Energy levels in a self-similar fractal cluster

H Yorikawa
Graduate School of Engineering, Utsunomiya University 7-1-2 Yoto, Utsunomiya, Tochigi, Japan
E-mail: yorikawa@cc.utsunomiya-u.ac.jp

Keywords: fractal cluster, energy level, spectrum, density of states, tight-binding method, graphene, Cantor set

Abstract

The energy spectrum of atomic clusters with a fractal structure corresponding to a Sierpiński triangle on a hexagonal lattice are studied theoretically using a simple tight-binding Hamiltonian. The evolution of the energy levels and degeneracy with the growing generation of the fractal cluster is investigated. The energy states are classified into two groups: growing states and temporary states. States belonging to the first group continue to grow after appearing at a certain generation, while those of the second group do not grow. The self-similar structure of the cluster model is reflected in the growing states, which consist of three distinct types. The energy levels of the growing states, whose degeneracy obeys a recurrence relation, can be expressed by an iterated or multi-nested function including the infinitely nested square root function.

1. Introduction

The mathematical concept of fractals has attracted great interest from mathematicians and scientists, who seek fractals in nature. Researchers in materials science have also developed an interest in building molecular fractals and predicting their properties.

The experimental techniques for the fabrication and analysis of fractal structured materials have evolved considerably since a fractal molecule was synthesized by Newkome et al using molecular self-assembly techniques [1]. Recently, several studies on atomic clusters with fractal geometry have been reported [2–6]. It is expected that further advances in nanotechnology will enable a variety of new fractal structured materials to be fabricated. There have been experimental and theoretical attempts to determine the characteristics of fractal clusters in terms of various parameters, such as cluster growth, spin, and atomic vibrations [7–9]. Several studies on electronic structure have been reported for the Koch curve with different self-energies on certain sites [10], a unique fractal aggregate of carbon atoms in the sp² hybridization [11], and a two-dimensional carbon cluster model with a hexagonal ring arrangement [12].

In this study, we propose a simple model to form a Sierpiński triangle on a hexagonal lattice. The model is a deterministic fractal with the Hausdroff dimension log 3/ log 2, and corresponds to a self-similar structured cluster of atoms. The energy spectrum, namely the energy levels and the degeneracy, of the fractal clusters is obtained by a tight-binding method and analyzed to clarify its relation with the size or generation, as quantitatively as possible. We are particularly interested in how the fractal geometry or self-similarity of the clusters is reflected in the energy spectrum.

In the following section we explain the model of fractal clusters and the framework of the calculations of the Hamiltonian. In section 3, the intrinsic states of the fractal clusters are identified by inspecting the results of numerical calculations, and are classified by their evolution with generation growth. The energy levels and the degeneracy are revealed explicitly. In section 4, the expression of the energy levels and the characteristic states are discussed from several different perspectives. Concluding remarks are presented in section 5.

2. Model

We consider a model of a two-dimensional fractal cluster that forms a Sierpiński triangle on a hexagonal lattice, as illustrated in figure 1. This self-similar fractal can be expressed by a recurrence relation characterized by an
integer $\alpha = 3$ because the $g$-th generation fractal structure is formed out of three structures of the $(g - 1)$-th generation. The number of atoms, $N(g)$, making up the $g$-th generation cluster is

$$\begin{align} N(g) &= \alpha N(g - 1) + \beta = \left(N(0) + \frac{\beta}{\alpha - 1}\right)\alpha^g - \frac{\beta}{\alpha - 1}, \tag{1} \end{align}$$

where $\beta = -3$ and the initial condition is $N(0) = 4$, that is,

$$\begin{align} N(g) &= \frac{5}{2}3^g + \frac{3}{2}. \tag{2} \end{align}$$

$\beta$ is needed to generate the $g$-th generation by connecting the preceding $\alpha$ clusters.

In constructing the tight-binding Hamiltonian for the fractal cluster, we used a one-site one-orbital approximation and included only the nearest-neighbor interactions. A $\pi$-electron approximation for graphene is a case of this treatment. Hereafter, energies will be measured in units of the nearest-neighbor hopping energy from the on-site energy.

For example, the tight-binding Hamiltonian matrix for the 0th generation cluster is

$$\begin{align} H_0 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{3} \end{align}$$

so that the secular determinant is

$$\begin{align} \det(H_0) = E^2(E^2 - 3) = 0. \end{align}$$

Therefore, the eigenvalues, $E = -\sqrt{3}$ (1), 0 (2), and $\sqrt{3}$ (1), can be obtained analytically, where the degeneracy is indicated in parentheses. The eigenvalues of the 1st generation cluster can be obtained analytically as well: $E = -\sqrt{5}$ (1), $-\sqrt{2}$ (2), 0 (3), $\sqrt{2}$ (2), $\sqrt{5}$ (1). The results for $g \geq 2$ are presented in the next section.

### 3. Results

Numerical calculations were performed for the fractal clusters up to the eighth generation to obtain the energy levels and the degeneracy. Some of the results are listed in table 1, where the energy level $E$ and its degeneracy $D$ are presented for $g = 2, 3, 4,$ and $5$. This table reveals that the energy levels can be classified into two groups: growing states and temporary states. The former appear at a certain generation ($s$) and continue to grow as the generation $g$ proceeds, while the latter are temporary and do not grow. In other words, the growing states are those whose degeneracy increases with increasing $g$. The energy levels of the growing states in table 1 are indicated by labels such as $c1$, $a3$, and $b4$, according to their properties, where the letters ‘$a$’, ‘$b$’ and ‘$c$’ distinguish three types of growing states ($a$-, $b$-, and $c$-states) and the following number indicates the starting generation $s$. The energy levels of the $a$- or $b$-states emerge at different energy positions as the generation $g$ increases, in addition to the energy levels of the preceding generation, while those of the $c$-states are always located at $E = 0$.
Table 1. Energy levels ($E$) and degeneracy ($D$) of fractal clusters for $g = 2, 3, 4, \text{ and } 5$. The energy levels of the growing states are labeled by a letter ($a$, $b$, or $c$) and a number representing the starting generation $s$. For the 5th generation cluster, only the energy levels of the growing states are listed, except those of the $a5$-states with $D = 1$.

| $g = 2$ | $E$ | $D$ |
|---------|-----|-----|
| 0.000 000 | 6 | $c1$ |
| $\pm 1.000 000$ | 1 | $a2$ |
| $\pm 1.211 574$ | 2 | |
| $\pm 1.505 971$ | 1 | |
| $\pm 1.628 712$ | 2 | |
| $\pm 2.208 933$ | 2 | |
| $\pm 2.394 170$ | 1 | |

| $g = 3$ | $E$ | $D$ |
|---------|-----|-----|
| 0.000 000 | 15 | $c1$ |
| $\pm 1.000 000$ | 4 | $a2$ |
| $\pm 1.061 683$ | 2 | |
| $\pm 1.235 786$ | 1 | |
| $\pm 1.262 364$ | 2 | |
| $\pm 1.414 214$ | 2 | |
| $\pm 1.543 362$ | 1 | $a3$ |
| $\pm 1.592 922$ | 1 | |
| $\pm 1.613 041$ | 2 | |
| $\pm 1.732 051$ | 3 | $b3$ |
| $\pm 2.148 961$ | 1 | $a3$ |
| $\pm 2.181 019$ | 2 | |
| $\pm 2.236 068$ | 1 | |
| $\pm 2.274 680$ | 2 | |
| $\pm 2.397 155$ | 2 | |
| $\pm 2.436 274$ | 1 | |

| $g = 4$ | $E$ | $D$ |
|---------|-----|-----|
| 0.000 000 | 42 | $c1$ |
| $\pm 1.000 000$ | 13 | $a2$ |
| $\pm 1.013 795$ | 2 | |
| $\pm 1.064 114$ | 1 | |
| $\pm 1.066 595$ | 2 | |
| $\pm 1.106 970$ | 2 | |
| $\pm 1.137 382$ | 1 | $a4$ |
| $\pm 1.232 850$ | 1 | |
| $\pm 1.255 407$ | 2 | |
| $\pm 1.302 776$ | 3 | $b4$ |
| $\pm 1.370 280$ | 1 | $a4$ |
| $\pm 1.389 968$ | 2 | |
| $\pm 1.426 537$ | 1 | |
| $\pm 1.440 343$ | 2 | |
| $\pm 1.518 560$ | 2 | |
| $\pm 1.543 362$ | 4 | $a3$ |
| $\pm 1.606 959$ | 1 | |
| $\pm 1.607 942$ | 2 | |
| $\pm 1.732 051$ | 12 | $b3$ |
| $\pm 2.148 961$ | 4 | $a3$ |
| $\pm 2.160 120$ | 2 | |
| $\pm 2.188 181$ | 1 | |
| $\pm 2.196 633$ | 2 | |
| $\pm 2.232 437$ | 2 | |
| $\pm 2.263 257$ | 1 | $a4$ |
| $\pm 2.264 847$ | 1 | |
| $\pm 2.271 664$ | 2 | |
| $\pm 2.302 776$ | 3 | $b4$ |
| $\pm 2.388 799$ | 1 | $a4$ |
| $\pm 2.393 444$ | 2 | |
| $\pm 2.403 669$ | 1 | |
| $\pm 2.413 500$ | 2 | |
| $\pm 2.438 435$ | 2 | |
The classification of the growing states are identified by three types of sequences of the degeneracy of the energy levels in table 2, as explained in section 3.1. As for the \( a \)-states, the degree of degeneracy increases in accordance with the sequence \( D_g \) of the degeneracy in table 2 as \( g \) proceeds. For example, the \( a_2 \)-states, starting with \( s = 2 \), constitute 2 levels at \( E = \pm 1.000 \ 000 \), the degeneracy \( D = 1 \) when \( g = 2 \), \( D = 4 \) when \( g = 3 \), \( D = 13 \) when \( g = 4 \), and so on. The \( a_3 \)-states (\( s = 3 \)) constitute 4 levels at \( E = \pm 1.543 \ 362 \) and \( \pm 2.148 \ 961 \), \( D = 1, 4, 13 \) for \( g = 3, 4, 5 \), respectively. The degeneracy of the \( b \)-states increases along the sequence \( D_b \) in table 2 as \( g \) proceeds. The \( b_3 \)-states (\( s = 3 \)) constitute 2 levels at \( E = \pm 1.732 \ 051 \), \( D = 3, 12, 39 \) for \( g = 3, 4, 5 \), respectively. The \( b_4 \)-states (\( s = 4 \)) constitute 4 levels at \( E = \pm 1.302 \ 776 \) and \( \pm 2.302 \ 776 \), \( D = 3, 12 \) for \( g = 4, 5 \), respectively. The \( c \)-states are nothing but the \( c_1 \)-states whose degeneracy obeys the sequence \( D_c \) in table 2. The energy levels with no label in table 1 belong to the temporary states.

The density of states (DOS) or energy spectrum, which is constituted of energy levels and their degeneracy, obtained by numerical calculations for the fractal clusters is shown in figure 2. This figure shows how the spectrum develops as the generation \( g \) proceeds. The spectrum preserves a shape that is symmetric with respect to \( E = 0 \), at which the energy level of the \( c \)-states is always located. However, the symmetric shape itself is not significant here as it depends on the tight-binding scheme used, that is, whether it has an orthogonal or non-orthogonal form. The DOS for \( g = 8 \) spreads almost from \(-\sqrt{6}\) to \(\sqrt{6}\), which is the limiting value when \( g \rightarrow \infty \), as explained in section 3.3. As \( g \) proceeds, the growing states become dominant in the DOS, while the contribution of the temporary states gradually disappears, and hence it is the former that characterizes the DOS. Thus, we focus on the structure of the energy levels of the growing states which resembles a Cantor-like structure.

### 3.1. Degeneracy of growing states

We consider the degeneracy of the growing states, which are regarded as intrinsic to the fractal clusters. In table 2, the degeneracy \( D \) of the energy levels for the \( a \)-, \( b \)-, and \( c \)-growing states is listed as a function of the age of the states, \( h (= g - s) \). All the data except for those in parenthesis were obtained from numerical calculations. It is observed that there is a correlation between \( D \) and \( h \). Namely, \( D \) obeys the following recurrence relation:

\[
D(h) = \alpha D(h - 1) + \gamma = \left(D(0) + \frac{\gamma}{\alpha - 1}\right)\alpha^h - \frac{\gamma}{\alpha - 1}.
\]  

### Table 1.
(Continued.)

| \( g = 5 \) | \( E \) | \( D \) |
|---|---|---|
| 0.000 000 | 123 | \( c_1 \) |
| \( \pm 1.000 \ 000 \) | 40 | \( a_2 \) |
| \( \pm 1.069 \ 377 \) | 3 | \( b_5 \) |
| \( \pm 1.137 \ 382 \) | 4 | \( a_4 \) |
| \( \pm 1.302 \ 776 \) | 12 | \( b_4 \) |
| \( \pm 1.370 \ 280 \) | 4 | \( a_4 \) |
| \( \pm 1.450 \ 714 \) | 3 | \( b_5 \) |
| \( \pm 1.543 \ 362 \) | 13 | \( a_3 \) |
| \( \pm 1.732 \ 051 \) | 39 | \( b_3 \) |
| \( \pm 2.148 \ 961 \) | 13 | \( a_3 \) |
| \( \pm 2.212 \ 562 \) | 3 | \( b_5 \) |
| \( \pm 2.263 \ 257 \) | 4 | \( a_4 \) |
| \( \pm 2.302 \ 776 \) | 12 | \( b_4 \) |
| \( \pm 2.388 \ 799 \) | 4 | \( a_4 \) |
| \( \pm 2.420 \ 007 \) | 3 | \( b_5 \) |
| (16 levels) | 1 | \( a_5 \) |

### Table 2.
Three types of sequences for the degeneracy \( D \) of growing states, where \( h = g - s \). The values in parenthesis are estimated by equations (7) or (6).

| \( h \) | 0 | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|---|
| \( D_a \) | 1 | 4 | 13 | 40 | 121 | 364 | 1093 | (3280) |
| \( D_b \) | 3 | 12 | 39 | 120 | 363 | 1092 | (3279) | (9840) |
| \( D_c \) | 3 | 6 | 15 | 42 | 123 | 366 | 1095 | 3282 |
By applying this relation to the data in Table 3, \( D(h) \) for the energy levels of the \( a \)-, \( b \)-, and \( c \)-states are obtained:

\[
D_a(h) = \frac{1}{2}(3^{h+1} - 1) = D_b(h - 1) + 1, \quad (5)
\]

\[
D_b(h) = \frac{1}{2}(3^{h+2} - 3) = D_c(h + 1) - 1. \quad (6)
\]

\[
D_c(h) = \frac{1}{2}(3^{h+1} + 3) = \frac{1}{5}N(g) + \frac{6}{5}. \quad (7)
\]

The sequences for the degeneracy of the \( a \)- and \( b \)-states resemble each other while their energy positions are obviously different.

Figure 2. Densities of states obtained by numerical calculations for the fractal clusters. The leading energy levels of the growing states are indicated by the same labels as those used in Table 1. The energy is measured in units of the nearest-neighbor hopping energy from the on-site energy.
3.2. Number of states

Figure 3 shows contributions of the growing states to the total states as a function of $g$. The contribution of the growing states increases, while that of the temporary states decreases, as $g$ proceeds. These results, which are based on numerical calculations, are interpreted analytically as follows.

First, we consider the number of energy levels of the growing states. The number of energy levels of $c$-states is always $M_c = 1$ since the $c$-states appear only at $E = 0$. The number of energy levels of type $a$- and $b$-states increases as $g$ proceeds, because new levels of these types appear in each generation. The number of new levels is twice as large as that of the previous generation cluster. For example, the number of $a_2$ levels is $2^2 = 4$, and those of $a_3$ and $a_4$ are 4 and 8, respectively, as seen in table 1. Thus, the numbers of new levels of $a$- and $b$-states in the $s$-th generation cluster can be expressed as

$$M_a(s) = 2M_a(s-1) = 2^{s-2}M_a(2) = 2^{s-1},$$

$$M_b(s) = 2M_b(s-1) = 2^{s-3}M_b(3) = 2^{s-2}.$$  

The total number of levels of the growing states is

$$M_g(s) = \sum_{s=2}^g M_a(s) + \sum_{s=3}^g M_b(s) + M_c = 3 \cdot 2^{s-1} - 3.$$  

Next, we calculate the number of growing states, which is given by the product of the number of levels and the degree of degeneracy. The total number of growing states $N_g(g)$ is

$$N_g(g) = M_g(g) \times (g+1).$$

Table 3. Specifications for three types of growing states for the $g$-th generation fractal cluster.

| Type | Parametersa | Number of energy levels | Number of states | Ratio ($g \to \infty$) | Energy position |
|------|-------------|-------------------------|-----------------|------------------------|----------------|
| $a$  | $s \geq 2$  | $D(0)$ $\gamma$ $\lambda$ $\eta$ | $2^s - 2$         | equation (13)  | $2/5$ equation (18) |
| $b$  | $s \geq 3$  | $3$ $3$ $3$ $3$         | $2^{s-1} - 2$    | equation (14)  | $2/5$ equation (18) |
| $c$  | $s = 1$     | $3$ $-3$ $0$ $0$        | $1$             | equation (15)  | $1/5$ 0          |
| Total|             |                         | $3(2^{s-1} - 1)$ | equation (12)  | 1                |

Note.

a See text.

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since the $c$-states appear only at $E = 0$. The number of energy levels of type $a$- and $b$-states increases as $g$ proceeds, because new levels of these types appear in each generation. The number of new levels is twice as large as that of the previous generation cluster. For example, the number of $a_2$ levels is $2(E = \pm 1)$, and those of $a_3$ and $a_4$ are 4 and 8, respectively, as seen in table 1. Thus, the numbers of new levels of $a$- and $b$-states in the $s$-th generation cluster can be expressed as

$$M_a(s) = 2M_a(s-1) = 2^{s-2}M_a(2) = 2^{s-1},$$

$$M_b(s) = 2M_b(s-1) = 2^{s-3}M_b(3) = 2^{s-2}.$$  

The total number of levels of the growing states is

$$M_g(g) = \sum_{s=2}^g M_a(s) + \sum_{s=3}^g M_b(s) + M_c = 3 \cdot 2^{s-1} - 3.$$  

Next, we calculate the number of growing states, which is given by the product of the number of levels and the degree of degeneracy. The total number of growing states $N_g(g)$ is

$$N_g(g) = M_g(g) \times (g+1).$$

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| Type | Parametersa | Number of energy levels | Number of states | Ratio ($g \to \infty$) | Energy position |
|------|-------------|-------------------------|-----------------|------------------------|----------------|
| $a$  | $s \geq 2$  | $D(0)$ $\gamma$ $\lambda$ $\eta$ | $2^s - 2$         | equation (13)  | $2/5$ equation (18) |
| $b$  | $s \geq 3$  | $3$ $3$ $3$ $3$         | $2^{s-1} - 2$    | equation (14)  | $2/5$ equation (18) |
| $c$  | $s = 1$     | $3$ $-3$ $0$ $0$        | $1$             | equation (15)  | $1/5$ 0          |
| Total|             |                         | $3(2^{s-1} - 1)$ | equation (12)  | 1                |

Note.

a See text.
\[ N_s(g) = N_a(g) + N_b(g) + N_c(g) \]
\[ = \frac{5}{2} \cdot 3^g - 5 \cdot 2^s + \frac{11}{2} = N(g) - (5 \cdot 2^s - 4), \]
where \( N_a(g), N_b(g), \) and \( N_c(g) \) are the numbers of \( a, b, \) and \( c \)-states, respectively:
\[ N_a(g) = \sum_{s=2}^{g} M_a(s)D_s(g - s) \]
\[ = 3^g - 2^{s+1} + 1 = \frac{2}{5}N(g) - 2^{s+1} + \frac{2}{5}, \]
\[ N_b(g) = \sum_{s=3}^{g} M_b(s)D_b(g - s) \]
\[ = 3^g - 3 \cdot 2^s + 3 = \frac{2}{5}N(g) - 3 \cdot 2^s + \frac{12}{5}, \]
\[ N_c(g) = M_cD_c(g - 1) \]
\[ = \frac{1}{2} \cdot 3^g + \frac{3}{2} = \frac{1}{5}N(g) + \frac{6}{5}. \]
The number of temporary states \( N_t(g) \) is obtained from equation (12) as
\[ N_t(g) = N(g) - N_b(g) = 5 \cdot 2^s - 4. \]

The contribution of all the growing states in the limit \( g \to \infty \) is \( N_t(g) / N(g) \to 1. \) The change of the contribution ratios with the generation growth agrees with the result shown in figure 3. The contribution of the temporary states is
\[ N_t(g) \sim \left( \frac{2}{3} \right)^g \left\{ 2 - \frac{8}{5} \left( \frac{1}{2} \right)^g - \frac{6}{5} \left( \frac{1}{3} \right)^g \right\} \to 0 \quad (g \to \infty). \]

Consequently, all the states of the fractal cluster are occupied by the growing states in the large size limit of the cluster: the \( a, b, \) and \( c \)-states occupy \( 2/5, 2/5, \) and \( 1/5 \) of the total states, respectively, and the \( a \)- and \( b \)-states are divided in half on the lower and higher energy sides of \( E = 0. \)

### 3.3. Energies of growing states

The energy levels of the \( c \)-states are always located at \( E = 0, \) as we already mentioned. The energies of the \( a \) - and \( b \)-states are not known explicitly except for \( E = \pm 1 \) for \( s = 2 \) and \( \pm \sqrt{3} \) for \( s = 3, \) though they can be numerically obtained with a limitation. Thus, we examined whether the energies could be expressed in an analytical form and were able to determine the analytical form.

The energies of the \( a \) - and \( b \)-states for \( s > s_0 \) can be represented in the form of nested square roots as follows:
\[ E_s(p) = \pm \sqrt{\sqrt{\ldots \sqrt{\pm \sqrt{\pm \ldots + \lambda}}}}, \]
where \( p = 7/2, q = 1/4, \) and \( r = p + q = 15/4, \) and \( \lambda = 1 \) \( (\pm \sqrt{3}) = a \)-states and \( \lambda = 3 \) \( (\pm \sqrt{5}) = c \)-states. Clearly, the energy levels \( E = \pm 1 \) and \( \pm \sqrt{3} \) are given by \( E_3(s) = \pm \sqrt{\lambda}. \) The plus-minus signs in equation (18) give different energy levels, in accord with equations (9) and (10). For example, the number of energy levels for the \( a3 \) growing states is \( M_a(3) = 4, \) so that \( E_3(3) = \pm \sqrt{(7 \pm \sqrt{5})/2} (= \pm 1.543 362 \) and \( \pm 2.148 961) \) is obtained. We confirmed 128 energy levels for \( a8 \)-states and 64 levels for \( b8 \)-states in the 8th generation cluster, e.g. \( E_1(8) = \pm 1.000 238, \) \( \pm 2.449 392, \) and \( E_1(8) = \pm 1.000 578, \) \( \pm 2.449 254, \) and so on. The maximum and minimum energies \( E(\infty) \) for \( g \to \infty \) are obtained when every plus-minus sign within the square root nesting infinitely in equation (18) takes a + sign:
\[ E(\infty) = \pm \sqrt{p + \sqrt{r + \sqrt{r + \sqrt{r + \ldots}}}} = \pm \sqrt{p + \phi_{(+)}(r)} = \pm \sqrt{6}, \]
where \( \phi_{(+)}(r) = 5/2 \) is derived from the mathematical function defined in the appendix.

Using a simple relation wherein the two constants \( p \) and \( q \) in equation (18) originate from a constant \( \eta = \alpha \) \( (= 3) \) and the function \( \phi_{(\pm)}(x) \) in the appendix, that is, \( p \pm \sqrt{q + \lambda} = \phi_{(\pm)}(\lambda) + \eta, \) we can rewrite equation (18) into the following iterative form:
\[ E_s(p) = \pm \sqrt{\sqrt{\ldots \sqrt{\phi_{(\pm)}(\ldots \phi_{(\pm)}(\phi_{(\pm)}(\sqrt{\pm \sqrt{\lambda} + \eta} + \eta \ldots + \eta) + \eta + \eta)}}}}, \]
where \( \phi_{(\pm)}(x) \) is either \( \phi_{(+)}(x) \) or \( \phi_{(-)}(x). \) Each of the energy levels is determined by the choice of the \( s-s_0 + 1 \) plus-minus sign in the equation.
By defining a function

\[ R_{\pm}(x) = \phi_{\pm}(x) + \eta \]  \hspace{1cm} (21)

and for a sequence of \( h \) signs,

\[ \sigma = (\sigma_1, \sigma_2, \ldots, \sigma_{h-1}, \sigma_h), \]  \hspace{1cm} (22)

where \( \sigma \) is either + or −, we can universalize equation (20) in an iterative form as follows:

\[ E_{h}(\sigma) = \begin{cases} \pm \sqrt{R_{\sigma_1}(\lambda) R_{\sigma_{h-1}}(\lambda) \cdots R_{\sigma_1}(\lambda)} & (h \geq 1) \\ \pm \sqrt{\lambda} & (h = 0) \end{cases} \]  \hspace{1cm} (23)

Of course, the infinite-size fractal cluster has all the energy levels from \( h = 0 \) to \( h \to \infty \). Because the inverse of equation (23) is \( R^{-1}(\lambda) \equiv (x - \eta)(x - \eta - 1) = (x - p)^2 - q \) (see appendix), a kind of affine self-similarity holds for the DOSs transformed by both iteratively applying the inverse function \( R^{-1}(\lambda) \) with the energy squared \( x = E^2 \) and scaling the number of states. An example is shown in figure 4, where \( E^2 \) and \( R^{-1}(E^2) \) are taken as abscissa axes, and the longitudinal axes differ by a factor of 1/3 owing to equations (5) and (6). In such a representation of the DOS, \( \varphi_{\pm}(\lambda) \) can be found in the distances between the energy levels, namely the golden ratio \( \tau_1 \) and \( \tau_3 \) in the appendix. Interestingly, the geometrical self-similarity of the fractal cluster appears as mathematical self-similarity of the recursion structure on the energy.

Figure 4. Example of self-affinity found in the DOS, plotted against \( E^2 \) (upper) and \( (E^2 - p)^2 - q \) (lower), for the 8th fractal cluster. See text for details. The separations between the major energy levels are related to \( \tau_1 \) or \( \tau_3 \) (see appendix).
4. Discussion

First, we focus on the characteristics of the energy levels of the growing states. It is already known that the energy obtained from the quadratic mapping Hamiltonian for a one-dimensional chain of inhomogeneous harmonic oscillators [13–16] is described by

\[
E = \pm \sqrt{\eta \pm \sqrt{\eta \pm \cdots}},
\]

where \(\eta\) is a constant. In comparison with equations (20) or (21), the infinitely nested square root function \(\varphi_{(\pm)}(x)\) is missing in equation (24). Therefore, we consider that the fractal structure or the fractal dimension of the cluster model is reflected in the existence of \(\varphi_{(\pm)}(x)\). The energy levels expressed by equation (23), which involves a multi-nested form of the function \(R_{(\pm),\lambda}(\lambda)\) containing \(\varphi_{(\pm),\lambda}(\lambda)\), are characterized by the constants \(\lambda = 1, 3, 0\), which correspond to the \(a\)-, \(b\)-, and \(c\)-states, respectively. With respect to \(E = 0\), the energy can be regarded as \(E = \varphi_{(\cdots),0}(0)\) or equation (23) with \(\eta = 0, \lambda = 0\), and \(\sigma = (-, -, \cdots, -)\) because the number of \(c\)-states is approximately half of the number of \(a\)- or \(b\)-states. However, there is another aspect of the \(c\)-states for \(E = 0\). It is known that clusters of graphene or AB bipartite lattices have zero-energy states due to a sublattice imbalance of \(N_A - N_B\) [17, 18]. This relation can be confirmed in the \(n\)-th generation fractal cluster of the model, that is, \(N_i(g) = N_i(g) - N_0(g)\) where \(N_i(g)\) is the number of \(c\)-states given by equation (15), and the number of \(A\)- and \(B\)-sublattice sites is \(N_i(g) = \frac{2}{3}(3^g + 1)\) and \(N_0(g) = 3^g\).

In fact, provided that the fractal clusters are made of carbon atoms and the \(\pi\)-electron approximation applies, the model can be considered as a triangular cluster of graphene containing vacancies. If the energies of the fractal cluster are mapped in the graphene Brillouin zone, \(E = 0\) corresponds to the K-points, \(E = \pm 1\) of the \(a\)-states, growing states corresponds to a straight contour line through the M-point, and \(E = \pm 3\) is at the \(\Gamma\)-point. Therefore, in the fractal cluster, there are a number of energy regions where no states exist, while states exist in the area around the \(\Gamma\)-point. The region \(\sqrt{3} < |E| < (7 + \sqrt{5})/2\) corresponds to the annular area around the \(\Gamma\)-point. Finally, we discuss the existence of energy states from the perspective of set theory. We consider again the \(c\)-states can be written as follows:

\[
\lim_{g \to \infty} \frac{N_i(g)}{N(g)} = \lim_{g \to \infty} \sum_{i=0}^{g} M_i(s) \frac{D_i(g-s)}{N(g)}
\]

\[
= \sum_{i=1}^{\infty} \frac{1}{2} \left(\frac{2}{3}\right)^{s-2} = 2 \left(\frac{1}{3} + \frac{2}{3^2} + \frac{2^2}{3^3} + \cdots\right)
\]

\[
= \frac{2}{5} \cdot \mathcal{C},
\]

where \(\mathcal{C}\) denotes the so-called complement of the Cantor ternary set:

\[
\mathcal{C} = \left(\frac{1}{3}\right) + \left(\frac{1}{3}\right)^2 + \left(\frac{1}{3}\right)^3 + \cdots = \frac{1}{3} \sum_{n=0}^{\infty} \left(\frac{2}{3}\right)^n,
\]

where the geometric progression corresponds to the sum of the products of the measure and the number, which continuously increases as \(g\) (or \(s\) proceeds. This holds also for \(b\)-states. Thus, both the \(a\)- and \(b\)-states form complements of the Cantor ternary set, with a contribution ratio of 1/5 to both the lower and higher energy sides of the energy of the \(c\)-states (\(E = 0\)) in the normalized DOS. Let the total set for the energy states of the fractal cluster be written as follows:

\[
X + 2 \cdot \frac{2}{5} \cdot \mathcal{C} + \frac{1}{5} \cdot \mathcal{C} = 1,
\]

where the first term \(X\) in the left side corresponds to the set for the temporary state, the second term corresponds to the sets for the \(a\)- and \(b\)-states, and the last term to the set for \(c\)-states, provided that the \(c\)-states form the complementary set \(\mathcal{C}\). Directly, \(X = \mathcal{C}\) from equation (27) and consequently, it is considered that the temporary states form the Cantor ternary set formally. In fact, equation (17) contains the term corresponding to the Cantor ternary set:

\[
\mathcal{C} = 1 - \mathcal{C} = \lim_{g \to \infty} \left(\frac{2}{3}\right)^g,
\]
5. Conclusions

The energy spectrum of a fractal cluster model that forms a Sierpiński triangle on a hexagonal lattice is investigated by considering the self-similar structure. The energy states are classified into temporary states and growing states. The former, resulting from a temporary size or structure of the cluster, have little effect on the spectrum, while the latter, whose degeneracy increases with increasing size of the cluster, make up the characteristic profile of the spectrum. The growing states consist of three types characterized by a constant $\lambda$.

One is the zero-energy states corresponding to $\lambda = 0$, which are attributed to the hexagonal lattice structure. The others appear in sequence at different energies, reflecting the self-similar structure, as the cluster size grows. These states have energy levels expressible in a multi-nested form including the infinitely nested square root function of $\lambda = 1$ or 3.

Acknowledgments

The author is deeply grateful to Professor S Muramatsu and Professor K Ozeki for their valuable advice.

Appendix. Infinitely nested square root function

We consider the mathematical function that represents the golden ratio in the form of infinitely nested square roots. The function is defined by

$$\phi_{++}(x) = \sqrt{x + \sqrt{x + \sqrt{x + \sqrt{x + \cdots}}} = \frac{1 + \sqrt{1 + 4x}}{2} = \tau_x$$  \hspace{1cm} (A.1)

or

$$\phi_{--}(x) = -\sqrt{-x - \sqrt{-x - \sqrt{-x - \sqrt{-x - \cdots}}} = \frac{1 - \sqrt{1 + 4x}}{2} = 1 - \tau_x,$$  \hspace{1cm} (A.2)

for $x > 0$. These are solutions of the equation $\phi^2 - \phi - x = 0$. It is important that $\phi_{++}(x) = y$ for $x = y(y - 1)$. Of course, $\tau_1 = \phi_{++}(1) = (1 + \sqrt{5})/2$ is the golden ratio. Further, $\tau_2 = \phi_{++}(2) = 2$, $\tau_3 = \phi_{++}(3) = (1 + \sqrt{13})/2$, and so on.

ORCID iDs

H Yorikawa  https://orcid.org/0000-0001-5181-618X

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