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The Forcing Polynomial of Catacondensed Hexagonal Systems*

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Abstract

Klein and Randić defined the innate degree of freedom of a graph G as the sum of the forcing numbers (innate degree of freedom) of perfect matchings of graph G. In this paper, we propose the forcing polynomial of a graph as a counting polynomial for perfect matchings with the same forcing number, from which the perfect matching count and innate degree of freedom of the graph can be easily obtained. We give recursive expressions for the forcing polynomial of hexagonal chains, and general catacondensed hexagonal systems as well. In particular, explicit expressions of the forcing polynomial and asymptotic behavior of the innate degree of freedom for zigzag hexagonal chains are obtained.

1. Introduction

The idea of innate degree of freedom was inspired by some practical studies in chemistry and is related to the concept of forcing number in graph theory. Klein and Randić proposed the innate degree of freedom in a graph for the study of resonance structures [11]. The same concept appeared in [9] of Harary et al. using the name 'forcing number', with specific reference to hexagonal systems.

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Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A *perfect matching* (or *Kekulé structure*) M of G, is a set of independent edges of G covering all vertices of G. A *forcing set* S of M is a subset of M such that S is contained in no other perfect matchings of G. The *forcing number* (or *innate degree of freedom*) *of* M, denoted by $f(G,M)$, is the smallest cardinality over all forcing sets of M. The *innate degree of freedom of* G, denoted by $IDF(G)$, is the sum over the forcing numbers of all perfect matchings of G. An edge of G is called a *forcing edge* if it is contained in exactly one perfect matching of G [4]. The minimum and maximum values of $f(G,M)$ over all perfect matchings M of G are denoted by $f(G)$ and $F(G)$, respectively.

One of the most interesting classes of graphs from the chemical point of view is the class of *hexagonal systems* (2-connected finite plane graphs such that every interior face is a regular hexagon of side length one) [5], since they represent the carbon skeletons of benzenoid hydrocarbons. Klein and Randić [11] gave a computation for the innate degree of freedom of a zigzag hexagonal chain by the transfer matrix, and Hansen and Zheng [8] derived an explicit expression. Zhang and Li [22,23], and Hansen and Zheng [7] independently characterized hexagonal systems with a forcing edge. Zhang and Zhang [24] gave a novel computation for perfect matching count of this kind of graphs. Recently Xu et al. [19] showed that the maximum forcing number of a hexagonal system equals the Clar number.

For fullerenes, the distribution of innate degree of freedom of Kekulé structures of C_{60}, C_{70} and C_{72} have been computed (see [12, 14–16]). Zhang et al. [26] showed that every fullerene has the minimum forcing number at least three, Jiang and Zhang [10] showed that every boron-nitrogen fullerene has the minimum forcing number at least two, and Wang et al. [18] determined the minimum forcing number of toroidal fullerenes. In recent years, some related concepts were put forward, such as global forcing number [3, 6, 17, 25] and complete forcing number [20].

In this paper, we propose the forcing polynomial of a graph G as a counting polynomial for perfect matchings of G with the same forcing number. We will see that the number of perfect matchings of G equals the sum of all coefficients of the forcing polynomial, and the innate degree of freedom of G can be obtained from the derivative of its forcing polynomial. From the forcing polynomial we confirm directly the derivative property of the innate degree of freedom of a graph first discovered by Klein and Randić [11]. In

Sections 3 and 5, we derive recursive expressions of the forcing polynomial for hexagonal chains and catacondensed hexagonal systems respectively. As corollaries, we obtain recursive expressions for their innate degree of freedom [8]. In particular, in Section 4 we derive an explicit expression for the forcing polynomial of zigzag hexagonal chains Z_n (or fibonacenes), and obtain explicit expressions and asymptotic behavior for the innate degree of freedom of Z_n.

2. The definition of forcing polynomial

First recall some basic results on forcing set and forcing number of a perfect matching of a graph. Let G be a graph with a perfect matching M. A cycle of G is called M-*alternating* if its edges appear alternately in M and $E(G) \setminus M$.

Lemma 2.1. [1, 13] *Let G be a graph with a perfect matching M. A subset $S \subseteq M$ is a forcing set of M if and only if each M-alternating cycle of G contains at least one edge of S.*

Here we propose the forcing polynomial of a graph. The *forcing polynomial* of a graph G is defined as the following counting polynomial,

$$F(G,x) = \sum_{M \in \mathcal{M}(G)} x^{f(G,M)}, \tag{1}$$

where $\mathcal{M}(G)$ denotes the set of all perfect matchings of G.

Note that if G has no perfect matchings, then $F(G,x) = 0$; if G has a unique perfect matching M, then $F(G,x) = 1$ since M has the forcing number 0; if G is an empty graph (no vertices), we assume that $F(G,x) = 1$, since G can be considered to have a unique perfect matching $\emptyset$.

Lemma 2.2. *The forcing polynomial of a graph G can be expressed as*

$$F(G,x) = \sum_{i=f(G)}^{F(G)} w(G,i)x^i,$$

where $w(G,i)$ denotes the number of perfect matchings of G with forcing number i.

Lemma 2.2 factually gives an equivalent definition for the forcing polynomial of a graph G. In fact, we just classify $\mathcal{M}(G)$ according to forcing number. The following result shows that $F(G,x)$ can produce the perfect matching count and the innate degree of freedom of G.

Lemma 2.3. *The forcing polynomial of a graph G has the following properties*:
(*i*) $F(G,x)|_{x=1} = \Phi(G)$, *the perfect matching count of* G,
(*ii*) $\frac{\mathrm{d}}{\mathrm{d}x}F(G,x)|_{x=1} = IDF(G)$, *the innate degree of freedom of* G.

As an example, we consider a linear hexagonal chain L_n with n hexagons (see Fig. 1). It is well known that $\Phi(L_n) = n+1$, and each perfect matching has only one 'vertical' edge illustrated heavy in Fig. 1, which is a forcing edge. This implies that every perfect matching has forcing number 1, so

$$F(L_n, x) = (n+1)x.$$

As second example, we consider coronene (see Fig. 1). There are 6 symmetry non-equivalent structures among the 20 perfect matchings of coronene. We list them along with the equivalent perfect matching count and forcing number in Table 1, in which a minimum forcing set is illustrated with heavy edges. Thus

$$F(\text{Coronene}, x) = x^3 + 6x^3 + 6x^3 + 2x^3 + 3x^2 + 2x^2 = 15x^3 + 5x^2.$$

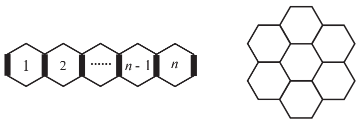
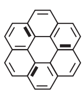
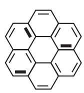
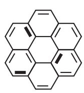
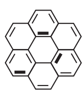
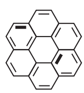
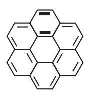


Fig. 1. Illustration of L_n (left) and coronene (right).

Table 1. Symmetry non-equivalent structures of coronene

symmetry non-equivalent structures						
structure counts	1	6	6	2	3	2
forcing numbers	3	3	3	3	2	2

In Refs. [12, 14, 16], the distributions of forcing numbers of perfect matchings for fullerenes C_{60}, C_{70} and C_{72} (see Fig. 2) were reported. These computation results can be expressed in the form of forcing polynomial as follows:

$$F(\mathrm{C}_{60},x) = x^{10} + 80x^9 + 2073x^8 + 4060x^7 + 3116x^6 + 3170x^5,$$
$$F(\mathrm{C}_{72},x) = x^{12}+100x^{11}+4096x^{10}+24037x^9+9196x^8+21604x^7+16809x^6+1557x^5.$$

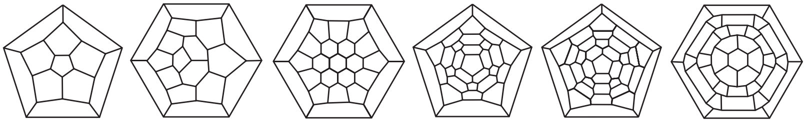


Fig. 2. Fullerenes C_{20}, C_{32}, C_{48}, C_{60}, C_{70} and C_{72} (from left to right).

Lately, Zeng [21] calculated some fullerene graphs as follows.

$$F(\mathrm{C}_{20},x) = 36x^3,\ F(\mathrm{C}_{32},x) = 30x^4 + 120x^3,$$
$$F(\mathrm{C}_{48},x) = x^7 + 244x^6 + 902x^5 + 519x^4,$$
$$F(\mathrm{C}_{70},x) = 32x^{11} + 680x^{10} + 4944x^9 + 12412x^8 + 18410x^7 + 13590x^6 + 2100x^5,$$

where the last one corrects the corresponding computation result in [12].

The following theorem shows that a disconnected graph can be partitioned into *components* (i.e. maximal connected subgraphs) to consider separately.

Theorem 2.4. *Let G be a graph with the components $G_1, G_2, \ldots, G_k$. Then*
(i) $F(G,x) = \prod_{i=1}^k F(G_i,x)$,
(ii) $IDF(G) = \sum_{i=1}^k IDF(G_i)\prod_{j=1,j\neq i}^k \Phi(G_j)$.

Proof. (*i*) If G has no perfect matchings, then the equality holds since both sides equal 0. So suppose that G has a perfect matching. From the definition it is evident that for each perfect matching M of G, a subset S of M is a forcing set of M if and only if the restriction of S on each component G_i is a forcing set of the restriction $M|_{G_i}$ of M on G_i, $i = 1, 2, \ldots, k$. Hence we can see that $f(G,M) = \sum_{i=1}^k f(G_i, M|_{G_i})$. These imply that

$$F(G,x) = \sum_{M\in\mathcal{M}(G)} x^{f(G,M)} = \sum_{M\in\mathcal{M}(G)} x^{\sum_{i=1}^k f(G_i,M|_{G_i})}$$
$$= \sum_{M_i\in\mathcal{M}(G_i),i=1,2,\ldots,k}\ \prod_{i=1}^k x^{f(G_i,M_i)} = \prod_{i=1}^k \sum_{M_i\in\mathcal{M}(G_i)} x^{f(G_i,M_i)} = \prod_{i=1}^k F(G_i,x).$$

(*ii*) Using Lemma 2.3, we can obtain

$$IDF(G) = \frac{\mathrm{d}}{\mathrm{d}x}F(G,x)|_{x=1} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\prod_{i=1}^{k}F(G_i,x)\right)\Bigg|_{x=1}$$
$$= \left(\sum_{i=1}^{k}\frac{\mathrm{d}}{\mathrm{d}x}F(G_i,x)\prod_{j=1,j\neq i}^{k}F(G_j,x)\right)\Bigg|_{x=1} = \sum_{i=1}^{k}IDF(G_i)\prod_{j=1,j\neq i}^{k}\Phi(G_j).$$

■

Now we generalize the theorem to a graph with elementary components. An edge of a graph G is *allowed* if it lies in some perfect matching of G, and *forbidden* otherwise. The subgraph of G formed by all the allowed edges may be disconnected and every component is called an *elementary component* of G. Then we have the following corollary.

Corollary 2.5. *Let G be a graph with a perfect matching and $G_1, G_2, \ldots, G_k$ the elementary components of G. Then*
(i) $F(G,x) = \prod_{i=1}^{k} F(G_i,x)$,
(ii) $IDF(G) = \sum_{i=1}^{k} IDF(G_i)\prod_{j=1,j\neq i}^{k}\Phi(G_j)$.

Proof. Let G' be the subgraph of G formed by its all allowed edges. That is, G' can be obtained from G by deleting all forbidden edges. For any perfect matching M of G, any forbidden edge of G does not belong to any M-alternating cycle of G. So $f(G,M) = f(G',M)$ from Lemma 2.1, which implies that $F(G,x) = F(G',x)$. Since G' has the components $G_1, G_2, \ldots, G_k$, the results follow immediately from Theorem 2.4. ■

In [11], Klein and Randić ever reported the second properties of Theorem 2.4 and Corollary 2.5, and revealed that $IDF(G)$ is derivative of $\Phi(G)$. We now show directly them by using the derivative of forcing polynomial and its multiplicative property.

3. Hexagonal chains

A hexagonal system is *catacondensed* if no three of its hexagons share a common vertex. Now we concentrate on *hexagonal chains*, i.e. non-branched catacondensed hexagonal systems, each hexagon of which is adjacent to at most two hexagons. Let H be a hexagonal chain possessing k maximal linear hexagonal chains with each no less than two hexagons (see Fig. 3), and in turn denote the numbers of hexagons of such maximal linear hexagonal chains by $r_1, r_2, \ldots, r_k$, for $r_i \geq 2,\ i = 1, 2, \ldots, k$. We use $Hl(r_1, r_2, \ldots, r_k)$ to denote such a hexagonal chain H [27]. For convenience, we make a convention that $Hl(r_1) = L_{r_1}$ and $Hl(r_1, r_2, \ldots, r_i, 1) = Hl(r_1, r_2, \ldots, r_i)$.

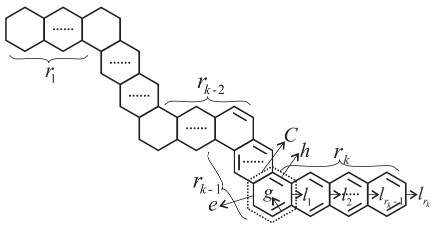


Fig. 3. Illustration of a hexagonal chain $Hl(r_1, r_2, \ldots, r_k)$.

For a perfect matching M of a graph G and an edge $e \in M$, let G_0 be the subgraph obtained from G by deleting e with the end vertices. If G_0 has a pendant edge (with an end of degree one), it must belong to M. From G_0 we delete recursively such pendant edges together with the ends with incident edges until the remaining graph has no pendant edges or is empty. Let G_e denote the remaining graph and M_e the set of pendant edges deleted. Then $M_e \subseteq M$ and M_e is *determined* by e.

Lemma 3.1. *Let G be a graph with a perfect matching M. If $e \in M$ is contained in a minimum forcing set of M, then*

$$f(G, M) = f(G_e, M|_{G_e}) + 1.$$

Proof. Let S be a minimum forcing set of M that contains e. It is obvious that every M-alternating cycle of G that does not contain e must be contained in G_e. By Lemma 2.1 this implies that $S \setminus \{e\}$ is a minimum forcing set of $M|_{G_e}$. ■

Theorem 3.2. *The forcing polynomial of a hexagonal chain $Hl(r_1, r_2, \ldots, r_k)$ $(r_i \geq 2,\ i = 1, 2, \ldots, k,\ k \geq 2)$ has the following recurrence relation:*

$$\begin{aligned} &F(Hl(r_1, r_2, \ldots, r_k), x) \\ =&F(Hl(r_1, r_2, \ldots, r_{k-2} - 1), x)x + r_k F(Hl(r_1, r_2, \ldots, r_{k-1} - 1), x)x, \end{aligned} \tag{2}$$

with initial conditions $F(Hl(r_1 - 1), x) = r_1 x$ and $F(Hl(r_0 - 1), x) = 1$.

Proof. Let e be the leftmost 'vertical' edge of the last maximal linear hexagonal chain. We classify $\mathcal{M}(Hl(r_1, r_2, \ldots, r_k))$ into two classes $\mathcal{M}_1 = \{M \in \mathcal{M}(Hl(r_1, r_2, \ldots, r_k)) \mid e \in$

$M\}$ and $\mathcal{M}_2 = \mathcal{M}(Hl(r_1, r_2, \ldots, r_k))\backslash\mathcal{M}_1$. In Fig. 3, we illustrate edges $e,\ g,\ h,\ l_1, \ldots, l_{r_k}$ and cycle C. Take any $M \in \mathcal{M}(Hl(r_1, r_2, \ldots, r_k))$.

Case 1. $e \in M$. Then $g,\ h \in M$. When $k = 2$, e is a forcing edge [23] and $|\mathcal{M}_1| = 1$. Then $\sum_{M\in\mathcal{M}_1} x^{f(Hl(r_1,r_2,\ldots,r_k),M)} = x$.

Let $k \geq 3$. By Lemma 2.1 every forcing set of M must contain at least one of the three edges e, g and h, since the hexagon C is M-alternating. And e lies in a minimum forcing set of M, since any M-alternating cycle containing g or h must contain e. In Fig. 3, we use double lines to mark the edges which e determines. So $Hl(r_1, r_2, \ldots, r_k)_e = Hl(r_1, r_2, \ldots, r_{k-2} - 1)$. By Lemma 3.1 we have

$$\sum_{M\in\mathcal{M}_1} x^{f(Hl(r_1,r_2,\ldots,r_k),M)} = \sum_{M\in\mathcal{M}_1} x^{f(Hl(r_1,r_2,\ldots,r_{k-2}-1),M|_{Hl(r_1,r_2,\ldots,r_{k-2}-1)})+1}$$
$$= \sum_{M\in\mathcal{M}(Hl(r_1,r_2,\ldots,r_{k-2}-1))} x^{f(Hl(r_1,r_2,\ldots,r_{k-2}-1),M)+1} = F(Hl(r_1, r_2, \ldots, r_{k-2} - 1), x)x.$$

Case 2. $e \notin M$. Then M has a unique 'vertical' edge in the last maximal linear hexagonal chain, say p, that is, an edge among the r_k edges $l_1, \ldots, l_{r_k}$ (see Fig. 3). Similar to the proof in Case 1, p lies in a minimum forcing set of M since the right side hexagon of p (if p is the rightmost 'vertical' edge, choose the left one) is an M-alternating cycle. And $|\mathcal{M}_2| = \sum_{i=1}^{r_k} |\mathcal{M}(Hl(r_1, r_2, \ldots, r_k)_{l_i})| = r_k|\mathcal{M}(Hl(r_1, r_2, \ldots, r_{k-1} - 1))|$. By Lemma 3.1 we have

$$\sum_{M\in\mathcal{M}_2} x^{f(Hl(r_1,r_2,\ldots,r_k),M)} = r_k F(Hl(r_1, r_2, \ldots, r_{k-1} - 1), x)x.$$

The proof is completed. ■

As special cases, we have

$$F(Hl(r_1, r_2), x) = F(Hl(r_0 - 1), x)x + r_2F(Hl(r_1 - 1), x)x$$
$$= x + r_1r_2x^2,\ r_1, r_2 \geq 2,$$
$$F(Hl(r_1, r_2, r_3), x) = F(Hl(r_1 - 1), x)x + r_3F(Hl(r_1, r_2 - 1), x)x$$
$$= \begin{cases} (r_1 + r_3)x^2 + r_1(r_2 - 1)r_3x^3, & \text{if } r_1, r_3 \geq 2, r_2 \geq 3, \\ (r_1 + r_3 + r_1r_3)x^2, & \text{if } r_1, r_3 \geq 2, r_2 = 2. \end{cases}$$

Corollary 3.3. *The innate degree of freedom of a hexagonal chain* $Hl(r_1, r_2, \ldots, r_k)$ $(r_i \geq 2,\ i = 1, 2, \ldots, k,\ k \geq 2)$ *has the following recurrence relation:*

$$IDF(Hl(r_1, r_2, \ldots, r_k)) = \Phi(Hl(r_1, r_2, \ldots, r_k))$$
$$+IDF(Hl(r_1, r_2, \ldots, r_{k-2} - 1)) + r_kIDF(Hl(r_1, r_2, \ldots, r_{k-1} - 1)),$$

with initial conditions $IDF(Hl(r_1-1)) = r_1$ *and* $IDF(Hl(r_0-1)) = 0$.

4. Zigzag hexagonal chains

In this section, we consider a zigzag hexagonal chain Z_n with n hexagons (see Fig. 4), or general fibonacene $Hl(\overbrace{2,2,\ldots,2}^{n-1})$. For the sake of simplicity, let $\Phi_n := \Phi(Z_n)$, $IDF_n := IDF(Z_n)$ and $F_n := F(Z_n, x)$.

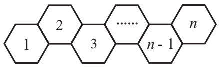


Fig. 4. Illustration of a zigzag hexagonal chain Z_n.

Theorem 4.1. *The forcing polynomial of a zigzag hexagonal chain* Z_n $(n \geq 4)$ *has the following recurrence relation:*

$$F_n = F_{n-3}x + 2F_{n-2}x, \tag{3}$$

with initial conditions $F_1 = 2x$, $F_2 = 3x$ *and* $F_3 = x + 4x^2$.

Proof. From Eq. (2), we have $F_n = F(Hl(\overbrace{2,2,\ldots,2}^{n-1}), x) = F(Hl(\overbrace{2,2,\ldots,2,1}^{n-3}), x)x + 2F(Hl(\overbrace{2,2,\ldots,2,1}^{n-2}), x)x = F(Hl(\overbrace{2,2,\ldots,2}^{n-4}), x)x + 2F(Hl(\overbrace{2,2,\ldots,2}^{n-3}), x)x = F_{n-3}x + 2F_{n-2}x$. Further, $F_1 = F(Hl(1), x) = 2x$, $F_2 = F(Hl(2), x) = 3x$, $F_3 = F(Hl(2,2), x) = x + 4x^2$. ■

By the above recursive expression for the forcing polynomial of zigzag hexagonal chains, we can obtain an explicit one as follows:

Theorem 4.2. *The forcing polynomial of a zigzag hexagonal chain* Z_n $(n \geq 2)$ *is*

$$F(Z_n, x) = \sum_{i=\lceil \frac{n}{3} \rceil}^{\lfloor \frac{n}{2} \rfloor} 2^{3i-n} \binom{i}{n-2i} x^i + \sum_{i=\lceil \frac{n+1}{3} \rceil}^{\lfloor \frac{n+1}{2} \rfloor} 2^{3i-1-n} \binom{i}{n-2i+1} x^i. \tag{4}$$

Proof. Adding the case '$F_0 = 1$' to the definition of F_n, we obtain the generating function of sequence $\{F_n\}_{n=0}^{\infty}$

$$\begin{aligned} P(t) &= \sum_{n=0}^{\infty} F_n t^n = F_0 t^0 + F_1 t^1 + F_2 t^2 + \sum_{n=3}^{\infty} F_n t^n \\ &= 1 + 2xt + 3xt^2 + \sum_{n=3}^{\infty} (F_{n-3}x + 2F_{n-2}x)t^n \\ &= 1 + 2xt + 3xt^2 + xt^3 P(t) + 2xt^2(P(t) - 1). \end{aligned}$$

So

$$\begin{aligned}
P(t) &= \frac{1+2xt+xt^2}{1-2xt^2-xt^3} = (1+2xt+xt^2)\sum_{i=0}^{\infty}(2xt^2+xt^3)^i \\
&= \sum_{i=0}^{\infty} x^i t^{2i}(2+t)^i + \sum_{i=0}^{\infty} x^{i+1}t^{2i+1}(2+t)^{i+1} \\
&= \sum_{i=0}^{\infty} x^i t^{2i} \sum_{j=0}^{i} 2^{i-j}\binom{i}{j} t^j + \sum_{i=0}^{\infty} x^{i+1}t^{2i+1} \sum_{j=0}^{i+1} 2^{i+1-j}\binom{i+1}{j} t^j \\
&= \sum_{i=0}^{\infty} x^i \sum_{n=2i}^{3i} 2^{3i-n}\binom{i}{n-2i} t^n + \sum_{i=0}^{\infty} x^{i+1} \sum_{n=2i+1}^{3i+2} 2^{3i+2-n}\binom{i+1}{n-2i-1} t^n \\
&= \sum_{n=0}^{\infty}\left(\sum_{i=\lceil \frac{n}{3}\rceil}^{\lfloor \frac{n}{2}\rfloor} 2^{3i-n}\binom{i}{n-2i} x^i + \sum_{i=\lceil \frac{n+1}{3}\rceil}^{\lfloor \frac{n+1}{2}\rfloor} 2^{3i-1-n}\binom{i}{n-2i+1} x^i\right) t^n.
\end{aligned}$$

From here we could obtain Eq. (4). ■

This explicit expression is not only convenient for calculating the forcing polynomial of a fibonacene of an arbitrary length, but also implies some topological indices. This can be seen in the following corollary.

Corollary 4.3. *The maximum and minimum forcing number of a zigzag hexagonal chain Z_n $(n \geq 1)$ are*

$$F(Z_n) = \left\lceil \frac{n}{2} \right\rceil, \quad f(Z_n) = \left\lceil \frac{n}{3} \right\rceil.$$

Lemma 4.4. [5] *The perfect matching count of a zigzag hexagonal chain Z_n $(n \geq 1)$ is*

$$\Phi_n = f(n+2), \tag{5}$$

where $\{f(n)\}$ denote the Fibonacci numbers with $f(n) = \frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^n$.

The following expression for the innate degree of freedom of a zigzag hexagonal chain was ever obtained by Hansen and Zheng. Here we present a short proof.

Corollary 4.5. [8] *The innate degree of freedom of a zigzag hexagonal chain Z_n $(n \geq 1)$ is*

$$\begin{aligned}
IDF_n =& \frac{25+3\sqrt{5}}{50}\left(\frac{1-\sqrt{5}}{2}\right)^n + \frac{3-\sqrt{5}}{10}\left(\frac{1-\sqrt{5}}{2}\right)^n n \\
&+ \frac{25-3\sqrt{5}}{50}\left(\frac{1+\sqrt{5}}{2}\right)^n + \frac{3+\sqrt{5}}{10}\left(\frac{1+\sqrt{5}}{2}\right)^n n + (-1)^{n+1}\ .
\end{aligned} \tag{6}$$

Proof. For $n \geq 4$, calculating the derivative and letting x be 1 for Eq. (3) results

$$IDF_n = IDF_{n-3} + 2IDF_{n-2} + \Phi_n.$$

One more step, using the relation $\Phi_{n+2} = \Phi_{n+1} + \Phi_n$, we have

$$IDF_{n+2} = IDF_{n+1} + 3IDF_n - IDF_{n-1} - 3IDF_{n-2} - IDF_{n-3}. \quad (7)$$

The homogeneous characteristics equation of recurrence relation (7) is $x^5 - x^4 - 3x^3 + x^2 + 3x + 1 = 0$. The solution is $x_1 = x_2 = \frac{1-\sqrt{5}}{2}$, $x_3 = x_4 = \frac{1+\sqrt{5}}{2}$, $x_5 = -1$. Let the general solution of (7) be $IDF_n = A_0(\frac{1-\sqrt{5}}{2})^n + A_1 n(\frac{1-\sqrt{5}}{2})^n + A_2(\frac{1+\sqrt{5}}{2})^n + A_3 n(\frac{1+\sqrt{5}}{2})^n + A_4(-1)^n$. The initial conditions $IDF_4 = 16$, $IDF_5 = 34$, $IDF_6 = 62$, $IDF_7 = 118$, $IDF_8 = 213$ imply that $A_0 = \frac{25+3\sqrt{5}}{50}$, $A_1 = \frac{3-\sqrt{5}}{10}$, $A_2 = \frac{25-3\sqrt{5}}{50}$, $A_3 = \frac{3+\sqrt{5}}{10}$, $A_4 = -1$. This obtains Eq. (6) for $n \geq 4$. By checking $IDF_1 = 2$, $IDF_2 = 3$, $IDF_3 = 9$, we know that the corollary holds for $n \geq 1$. ■

Corollary 4.6. *For a zigzag hexagonal chain Z_n $(n \geq 1)$, we have*

$$\frac{IDF_n}{n\Phi_n} \sim \frac{\sqrt{5}}{5}.$$

Proof. By Eqs. (5) and (6), we have

$$\begin{aligned}
&\lim_{n\to\infty} \frac{IDF_n}{n\Phi_n} \\
&= \lim_{n\to\infty} \frac{\frac{25+3\sqrt{5}}{50}\left(\frac{1-\sqrt{5}}{2}\right)^n + \frac{3-\sqrt{5}}{10}\left(\frac{1-\sqrt{5}}{2}\right)^n n + \frac{25-3\sqrt{5}}{50}\left(\frac{1+\sqrt{5}}{2}\right)^n + \frac{3+\sqrt{5}}{10}\left(\frac{1+\sqrt{5}}{2}\right)^n n + (-1)^{n+1}}{n\left[\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^{n+2} - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^{n+2}\right]} \\
&= \lim_{n\to\infty} \frac{\frac{25+3\sqrt{5}}{50}\left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^n + \frac{3-\sqrt{5}}{10}\left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^n n + \frac{25-3\sqrt{5}}{50} + \frac{3+\sqrt{5}}{10} n - \left(\frac{-2}{1+\sqrt{5}}\right)^n}{n\left[\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^2 - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^2 \cdot \left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^n\right]} \\
&= \lim_{n\to\infty} \frac{\frac{3-\sqrt{5}}{10}\left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^n n + \frac{3+\sqrt{5}}{10} n}{n\left[\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^2 - \frac{1}{\sqrt{5}}\left(\frac{1-\sqrt{5}}{2}\right)^2 \cdot \left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^n\right]} = \frac{\frac{3+\sqrt{5}}{10}}{\frac{1}{\sqrt{5}}\left(\frac{1+\sqrt{5}}{2}\right)^2} = \frac{\sqrt{5}}{5}.
\end{aligned}$$

■

By the previous conclusions we have calculated perfect matching count Φ_n, forcing spectrum $\text{Spec}(Z_n) = \{f(Z_n, M) \mid M \in \mathcal{M}(Z_n)\}$ [2], innate degree of freedom IDF_n and forcing polynomial F_n of zigzag hexagonal chains Z_n for n up to 14 (see Table 2).

Table 2. Φ_n, Spec(Z_n), IDF_n and F_n

n	Φ_n	Spec(Z_n)	IDF_n	F_n
1	2	{1}	2	$2x$
2	3	{1}	3	$3x$
3	5	{1,2}	9	$4x^2 + x$
4	8	{2}	16	$8x^2$
5	13	{2,3}	34	$8x^3 + 5x^2$
6	21	{2,3}	62	$20x^3 + x^2$
7	34	{3,4}	118	$16x^4 + 18x^3$
8	55	{3,4}	213	$48x^4 + 7x^3$
9	89	{3,4,5}	387	$32x^5 + 56x^4 + x^3$
10	144	{4,5}	688	$112x^5 + 32x^4$
11	233	{4,5,6}	1220	$64x^6 + 160x^5 + 9x^4$
12	377	{4,5,6}	2140	$256x^6 + 120x^5 + x^4$
13	610	{5,6,7}	3738	$128x^7 + 432x^6 + 50x^5$
14	987	{5,6,7}	6487	$576x^7 + 400x^6 + 11x^5$

Remark 4.7. By transfer matrix due to Klein and Randić [11] we can obtain the forcing polynomial of a zigzag hexagonal chain Z_n $(n \geq 2)$ as follows.

$$F_n = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \boldsymbol{X}^{n-1} \begin{pmatrix} 0 & x & x \end{pmatrix}^{\mathrm{T}}.$$

From this, we can obtain

$$\Phi_n = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \boldsymbol{T}^{n-1} \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}^{\mathrm{T}},$$

$$IDF_n = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix} \left(\boldsymbol{T}^{n-1} + \sum_{i=0}^{n-2} \boldsymbol{T}^i \boldsymbol{C} \boldsymbol{T}^{n-2-i} \right) \begin{pmatrix} 0 & 1 & 1 \end{pmatrix}^{\mathrm{T}},$$

where $\boldsymbol{T} = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}$, $\boldsymbol{C} = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$, and $\boldsymbol{X} = \begin{pmatrix} 0 & 1 & 1 \\ x & 0 & 0 \\ x & 1 & 0 \end{pmatrix}$.

Remark 4.8. Another expression for forcing polynomial of a zigzag hexagonal chain Z_n $(n \geq 1)$ can be produced in exponential generating function. The exponential generating function of sequence $\{F_n\}_{n=0}^{\infty}$ is

$$p(t) = \sum_{n=0}^{\infty} \frac{F_n}{n!} t^n = \frac{F_0}{0!} t^0 + \frac{F_1}{1!} t^1 + \frac{F_2}{2!} t^2 + \sum_{n=3}^{\infty} \frac{F_n}{n!} t^n$$
$$= 1 + 2xt + \frac{3xt^2}{2} + \sum_{n=3}^{\infty} \left(\frac{F_{n-3}x + 2F_{n-2}x}{n!} \right) t^n$$

$$= 1 + 2xt + \frac{3xt^2}{2} + \sum_{n=0}^{\infty} \frac{F_n x}{(n+3)!} t^{n+3} + \sum_{n=1}^{\infty} \frac{2F_n x}{(n+2)!} t^{n+2}.$$

So

$$\frac{\partial^3 p(t)}{\partial t^3} = xp(t) + 2x \frac{\partial p(t)}{\partial t}.$$

Let $\frac{\partial p(t)}{\partial t} = q(t)$ and $\frac{\partial q(t)}{\partial t} = \xi(t)$, then $p(0) = 1$, $q(0) = 2x$, $\xi(0) = 3x$ and

$$\frac{\partial}{\partial t} \begin{pmatrix} p(t) \\ q(t) \\ \xi(t) \end{pmatrix} = \begin{pmatrix} q(t) \\ \xi(t) \\ xp(t) + 2xq(t) \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ x & 2x & 0 \end{pmatrix} \begin{pmatrix} p(t) \\ q(t) \\ \xi(t) \end{pmatrix} := \boldsymbol{W} \begin{pmatrix} p(t) \\ q(t) \\ \xi(t) \end{pmatrix},$$

which deduces that

$$\begin{pmatrix} p(t) \\ q(t) \\ \xi(t) \end{pmatrix} = e^{\boldsymbol{W}t} \begin{pmatrix} 1 \\ 2x \\ 3x \end{pmatrix} = \sum_{n=0}^{\infty} \frac{(\boldsymbol{W}t)^n}{n!} \begin{pmatrix} 1 \\ 2x \\ 3x \end{pmatrix}.$$

Then the first row of $\boldsymbol{W}^n$ multiplies $\begin{pmatrix} 1 & 2x & 3x \end{pmatrix}^{\mathrm{T}}$ equals forcing polynomial F_n.

5. Catacondensed hexagonal systems

To compute the forcing polynomial of catacondensed hexagonal systems, our approach is to decrease recursively *kinks* (hexagons glued to two hexagons along two non-parallel edges) and *branched hexagons* (adjacent to three hexagons), then come down to a series of hexagonal chains, which have been already treated in Section 3.

Let H be a catacondensed hexagonal system and s an end hexagon (with only one neighboring hexagon) (see Fig. 5). Let $H(s)$ be the maximal linear chain of H with r (≥ 2) hexagons, and s and s' as the pair of end hexagons. Note that H may be a linear hexagonal chain or s' is a kink or branched hexagon. Let H_s be the graph consisting of the hexagons of H not in $H(s)$. Let $H*s$ be the graph obtained from H_s by deleting the edges of s' together with their end vertices, deleting consecutively the pendant edges with their vertices and finally deleting the edges which do not belong to any remaining hexagon [8]. Note that H_s and $H*s$ may be empty or each component of which is a catacondensed hexagonal system. Then we generalize Theorem 3.2 in the following theorem.

Theorem 5.1. *Let H be a catacondensed hexagonal system and s an end hexagon. Then*

$$F(H, x) = F(H*s, x)x + rF(H_s, x)x. \tag{8}$$

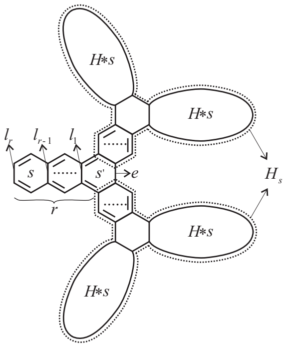


Fig. 5. Illustration of a catacondensed hexagonal system H.

Proof. Let e be the right 'vertical' edge of s'. We classify $\mathcal{M}(H)$ into two classes $\mathcal{M}_1 = \{M \in \mathcal{M}(H) \mid e \in M\}$ and $\mathcal{M}_2 = \mathcal{M}(H) \setminus \mathcal{M}_1$. In Fig. 5, we illustrate edges $e,\ l_1, \ldots, l_r$. Take any $M \in \mathcal{M}(H)$.

Case 1. $e \in M$. When $H * s$ or H_s is an empty graph, e is a forcing edge. Then $\sum_{M \in \mathcal{M}_1} x^{f(H,M)} = x$. Otherwise, similar to Case 1 in the proof of Theorem 3.2, e lies in a minimum forcing set of M. In Fig. 5, we use double lines to mark the edges which e determines. By Lemma 3.1 we have

$$\sum_{M \in \mathcal{M}_1} x^{f(H,M)} = F(H * s, x)x.$$

Case 2. $e \notin M$. Let p be the 'vertical' edge of $H(s)$ in M (see Fig. 5). Then p could only be one of the r edges $l_1, \ldots, l_r$. When H_s is an empty graph, p is a forcing edge. Then $\sum_{M \in \mathcal{M}_2} x^{f(H,M)} = rx$. Otherwise, similar to Case 2 in the proof of Theorem 3.2, we have

$$\sum_{M \in \mathcal{M}_2} x^{f(H,M)} = rF(H_s, x)x.$$

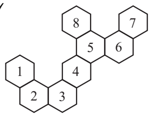
The proof is completed. ∎

By applying Lemma 2.3 to Eq. (8), we immediately obtain

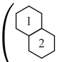
Corollary 5.2. [8] *Let H be a catacondensed hexagonal system and s an end hexagon. Then*

$$IDF(H) = \Phi(H) + IDF(H * s) + rIDF(H_s).$$

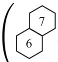
We give some examples as follows:

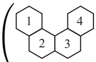
$F\Big($ 

$, x\Big) = F\big($ 

$, x\big)\, F\big($ 

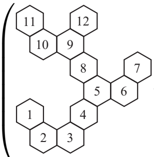
$, x\big)\, x$

$+2F\big($ 

$, x\big)\, F\big($ 

$, x\big)\, x$

$$=2x \cdot 3x \cdot x + 2 \cdot 3x \cdot 8x^2 \cdot x = 6x^3 + 48x^4.$$

$F\Big($ 

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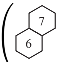
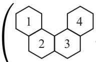
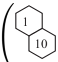
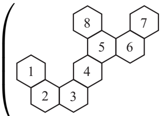
$, x\big)\, F\big($ 

$, x\big)\, F\big($ 

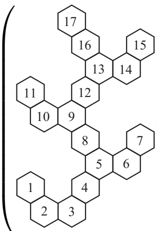
$, x\big)\, x$

$+2F\big($ 

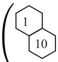
$, x\big)\, F\Big($ 

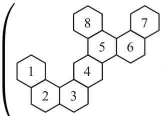
$, x\Big)\, x$

$$=2x \cdot 3x \cdot 8x^2 \cdot x + 2 \cdot 3x \cdot (6x^3 + 48x^4) \cdot x = 84x^5 + 288x^6.$$

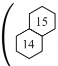
$F\Big($ 

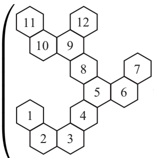
$, x\Big) = F\big($ 

$, x\big)\, F\big($ 

$, x\big)\, F\Big($ 

$, x\Big)\, x$

$+3F\big($ 

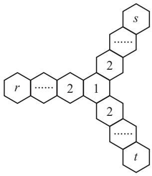
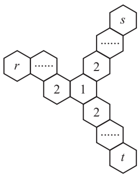
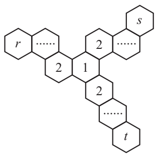
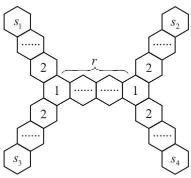
$, x\big)\, F\Big($ 

$, x\Big)\, x$

$$=2x \cdot 3x \cdot (6x^3 + 48x^4) \cdot x + 3 \cdot 3x \cdot (84x^5 + 288x^6) \cdot x$$
$$=36x^6 + 1044x^7 + 2592x^8.$$

Below we present some forcing polynomials of special catacondensed hexagonal systems (see Table 3).

Table 3. Some forcing polynomials, for $r, s, t, s_1, s_2, s_3, s_4 \geq 2$

catacondensed hexagonal systems	forcing polynomials
	$rstx^3 + x$
	$stF_{r-1}x^2 + F_{r-2}x$, with initial condition $F_0 = 1$
	$tF_{r-1}F_{s-1}x + F_{r-2}F_{s-2}x$, with initial condition $F_0 = 1$
	$(s_1s_3 + s_2s_4)x^3 + s_1s_2s_3s_4(r-1)x^5$, if $r \geq 3$, $(s_1s_3 + s_2s_4)x^3 + s_1s_2s_3s_4x^4$, if $r = 2$

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