On the matching properties of three fence graphs

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Supplementing the construction of a Möbius ladder graph derived from a ladder graph, the linear fence graph and cyclic fence graph are introduced. These have neater mathematical expressions for the perfect matching numbers and the matching and characteristic polynomials than the graphs in the previous families.

1. Introduction

It is well known [1] that *ladder graphs* are defined as $P_2 \times P_n$ and *prisms* (cyclic ladder graphs) as $P_2 \times C_n$. Following the notation of ref. [1], P_n is the path and C_n the cycle of order n nodes. One defines a *Möbius ladder graph* as in fig. 1

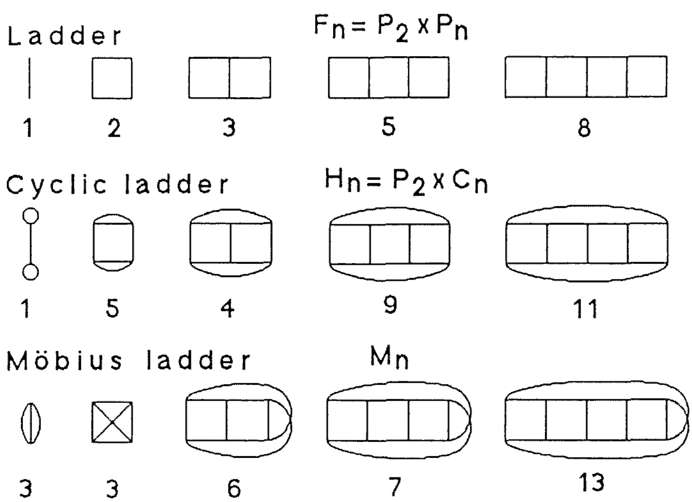

Fig. 1. Conventional definitions of ladder, prism, and Möbius ladder graphs. Below each graph is its Kekulé number.

just by a physical twist of a cyclic ladder graph. Accordingly, several interesting mathematical features including the crossing number have been discussed [2]. That this structure is a natural phenomenon can be supported by the existence of chemical compounds corresponding to the Möbius ladder graphs [3,4]. For another chemical reason, the prism or cyclic ladder graph has been called the *Hückel ladder graph* [5].

From a graph-theoretic point of view, the *Kekulé number* (or the number of perfect matchings or 1-factors) for these families of graphs presents an interesting question. One of us (HH) has enumerated the Kekulé numbers for many series of graphs by proposing the topological index, and found their interesting mathematical properties [5–11]. Based on these results, it was found that the two series of Hückel ladder and Möbius ladder graphs are entangled with each other [5]. Our present purpose is to introduce the fence graph, cyclic fence graph, and Möbius-cyclic fence graph to disentangle the vexing properties of the previous families of graphs.

2. Perfect matching numbers

All the graphs treated here have at least one 1-factor or perfect matching. Hence, they have been called *Kekuléan* [12]. In fig. 1, the Kekuléan numbers of the displayed graphs are given. As is well known, the perfect matching numbers for the ladder (or fence) graphs form the Fibonacci numbers [9],

$$F_n = F_{n-1} + F_{n-2}, \qquad (n \geq 2) \tag{1}$$

$$F_1 = 1 \text{ and } F_2 = 2.$$

It is very well known that F_n can be expressed explicity as

$$F_n = (A^{n+1} - B^{n+1})/\sqrt{5}, \tag{2}$$

with $A = (1+\sqrt{5})/2$ and $B = (1-\sqrt{5})/2$. Denoting the shift-up operator of F_n by $\hat{A}$ [8], we have

$$\hat{A}F_n = F_{n+1}. \tag{3}$$

Equation (1) can be expressed by an operator polynomial as

$$\hat{A}^2 - \hat{A} - 1 = 0, \tag{4}$$

whose zeros are A and B.

On the other hand, the 1-factors (or perfect matching numbers or Kekulé numbers) $f_1(\mathrm{H}_n)$ and $f_1(\mathrm{M}_n)$, respectively, of the Hückel ladder H_n and Möbius ladder M_n graphs can be expressed by

$$f_1(\mathrm{H}_n) = A^n + B^n + 1 + (-1)^n \tag{5}$$

and

$$f_1(\mathrm{M}_n) = A^n + B^n + 1 - (-1)^n, \tag{6}$$

which are derived by using the zeros of the common operator polynomials for the two series of graphs:

$$\hat{A}^4 - \hat{A}^3 - 2\hat{A}^2 + \hat{A} + 1 = (\hat{A}^2 - 1)(\hat{A}^2 - \hat{A} - 1) = 0. \tag{7}$$

The expressions of eqs. (5)–(7) are rather awkward. This might be due to the fact that the graphs in each of the two series H_n and M_n are alternately bipartite and nonbipartite.

For this reason, we now rearrange the two families of graphs alternately to obtain two new series of graphs E_n and L_n, as shown in fig. 2. Now the new families E_n and L_n are, respectively, bipartite and nonbipartite. A graph with a loop such as

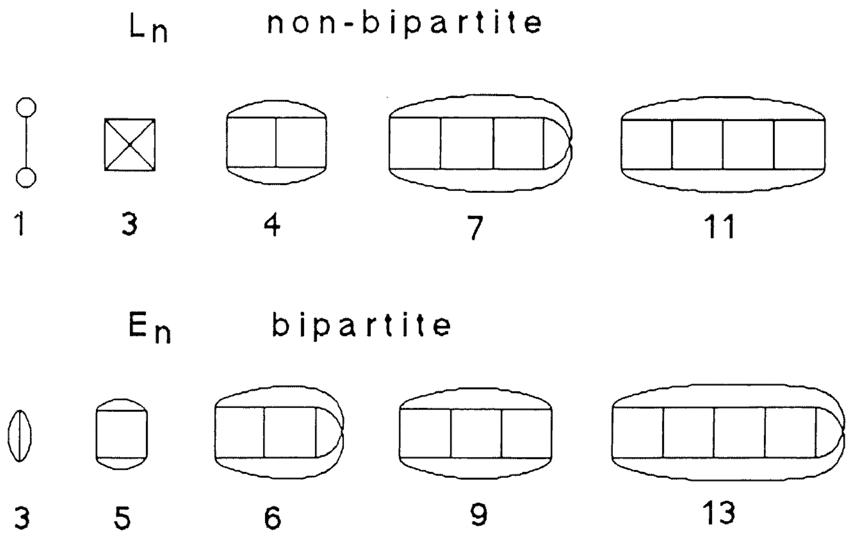

Fig. 2. Alternate interchange of H_n and M_n ladder graphs gives the nonbipartite L_n and bipartite E_n families.

L_1 is considered nonbipartite, since a loop is interpreted as an edge joining two nodes belonging to the same class (starred or unstarred). It is straightforward that the Kekulé numbers of L_n, $f_1(L_n)$, form the Lucas numbers

$$f_1(L_n) = f_1(L_{n-1}) + f_1(L_{n-2}), \tag{8}$$

$$f_1(L_1) = 1 \text{ and } f_1(L_2) = 3$$

and that

$$f_1(E_n) = f_1(L_n) + 2 \text{ (for all positive integers } n). \tag{9}$$

3. Definitions of fence graphs

Now the three series of graphs in figs. 1 and 2 can be redrawn as shown in figs. 3(a)–(c). The linear ladder graph F_n may be called the *linear fence graph*, while E_n and L_n may be called the *cyclic fence graph* and the *Möbius-cyclic fence graph*, respectively. It is clear that the definitions of these two graphs, the linear

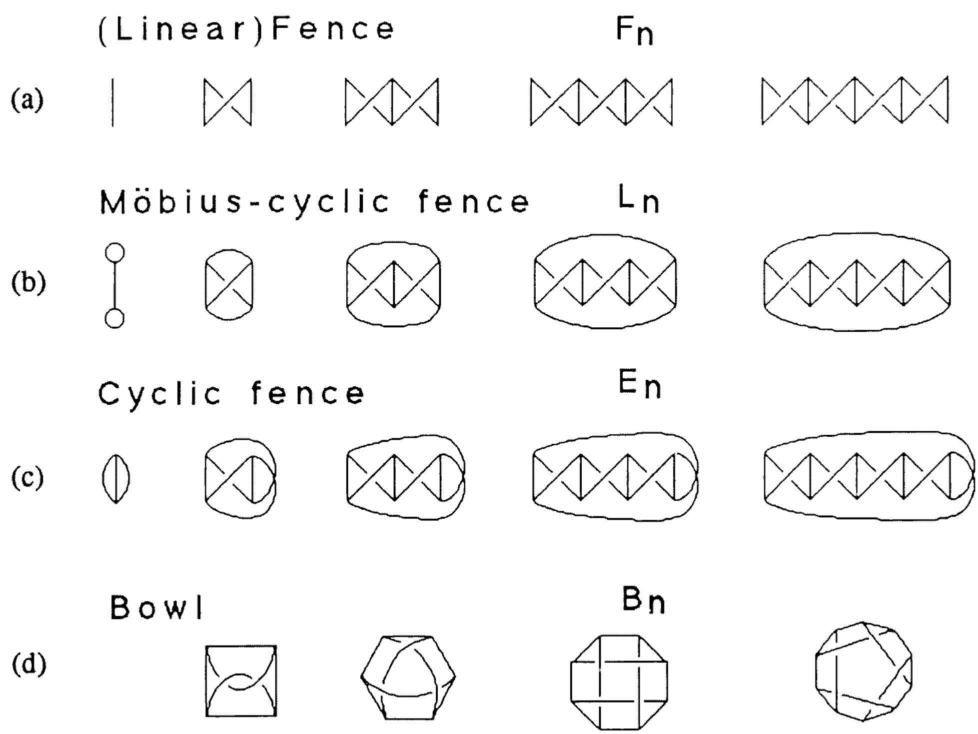

Fig. 3. Three families of fence graphs F_n, L_n, and E_n. The cyclic fence graph E_n is also the bowl graph B_n.

fence F_n and the cyclic fence graphs E_n, are natural, both being bipartite and with a simple perfect matching number expression. Note that the perfect matching numbers of F_n are Fibonacci numbers as expressed by eq. (1) or (2). Further, the cyclic fence graph can be drawn as in fig. 3(d) and may be called *bowl graphs*, B_n, because of their appearance. Incidentally, $B_4 = E_4 = Q_3$ (cube graph). We already know that $B_3 = E_3 = K_{3,3}$ and $L_2 = K_4$.

4. Matching polynomials of fence graphs

The matching polynomials $\alpha_G(x)$ of the fence graphs are fully discussed elsewhere [9]. Table 1 gives the matching polynomials of the smaller members of

Table 1

The matching polynomials of cyclic and Möbius-cyclic fence graphs

n	$E_n(x)$ / $L_n(x)$	Z_G
1	$x^2 - \begin{cases} 3 \\ 1 \end{cases}$	4 2
2	$x^4 - 6x^2 + \begin{cases} 5 \\ 3 \end{cases}$	12 10
3	$x^6 - 9x^4 + 18x^2 - \begin{cases} 6 \\ 4 \end{cases}$	34 32
4	$x^8 - 12x^6 + 42x^4 - 44x^2 + \begin{cases} 9 \\ 7 \end{cases}$	108 106
5	$x^{10} - 15x^8 + 75x^6 - 145x^4 + 95x^2 - \begin{cases} 13 \\ 11 \end{cases}$	344 342

cyclic fence and Möbius-cyclic fence graphs. By using the operator technique [8,9], the following recursion formula is obtained for the matching polynomials of both E_n and L_n [5]:

$$\hat{O}^4 - (x^2-3)\hat{O}^3 + 2\hat{O}^2 + (x^2-1)\hat{O} - 1 = 0, \tag{10}$$

where the operator $\hat{O}$ is defined to shift-up the matching polynomial $\alpha_n(x)$ of the nth member to that of the next member:

$$\hat{O}\alpha_n(x) = \alpha_{n+1}(x). \tag{11}$$

The operator polynomial for the matching polynomial of the graphs F_n has already been obtained in ref. [9]:

$$\hat{O}^3 - (x^2-2)\hat{O}^2 + x^2\hat{O} - 1 = 0. \tag{12}$$

Note that eq. (10) may be factored as the product of $(\hat{O}+1)$ with the polynomial in eq. (12). Since the *topological index* Z_G [6,7] of a graph G which is composed of N points and whose matching polynomial is expressed as $\alpha_G(x)$ is defined as

$$Z_G = \mathrm{i}^N \alpha_G(\mathrm{i}) \quad (\mathrm{i}^2 = -1), \tag{13}$$

the operator polynomial for the topological index of the series of graphs F_n is given by

$$\hat{A}^3 - 3\hat{A}^2 - \hat{A} + 1 = 0 \tag{14}$$

and that for both series E_n and L_n is

$$\hat{A}^4 - 4\hat{A}^3 + 2\hat{A}^2 + 2\hat{A} - 1 = (\hat{A} - 1)(\hat{A}^3 - 3\hat{A}^2 - \hat{A} + 1) = 0. \tag{15}$$

Note that eqs. (14) and (15) are, respectively, derived by putting $\hat{O} \to -\hat{A}$ and $x \to \mathrm{i}$ into eqs. (12) and (10).

5. Characteristic polynomials of cyclic fence graphs

Among the three series of graphs F_n, L_n, and E_n, only the cyclic fence graph E_n has cyclic symmetry. Thus, its characteristic polynomial can be factored systematically [5] by a standard technique in solid state physics [13,14] as

$$E_n(x) = \prod_{k=1}^{n} f_k, \tag{16}$$

where

$$f_k = x^2 - [1 + 2\cos(2k\pi/n)]^2.$$

The highly factored characteristic polynomials of the smaller members of the cyclic fence graphs are given in table 2. This property also supports the proposed definition of the cyclic fence graphs.

Table 2

Characteristic polynomials of the smaller members of the cyclic fence graph.

n	$E_n(x)$
1	(x^2-9)
2	$(x^2-1)(x^2-9)$
3	$x^4(x^2-9)$
4	$(x^2-1)^3(x^2-9)$
5	$(x^2-9)(x^4-3x^2+1)^2$
6	$x^4(x^2-1)(x^2-4)^2(x^2-9)$

From the structure of eq. (16), one can conclude that the characteristic polynomials $E_n(x)$ of the cyclic fence graphs E_n (n = 1, 2, 3, 4, and 6) are all integers and no other member of this family has this property.

Factorizability of the characteristic polynomial of a given graph is important in the discussion of the electronic properties of the corresponding conjugated molecule. Although no real molecule exists corresponding to the three series of fence graphs in fig. 3, the F_n and E_n families are known to be important in the discussion of the infinitely large conjugated hydrocarbon polymer networks [14,15].

6. Iso-Kekuléan graph

It is obvious that replacing any edge P_2 by the longer path P_4 does not change the perfect matching number (see fig. 4). By definition, two graphs are *iso-Kekuléan* if they have the same Kekulé number. By using this strategy, one can construct from

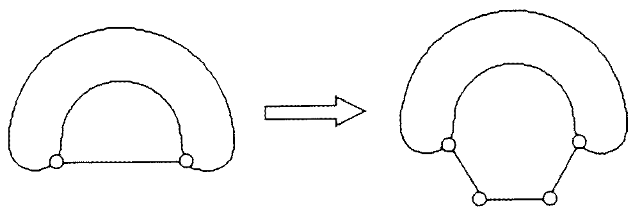

Fig. 4. Substitution of an edge does not affect the number of perfect matchings.

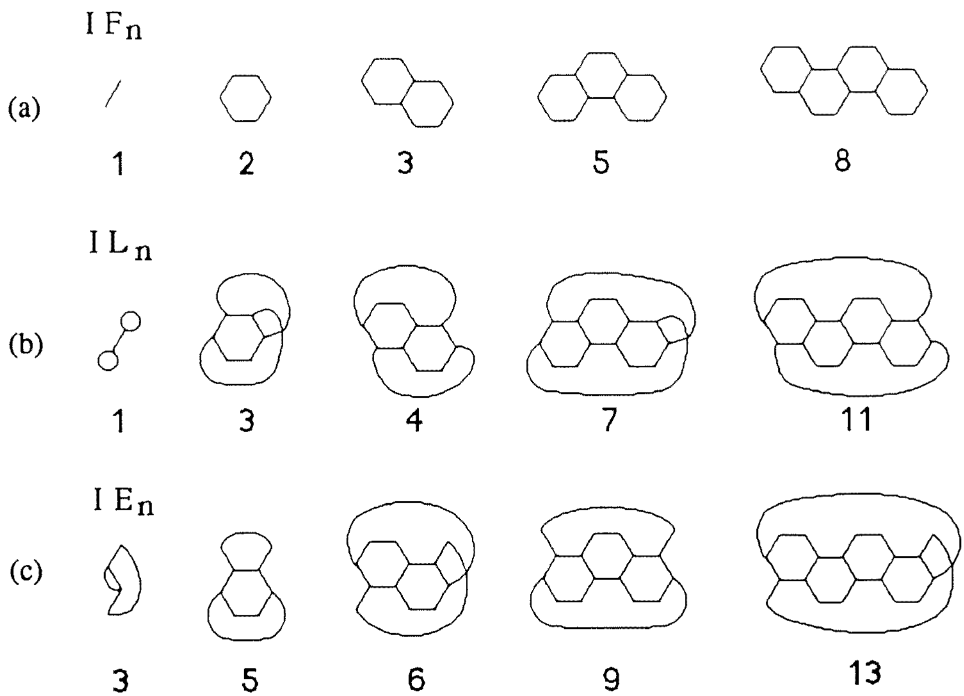

Fig. 5. Three families of graphs iso-Kekuléan to the graphs in fig. 3.

a given graph as many iso-Kekuléan graphs as one wishes. Figures 5(a)–(c) give examples of the three series of graphs IF_n, IL_n, and IE_n, respectively, iso-Kekuléan with the three different fence graphs F_n, L_n, and E_n in fig. 3. The IF_n series, called *zigzag polyacenes* [8], form one of the typical families of polyhex graphs, and have been shown to have Kekulé numbers in the Fibonacci sequences. No real hydrocarbon molecule exists corresponding to the cyclic benzenoid graphs IL_n and IE_n. However, the hypothetical molecular graphs IE_n have been shown to be important when one considers the density of states of infinitely large zigzag polyacene networks IF_n [14]. Note that although any member of the linear IF_n has no $4n$-membered cycle, the cyclic counterpart IE_n has at least two $4n$-membered cycles. Since the IL_n series has at least two odd cycles, they are not polyhex graphs nor do they have any important role in theoretical chemistry.

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