Eur. Phys. J. B **39**, 475–481 (2004)
DOI: 10.1140/epjb/e2004-00220-0

THE EUROPEAN PHYSICAL JOURNAL B

Splitting rules for the 2nd hierarchy structure of the electronic spectra of 2D FC(n) quasicrystals

Feng Li and Xiangbo Yang[a]

Institute of Laser Life Science, South China Normal University, Guangzhou 510631, P.R. China

Received 18 March 2004
Published online 23 July 2004 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2004

Abstract. On the basis of our former work and by means of the decomposition-decimation method, we study the splitting rules for the second hierarchy of the electronic energy spectra for two-dimensional Fibonacci-class quasicrystals with one kind of atom and two bond lengths. It is found that every line of the sub-spectra for $n \times n$ and $(n+1) \times (n+1)$ clusters of FC(n) ($n \geq 2$) splits according to the type $Y'_{(n-1)-2-1}$ and type Y_{n-2-1} respectively. The one for $n \times (n+1)$ clusters of FC(n) consists of three sub-subbands when $n \leq 2$, and five sub-subbranches when $n \geq 3$. The general formulae of the number of energy levels for the spectra of the second hierarchy are obtained. The analytical results are confirmed by numerical simulations.

PACS. 71.23.Ft Quasicrystals – 63.90.+t Other topics in lattice dynamics (restricted to new topics in section 63) – 33.70.Jg Line and band widths, shapes, and shifts

1 Introduction

There have been a large number of studies on the properties of quasicrystals and quasiperiodic systems since the leading experiment made by Schechtman et al. [1] in 1984, which demonstrated the existence of quasicrystals and opened up an interesting field of solid-state physics—quasicrystal physics. The one-dimensional (1D) Fibonacci chain [FC(1)] has attracted much attention from both physicists and mathematicians, because its structure is not only relatively simple but also possesses the main characteristics of quasicrystals. Huang and co-workers [2] proposed a so-called intergrowth quasiperiodic model [FC(2)] in 1992. In 1997 based on research concerning FC(1) and FC(2), Fu et al. [3] designed a class of flawless quasiperiodic models, which contain FC(1) and FC(2) and have been called as Fibonacci-class quasilattices [FC(n)].

For 2D FC(1) with one kind of atom and two bond lengths, Ueda et al. [4] investigated the energy spectrum and conductance numerically. Ashraff et al. [5] have analytically studied the energy spectrum, density of states and the dynamical response function. By means of a decomposition-decimation (DD), Fu et al. [6] studied the splitting rules. Yang et al. [7] have found the branching rules for spectra of 2D FC(1) with three kinds of atoms and one bond length. For 2D FC(n) with one kind of atom and two bond lengths Yang et al. [8] recently obtained the rules for the first hierarchy of the spectra. However, the studies of the properties of the second hierarchy, as far as we know, have not been reported yet.

The DD method was created by Liu and Sritrakool [9] on the basis of researches of Niu and Nori [10], 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. So 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 calculation. By means of this method, in this paper, we have focused our study on the splitting rules for the spectra of the second hierarchy of 2D FC(n) with one kind of atom and two bond lengths, and obtain general formulae for the number of energy levels and some splitting types. In Section 2, the construction of 2D FC(n) is introduced. The splitting rules for the second hierarchy of the spectra are given in Section 3. In Section 4, the influences of different clusters on the positions of sub-spectra are studied analytically. Section 5 is a brief summary.

2 Construction of 2D FC(n)

In reference [8] it is proposed that a 2D FC(n) with one kind of atom and two bond lengths can be composed as follows: (1) create one FC(n) chain in a horizontal direction by the substitution rules

$$S_0 = B, B \rightarrow B^{n-1}A, A \rightarrow B^{n-1}AB, \qquad (1)$$

[a] e-mail: xbyang@scnu.edu.cn

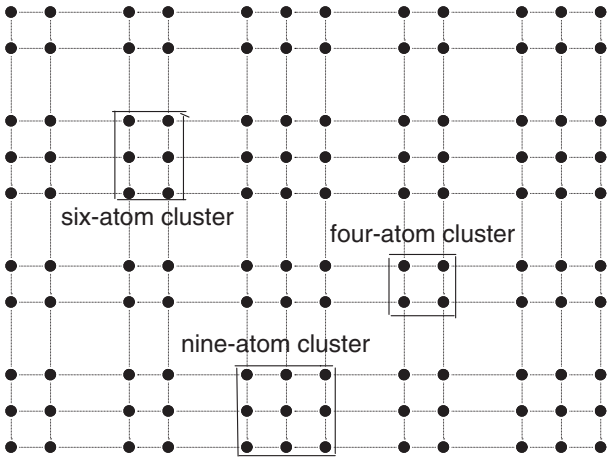

Fig. 1. The structure of FC(2) with one kind of atom and two kinds of bond lengths.

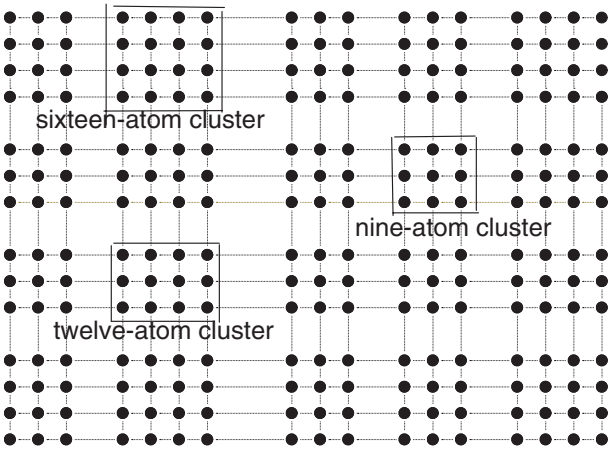

Fig. 2. The structure of FC(3) with one kind of atom and two kinds of bond lengths.

which shows the following sequence:

$$\underbrace{B\cdots\cdots B}_{n-1}A\cdots\cdots\underbrace{B\cdots\cdots B}_{n-1}AB\cdots$$
$$\cdots\underbrace{B\cdots\cdots B}_{n-1}A\cdots\cdots; \quad (2)$$

(2) make "B" units in equation (2) such that there are "short" bond lengths between atoms for the horizontal lattices, and order "A" units to define "long" bond lengths, respectively; (3) by the same step as that for horizontal chains, we can obtain a vertical sequence with the same order of bond lengths; from which the 2D FC(n) can be obtained.

Figures 1 and 2 show a 2D FC(2) and a 2D FC(3), respectively.

3 Splitting rules for the spectra of the second hierarchy of 2D FC(n)

3.1 Spectra for the second hierarchy of 2D FC(2)

3.1.1 Numerical simulations

In the framework of the single-particle tight-binding transfer model, atomic orbits 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

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

where $|i\rangle$ is the ith Wannier state, $\sum_{i,j}{}'$ is the sum over the nearest-neighbor atoms, and t_{ij} is the transfer-matrix element, which contains two kinds of elements t_s (strong) and t_w (weak) corresponding to short and long bonds, respectively. 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. The numerical results for the spectra of FC(2) illustrated in Figure 1 are shown in Figure 3, where from top to bottom we refer to the subbands as E_1 to E_{13}, respectively.

3.1.2 Analyses of the spectra

Making use of the DD method [9], we presume that

(a) in the zeroth approximation there exists no interaction among the atoms (i.e., $t_{ij} = 0$), the 2D FC(2)'s are broken into isolated atoms, and there is only one highly degenerate energy 0.0 in the systems;
(b) in the first approximation only the interactions between the nearest-neighbor atoms are calculated and weak bonds are absent (i.e., $t_{ij} = t_{nearest-neighbor} = -1.0$ and $t_{ij} = t_{others} = 0.0$), then the 2D FC(2) contain only three kinds of isolated clusters: nine-atom clusters, four-atom clusters, and six-atom clusters, and its spectra consist of thirteen subbands. In Figure 3, (1) subbands E_1, E_4, E_{10}, and E_{13} are for the nine-atom clusters, (2) E_3 and E_{11} are for the four-atom clusters, (3) E_2, E_5, E_6, E_8, E_9, and E_{12} are for the six-atom clusters, and (4) E_7 consists of degenerate energy levels of nine-atom clusters and four-atom clusters. Thus there only exist four splitting types for the second hierarchy sub-spectra;
(c) in the second approximation, the interactions between the nearest-neighbor atoms and those between the next-nearest-neighbor atoms are taken into account. The interactions between atoms with the same energy are the dominant factors affecting the spectra splitting of the sub-subbands; the interactions between atoms with different levels can be regarded as perturbations.

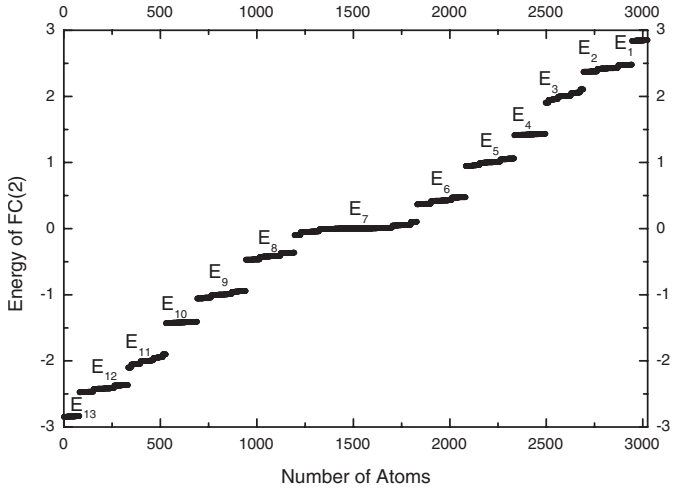

Fig. 3. The electronic energy spectra of 2D FC(2) vs. atom numbers with 3025 atoms.

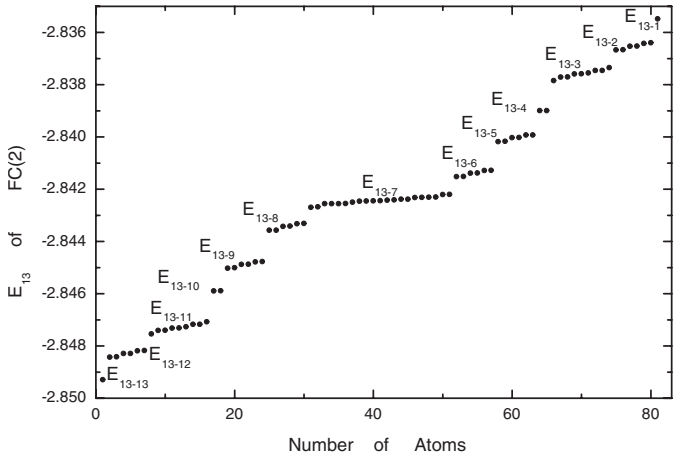

Fig. 4. Subband E_{13} of 2D FC(2).

(a) *Nine-atom clusters' spectra (E_1, E_4, E_{10}, and E_{13})*

For the nine-atom clusters in Figure 1, in the second approximation, there exist three kinds of isolated sub-clusters: four nearest-neighbor nine-atom sub-clusters, six nearest-neighbor nine-atom sub-clusters, and nine nearest-neighbor nine-atom sub-clusters. The structure of the nine-atom sublattice is that of a FC(2) and each of its spectra (E_1, E_4, E_{10}, and E_{13}) splits into thirteen sub-subbands as type Y_{2-2-1} [8]. The picture of the sub-spectra for level E_{13} is shown in Figure 4.

(b) *Four-atom clusters' spectra (E_3 and E_{11})*

For the four-atom clusters in Figure 1, in the second approximation, the structure is different from that of 2D FC(1) though there exist three kinds of isolated sub-clusters: one nearest-neighbor four-atom sub-clusters, two nearest-neighbor four-atom sub-clusters, and four nearest-neighbor four-atom sub-clusters. The sub-spectra (E_3 and E_{11}) split into five branches, and we denote this

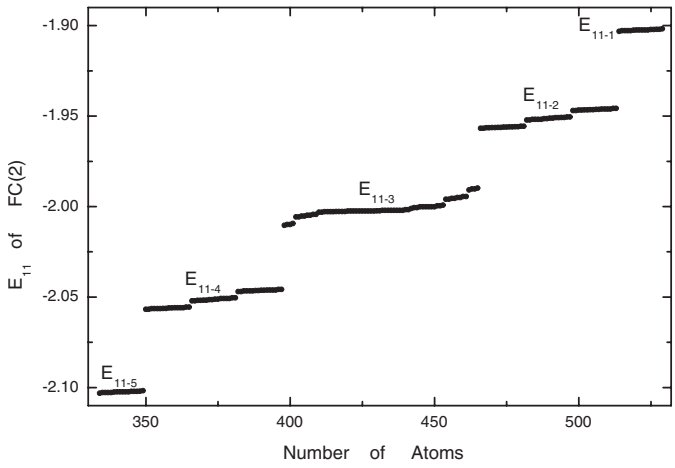

Fig. 5. Sub-spectra E_{11} of 2D FC(2).

kind of structure as type F'. The branch E_{11} is shown in Figure 5.

(c) *Six-atom clusters' spectra (E_2, E_5, E_6, E_8, E_9, and E_{12})*

For the six-atom clusters in Figure 1, the case is more complicated than the aforementioned ones and there exist six kinds of coupling interactions as shown in Figure 6. If the mth molecular denotes the six-atom cluster with atoms 1, 2, 3, 4, 5, and 6, and the nth one the six-atom cluster with atoms $1'$, $2'$, $3'$, $4'$, $5'$, and $6'$. The mth state for the two six-atom sub-clusters in Figure 6a is

$$|\Psi_m\rangle = \sum_{i=1}^{6} C_i |\psi_i\rangle, \tag{4}$$

where C_i is the coupling interaction coefficient for every atom and for atom 1 we have

$$E\psi_1 = \sum_{j=1}^{6} B_j t_{1j} \psi_j, \tag{5}$$

where B_i is the coupling interaction coefficient for atom 1. Then one can obtain

$$T_1 = \frac{t_w}{2}, T_2 = -\frac{{t_w}^2}{2t_s}, T_3 = \frac{t_w^2}{3t_s}, T_4 = \frac{t_w^3}{3t_s^2}, T_5 = 0, T_6 = 0. \tag{6}$$

Formula (6) shows that $|T_2|, |T_3|$ and $|T_4| \ll |T_1|$, and so T_2, T_3 and T_4 can be ignored, then every line of the sub-spectra (E_2, E_5, E_6, E_8, E_9 and E_{12}) will divide into three sub-branches whereas the splitting type is unknown. The graph for the sub-spectra of E_{12} is illustrated in Figure 7.

(d) *The middle spectrum (E_7) of FC(2)*

In the second approximation, because the interactions between nine-atom clusters are much weaker than those between four-atom clusters, the splitting rules for the middle

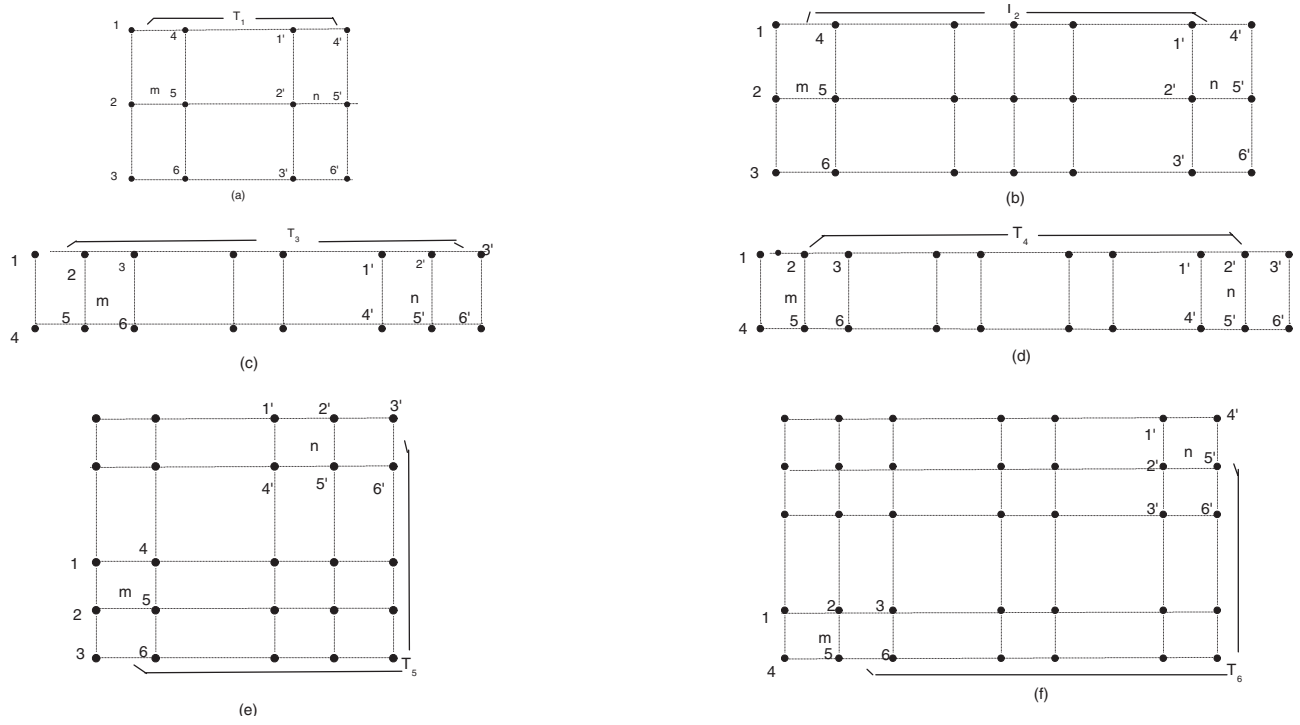

Fig. 6. Coupling interactions between six-atom clusters for 2D FC(2).

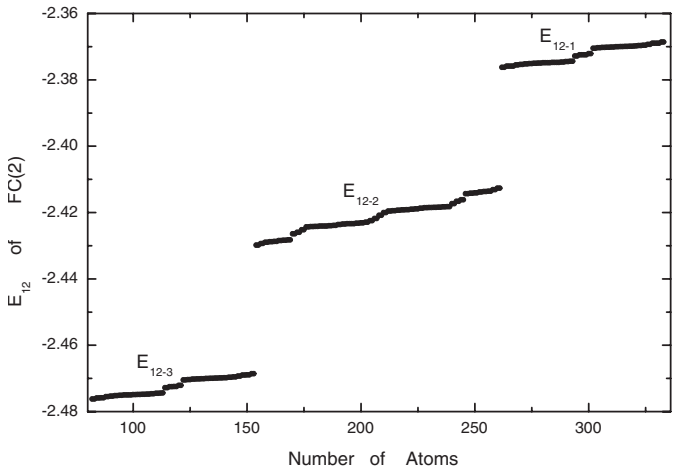

Fig. 7. Subband E_{12} of 2D FC(2).

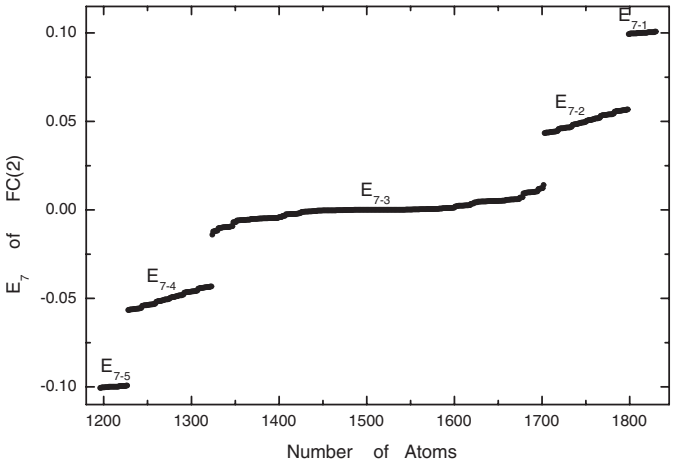

Fig. 8. Sub-spectra E_7 of 2D FC(2).

subband E_7 are mainly controlled by four-atom clusters, and E_7 splits into five sub-subbands. The figure for the sub-spectra of E_7 is illustrated in Figure 8.

3.2 Spectra of 2D FC(3)

The numerical results for the spectra of FC(3) illustrated in Figure 2 are shown in Figure 9, where from top to bottom we refer to the twenty-five subbands as E_1 to E_{25}, respectively. By means of the DD method and in the first approximation there exist three kinds of isolated clusters: sixteen-atom clusters, nine-atom clusters, and twelve-atom clusters. Here we only present the results for the sub-spectra (E_2, E_5, E_6, E_{10}, E_{11}, E_{12}, E_{14}, E_{15}, E_{16}, E_{20}, E_{21}, and E_{24}) of twelve-atom clusters in detail. In the second approximation, there exist six kinds of coupling interactions as shown in Figure 10, and the corresponding six renormalized transfer-matrix elements are obtained as follows

$$T_1 = \frac{t_w}{3}, T_2 = \frac{1}{\sqrt{2}}T_1, T_3 = \frac{-{t_w}^2}{3t_s}, T_4 = \frac{{t_w}^3}{4t_s^2}, \\ T_5 = 0, T_6 = 0. \quad (7)$$

It shows that $|T_3|$and $|T_4| \ll |T_1|$ and $|T_2|$, and so T_3 and T_4 can be ignored. The sub-spectrum for twelve-atom clusters divides into five branches. Figure 11 shows the picture for the sub-spectra of E_{21}.

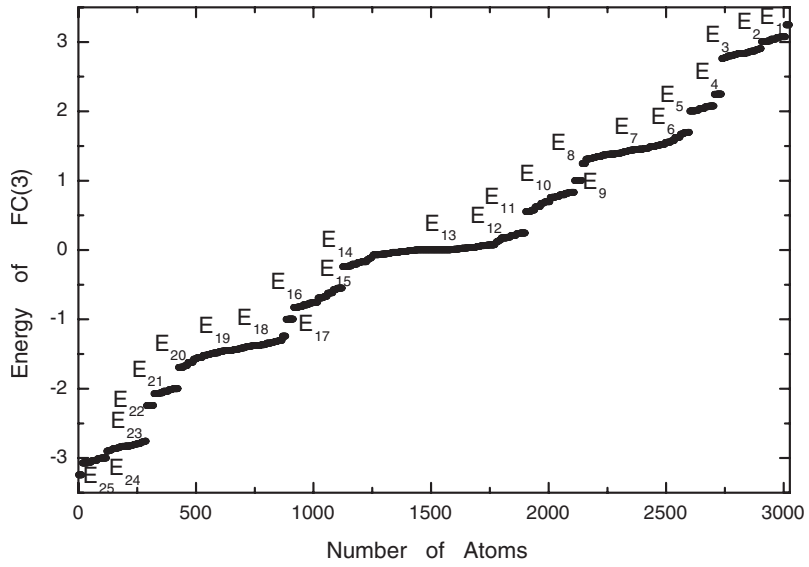

Fig. 9. The electronic energy spectra of 2D FC(3) vs. atom numbers with 3025 atoms.

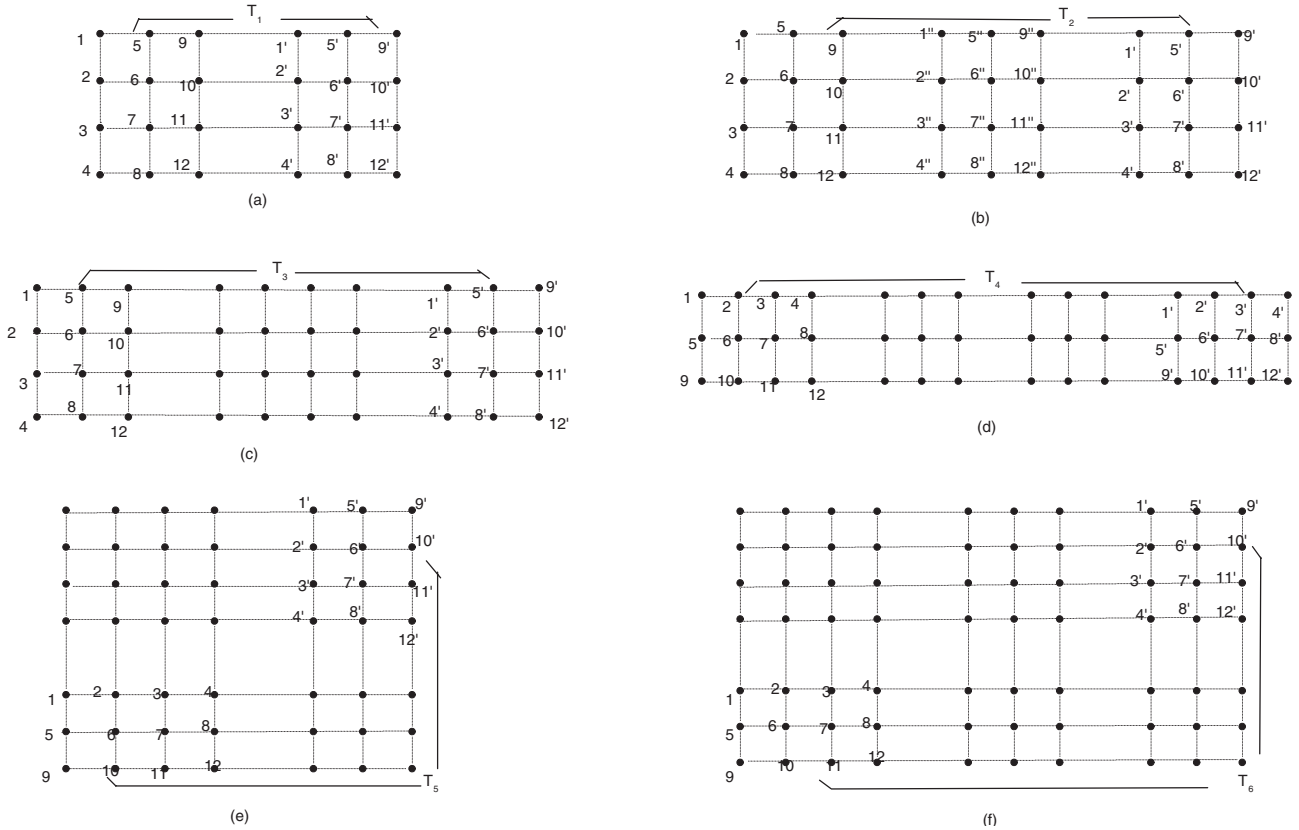

Fig. 10. Coupling interactions between twelve-atom clusters for 2D FC(3).

3.3 Spectra of 2D FC(n)

3.3.1 $(n+1)\times(n+1)$ clusters' spectra

In the second approximation the structures of $(n+1)\times(n+1)$ clusters for FC(n)$(n\geq 2)$ are that of FC(n). From reference [8], one knows that every line of the sub-spectra splits according to the type Y_{n-2-1} and the number of the sub-spectra lines with different energy values is given by

$$l_{(n+1)\times(n+1)} = N'_{FC(n)}, \tag{8}$$

and the total number of this kind of sub-spectra is

$$L_{(n+1)\times(n+1)} = (n^2-n+2)\times N'_{FC(n)}. \tag{9}$$

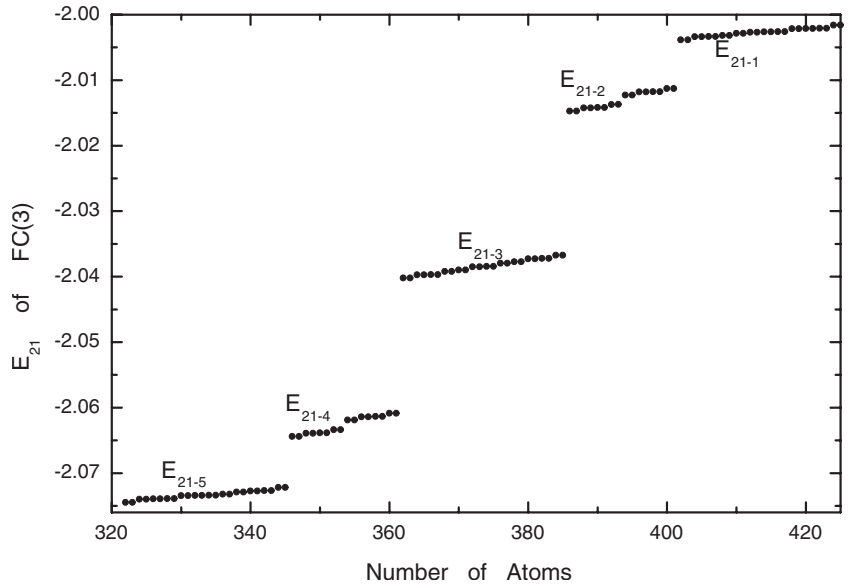

Fig. 11. Subband E_{21} of 2D FC(3).

3.3.2 n × n clusters' spectra

Similarly, it is found that the sub-spectrum for $n \times n$ clusters of FC(n)($n \geq 2$) splits according to the type $Y'_{(n-1)-2-1}$ and the number of lines with different energy values is given by

$$l_{n\times n} = N'_{FC(n-1)}, \tag{10}$$

and the total number is

$$L_{n\times n} = 2(n-1) \times N'_{FC(n-1)}. \tag{11}$$

3.3.3 n × (n + 1) clusters' spectra

In the second approximation, when $n \geq 3$ there exist only two kinds of relatively strong coupling interactions for $n \times (n+1)$ clusters of FC(n), and the sub-spectrum splits into five branches. In conclusion, the number of the sub-spectra with different energy values for FC(n) can be given as follows:

$$l_{n\times(n+1)} = \begin{cases} 3, & n \leq 2 \\ 5, & n \geq 3, \end{cases} \tag{12}$$

and the total number is

$$L_{n\times(n+1)} = \begin{cases} 3 \times (n^2+n), & n \leq 2 \\ 5 \times (n^2+n), & n \geq 3. \end{cases} \tag{13}$$

3.3.4 The middle spectrum of FC(n)

It can be demonstrated that the interactions between $n \times n$ clusters are the most significant effects for the sub-spectra splitting of the middle line and the number of the sub-spectra can be obtained as follows:

$$l_{Middle\ Line} = N'_{FC(n-1)} \quad (n \geq 2). \tag{14}$$

3.3.5 Total spectra number for the second hierarchy of 2D FC(n)

By means of equations (9), (11), (13) and (14), one can obtain the following formula for the total number of the second hierarchy sub-spectra of FC(n) ($n \geq 2$):

$$\begin{aligned} L_{FC(n)} &= L_{(n+1)\times(n+1)} + L_{n\times n} + L_{n\times(n+1)} \\ &\quad + l_{Middle\ Line} \\ &= \left(n^2 - n + 2\right) \times N'_{FC(n)} \\ &\quad + (2n-1) \times N'_{FC(n-1)} \\ &\quad + L_{n\times(n+1)} \ (n \geq 2). \end{aligned} \tag{15}$$

(a) When $n = 2$ the total number is

$$\begin{aligned} L_{FC(n)} &= \left(n^2 - n + 2\right) \times \left(2n^2 + 2n + 1\right) + 3\left(n^2 + n\right) \\ &\quad + (2n-1)\left[2(n-1)^2 + 2(n-1) + 1\right] \\ &= 85. \end{aligned} \tag{16}$$

(b) When $n \geq 3$ the number of the levels is

$$\begin{aligned} L_{FC(n)} &= \left(n^2 - n + 2\right) \times \left(2n^2 + 2n + 1\right) + 5\left(n^2 + n\right) \\ &\quad + (2n-1)\left[2(n-1)^2 + 2(n-1) + 1\right] \\ &= 2n^4 + 4n^3 + 2n^2 + 12n + 1. \end{aligned} \tag{17}$$

The number of the sub-spectra for the second hierarchy of FC(n) and some splitting types are also shown in Table 1.

Table 1. The number and some splitting types of the sub-spectra for the second hierarchy of FC(n) ($n \geq 2$).

item	FC(2)	FC(3)	FC(n)
$n \times n$ cluster	5 (*type* F')	13 (*type* Y'_{2-2-1})	$\mathrm{N}'_{\mathrm{FC(n-1)}}$ (*type* $Y'_{(n-1)-2-1}$)
$(n+1) \times (n+1)$ cluster	13 (*type* Y_{2-2-1})	25 (*type* Y_{3-2-1})	$\mathrm{N}'_{\mathrm{FC(n)}}$ (*type* Y_{n-2-1})
$n \times (n+1)$ cluster	3 (*Unknown*)	5 (*Unknown*)	5 (*Unknown*)
$n \times n$ & $(n+1) \times (n+1)$ clusters	5 (*Unknown*)	13 (*Unknown*)	$\mathrm{N}'_{\mathrm{FC(n-1)}}$(*Unknown*)
quasilattice	85 (*Unknown*)	325 (*Unknown*)	$\mathrm{L}_{FC(n)}$ (*Unknown*)

4 Influences on the positions of energy spectra

In the first-order approximation, the number and the polarities of the three kinds of clusters for FC(n) are quite different. Although the volume of $n \times n$ clusters is nearly equal to that of $n \times (n+1)$ clusters, the former is nonpolar and the later is polar. On the other hand, the number of $(n+1) \times (n+1)$ clusters is much smaller than that of the two kinds of aforementioned clusters and is also nonpolar. So we think that the interactions of $n \times (n+1)$ clusters are the most dominant effect influencing the sub-spectra.

The center [8] of the subband with the lowest energy values for nine-atom clusters is located at $E_{13} = -2\sqrt{2} \approx -2.828$, but the realistic range for E_{13} values as shown in Figure 4 is from -2.849 to -2.835. It shows that in practice spectrum shifts downward obviously because of the repelling actions of the polar six-atoms clusters. For the symmetry, the line E_1 will shift upward. For FC(n) the same conclusion can be drawn out.

5 Summary

We have investigated the spectra for the second hierarchy of 2D FC(n) ($n \geq 2$) with the DD method. In the first approximation, there exist three kinds of isolated clusters: $n \times n$, $n \times (n+1)$, and $(n+1) \times (n+1)$ clusters, and the sub-spectra split into four types. The sub-spectra for $n \times n$ and $(n+1) \times (n+1)$ clusters split according to the type $Y'_{(n-1)-2-1}$ and Y_{n-2-1}, respectively. The one for $n \times (n+1)$ clusters splits from one to three when $n \leq 2$, and one to five when $n \geq 3$. The number of the sub-spectrum of the middle line is the same as that of type $Y'_{(n-1)-2-1}$ but the structure is unknown. We also obtain the number of the total spectra for the second hierarchy of 2D FC(n) ($n \geq 2$) and analyse the influences of the number and polarities of clusters on the positions of the sub-spectra. The analytical results are confirmed by the numerical simulations.

This work was supported by the National Natural Science Foundation of China, Grant No. 10004003, and the Doctoral Foundation of South China Normal University. Yang acknowledges the International Center for Theoretical Physics (Trieste, Italy) and Physics Department of Hong Kong University of Science and Technology, for part of the computations were accomplished there.

References

1. D. Shechtman, I. Blech, D. Gratias, J.W. Cahn, Phys. Rev. Lett. **53**, 1951 (1984)
2. X. Huang, Y. Liu, Chin. Phys. Lett. **9**, 609 (1992)
3. X. Fu, Y. Liu, P. Zhou, W. Sritrakool, Phys. Rev. B **55**, 2882 (1997)
4. K. Ueda, H. Tsunetsugu, Phys. Rev. Lett. **58**, 1272 (1987)
5. J.A. Ashraff, J.-M. Luck, R.B. Stinchcombe, Phys. Rev. B **41**, 4314 (1990)
6. X. Fu, Y. Liu, B. Cheng, D. Zhang, Phys. Rev. B **43**, 10808 (1991)
7. X. Yang, Y. Liu, Phys. Rev. B **56**, 8054 (1997)
8. X. Yang, D. Xing, Phys. Rev. B **65**, 134205 (2002)
9. Y. Liu, W. Sritrakool, Phys. Rev. B **43**, 1110 (1991)
10. Q. Niu, F. Nori, Phys. Rev. Lett. **57**, 2057 (1986)