∼ Figure 8c2 are that of n-atom C chain for FC(2), FC(3) and FC(5), respectively; Figure 8d1 and Figure 8d2 are that of 1D periodic lattice.
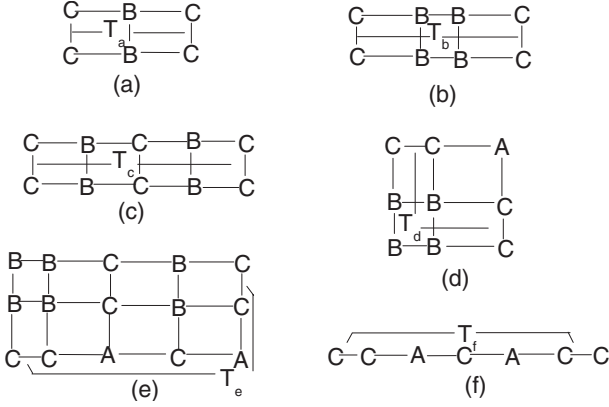
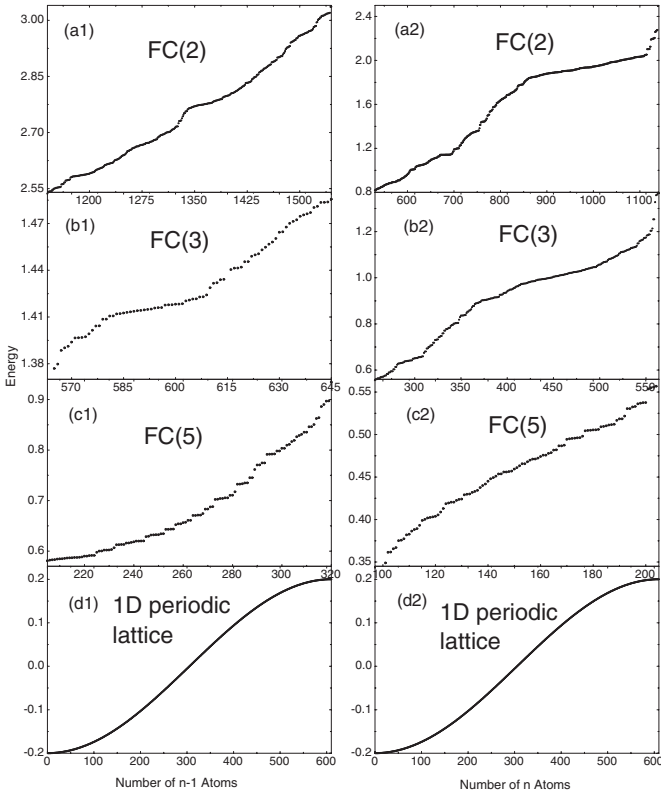**Fig. 7.** Coupling interactions between diatomic C clusters of 2D FC(2).

Fig. 8. Spectra of 1D C-atom chains and 1D periodic lattice. (a1) $\sim$ (c1) are for the $n-1$-atom chain, the systems are FC(2), FC(3) and FC(5), respectively. (a2) $\sim$ (c2) are for n-atom chain. (d1) and (d2) are for 1D periodic lattice (see context).

From Figure 8 one can see that their sub-spectra are different from each other, even if n becomes large enough so as to the former changes to very long 1D chain, but the sub-spectra of the former will not be the same as that of the latter. The reason is that there are only two boundaries for the latter, i.e., the originating point and the endpoint, and there are not any other affections to the total body of the periodic chain, so its sub-spectra are perfectly continuous and smooth when n is large enough. But the

case to the former is quite different. These two kinds of 1D chains are all located among other clusters. Not only are they influenced by their two boundaries, but also are impacted by other clusters at many points of their body, including the interactions between themselves each other. The boundaries for them are all over the total chains. By means of a DD method, one knows that under the second approximation the interactions between the same kind of atoms are the dominant factors to affect the spectra splitting of the subband, and that between the different kinds of atoms can be regarded as perturbations, so the interactions between these two kinds of 1D chains will strongly affect the shape of their sub-spectra.

In a word, the sub-spectra of the former will only tend to be continuous, but not perfectly continuous, even if the number n tends to be infinite.

Summing up all of the results, we finally obtain the spectrum structure for the 2D FC(n) with three kinds of atoms and one bond length, which is schematically shown in Figure 3. The detail data are shown in Table 3.

4 Influence on the energy spectra

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

4.1 Change of the position of energy spectra

4.1.1 Downward shift of energy spectra of A atoms

The "bare energy" of A atoms is $E_A = -5.0$, but numerical calculation for FC(2) in Figure 2 shows that the center of the corresponding sub-band is located at -5.45, i.e., the energy level shifts downward. In the class of FC(n) and under the first approximation, there only exist isolated A atoms and they are all enwrapped by C atoms, so the Hamiltonian of the isolated A atoms can be written as

$$H = \begin{pmatrix} E_C & 0 & -1 & 0 & 0 \\ 0 & E_C & -1 & 0 & 0 \\ -1 & -1 & E_A & -1 & -1 \\ 0 & 0 & -1 & E_C & 0 \\ 0 & 0 & -1 & 0 & E_C \end{pmatrix}. \tag{7}$$

The secular equation is

$$\lambda I - H = 0, \tag{8}$$

where I is a unit matrix. When we choose $E_A = -5.0$ and $E_C = 3.0$, by formula (8) we get the energy eigenvalues

$$\lambda_A = -5.47214. \tag{9}$$

Table 3. Spectral rules of FC(n) ($n \geq 2$) with three kinds of atoms and one bond length.

	item	FC(2)	FC(n)
first hierarchy	A atoms	1 (type Y_{2-2-A})	1 (type Y_{n-2-A})
	B atoms	5 (type F')	$N'_{FC(n-1)}$ (type $Y'_{(n-1)-2-1}$)
	C atoms	3 (type Y_{2-2-C})	$2n-1$ (type Y_{n-2-C})
	sum	9	$2n + N'_{FC(n-1)}$
second hierarchy	isolated A atoms	13 (type Y_{2-2-1})	$N'_{FC(n)}$ (type Y_{n-2-1})
	$n \times n$ B clusters	13 (type Y_{2-2-1})	$N'_{FC(n)}$ (type Y_{n-2-1})
	$n \times (n-1)$ B clusters	3 (type unknown)	5 (type unknown)
	$(n-1) \times (n-1)$ B clusters	5 (type F')	$N'_{FC(n-1)}$ (type $Y'_{(n-1)-2-1}$)
	mixing nonpolar B clusters	5 (type unknown)	$N'_{FC(n-1)}$ (type unknown)
	$n-1$ C chains	4 (quasi $-$ continuous)	continuous
	n C chains	7 (quasi $-$ continuous)	continuous

That is to say the center of the energy spectra of A atoms shifts downward from $E_A=-5.0$. The main reason is that the polarity of A atoms is quite less than that of C atoms, for all of the two types of C-atom chains are strongly polarized, but only very few A-atom clusters ($n \times (n-1)$ molecules) are polarized. On the other hand, the number of A atoms is smaller than that of C atoms, and with the increase of n the case becomes more and more seriously. By the way, B-atom clusters will also repulse A-atom molecules slightly.

4.1.2 Upward shift of energy spectra of B atoms

The case for B atoms is different from that of A atoms, the center for the former will shift upward and the reason is also caused by the repellency of C atoms.

4.2 Change of the shape of energy spectra

The interactions between atoms change not only the position of energy sub-bands, but also the shape of the energy spectra structure.

4.2.1 Energy spectra of A atoms

Repelled by the large number of strong polarized 1D C-atom chain, the shape of the sub-spectra of A atoms are changed. The lower the energy spectra, the narrower the gaps of the energy spectra and the less the number of the atoms will be. Some of the super-atoms with lower energy in the third or higher hierarchies are excited to higher energy levels. It breaks the symmetry of the energy spectra in the third, fourth and higher hierarchies.

4.2.2 Energy spectra of B atoms

The symmetry of the energy spectra structure of B atoms is broken and the spectra is also compressed because of the same reason as that of A atoms. The case of FC(2) can be seen in Figure 2.

4.2.3 Energy spectra of C atoms

Being 1D periodic chain the spectra of two kinds of C-atom clusters should be more and more continuous and smooth with the increase of n, but in fact, the result is not so perfect. We analyzed it in detail in Section 3.2.3.

5 Summary

In this paper, we present the construction method of the 2D FC(n) with three kinds of atoms and one kind of bond length and analyze the splitting rulers for the energy spectra by means of the DD method based on the renormalization-group technique. The splitting types and spectra lines for total first-hierarchy, spectra lines for total second-hierarchy are all obtained, although some of the splitting types for second-hierarchy are unknown yet.

Under the first approximation, there are only six kinds of isolated clusters and the electronic energy spectra split in the way of one into $N'_{FC(n)-3atoms}=2n + N'_{FC(n-1)}$, where the splitting types for A, B, and C atoms are Y_{n-2-A}, $Y'_{(n-1)-2-1}$, and Y_{n-2-C}, respectively.

Under the second-order approximation, (1) the sublattices for all of A atoms, which are isolated under first-approximation, form $FC(n)$, the corresponding splitting type for spectra is Y_{n-2-1} ($1 \to N'_{FC(n)}$, see Ref. 14). (2) For B atoms, there exist three kinds of clusters and four types of splitting manners for spectra. The sublattices and splitting manners of spectra for $n \times n$ B clusters are the same as the ones of A atoms; the subquasilattices for $(n-1) \times (n-1)$ B clusters are FC(n)$'$, and the spectra split as type $Y'_{(n-1)-2-1}$ ($1 \to N'_{FC(n-1)}$, but the structure of $Y'_{(n-1)-2-1}$ and $Y_{(n-1)-2-1}$ are different from each other); for $n \times (n-1)$ B clusters, each sub-band splits into three and five when $n = 2$ and $n \geq 3$, respectively; the spectra for mixing nonpolar B clusters (the mixing clusters of $n \times n$ and $(n-1) \times (n-1)$) split in the way of $1 \to N'_{FC(n-1)}$. (3) For C atoms, there are two kinds of 1D periodic chains, their spectra tend to be continuous in different way.

The modifications for the positions and shapes of the spectra are also analyzed. The analytic results are confirmed by numerical simulations.

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