Forcing and anti-forcing polynomials of perfect matchings of a pyrene system *

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Abstract

The forcing number of a perfect matching of a graph was introduced by Harary et al., which originated from Klein and Randić’s ideal of innate degree of freedom of Kekulé structure in molecular graph. On the opposite side in some sense, Vukičević and Trinajšić proposed the anti-forcing number of a graph, afterwards Lei et al. generalized this idea to single perfect matching. Recently the forcing and anti-forcing polynomials of perfect matchings of a graph were proposed as counting polynomials for perfect matchings with the same forcing number and anti-forcing number respectively. In this paper, we obtain the explicit expressions of forcing and anti-forcing polynomials of a pyrene system. As consequences, the forcing and anti-forcing spectra of a pyrene system are determined.

Key words: Perfect matching; Forcing polynomial; Anti-forcing polynomial; Hexagonal system

1 Introduction

Let \( G \) be a simple graph with vertex set \( V(G) \) and edge set \( E(G) \). A perfect matching of \( G \) is a set of independent edges which covers all vertices of \( G \). A perfect

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matching coincides with a Kekulé structure of a conjugated molecule graph (the graph representing the carbon-atoms), Klein and Randić [17, 24] discovered the phenomenon that a Kekulé structure can be determined by a few number of fixed double bonds, and they defined the innate degree of freedom of a Kekulé structure as the minimum number of fixed double bonds required to determine it. Further, the sum over innate degree of freedom of all Kekulé structures of a graph was called the degree of freedom of the graph, which was proposed as a novel invariant to estimate the resonance energy. In 1991, Harary, Klein and Živković [12] extended the concept “degree of freedom” to a graph $G$ with a perfect matching, and renamed it as the forcing number of a perfect matching $M$, denoted by $f(G, M)$. Over the past 30 years, many researchers were attracted to the study on the forcing numbers of perfect matchings of a graph [3], in addition, the anti-forcing number [20, 32, 33] was proposed from the point of opposite view of forcing number. In general, to compute the forcing number of a perfect matching of a bipartite graph with the maximum degree 3 is an NP-complete problem [1], and to compute the anti-forcing number of a perfect matching of a bipartite graph with the maximum degree 4 is also an NP-complete problem [8]. But the particular structure of a graph enables us to do much better. In this paper, we will calculate the forcing and anti-forcing polynomials of a pyrene system, as consequences, the exact values of forcing and anti-forcing numbers of a perfect matching of the pyrene system are determined.

A forcing set $S$ of a perfect matching $M$ of a graph $G$ is a subset of $M$ such that $S$ is contained in no other perfect matchings of $G$. Therefore, $f(G, M)$ equals the smallest cardinality over all forcing sets of $M$. The minimum (resp. maximum) forcing number of $G$ is the minimum (resp. maximum) value over forcing numbers of all perfect matchings of $G$, denoted by $f(G)$ (resp. $F(G)$). Afshani et al. [2] proved that the smallest forcing number problem of graphs is NP-complete for bipartite graphs with maximum degree four. In order to investigate the distribution of forcing numbers of all perfect matchings of a graph $G$, the forcing spectrum $\text{Spec}_f(G)$ of $G$ is proposed, denoted by $\text{Spec}_f(G)$, which is the collection of forcing numbers of all perfect matchings of $G$. Further, Zhang et al. [42] introduced the forcing polynomial of a graph, which can enumerate the number of perfect matchings with the same forcing number.

A hexagonal system (or benzenoid) is a finite 2-connected planar bipartite graph in which each interior face is surrounded by a regular hexagon of side length one. Hexagonal systems are extensively used in the study of benzenoid hydrocarbons [5], as they properly represent the skeleton of such molecules. Zhang and Li [38] and Hansen and Zheng [11] characterized independently the hexagonal systems with minimum forcing number 1, and the forcing spectrum of such a hexagonal system was determined by Zhang and Deng [39]. Afterwards Zhang and Zhang [41] characterized plane elemen-
tary bipartite graphs with minimum forcing number 1. Xu et al. [35] proved that the maximum forcing number of a hexagonal system equals its Clar number (i.e. the number of hexagons in a maximum resonance set), which is an invariant used to measure the stability of benzenoid hydrocarbons. Similar results also hold for polyomino graphs [43] and (4,6)-fullerenes [28]. Zhang et al. [40] proved that the minimum forcing number of a fullerene graph is not less than 3, and the lower bound can be achieved by infinitely many fullerene graphs. Randić, Vukičević and Gutman [25, 30, 31] determined the forcing spectra of fullerene graphs $C_{60}$, $C_{70}$ and $C_{72}$, in particular there is a single Kekulé structure of $C_{60}$ that has the highest degree of freedom 10 such that all hexagons of $C_{60}$ have three double CC bonds, which represents the Fries structure of $C_{60}$ and is the most important valence structure. For forcing polynomial, only a few types of hexagonal systems have been studied, such as catacondensed hexagonal systems [42] and benzenoid parallelogram [45]. For more results on forcing number, we refer the reader to see [4, 15, 16, 18, 19, 23, 26, 27, 34, 47–49].

Given a perfect matching $M$ of a graph $G$. A subset $S \subseteq E(G) \setminus M$ is called an anti-forcing set of $M$ if $M$ is the unique perfect matching of $G - S$. The smallest cardinality over all anti-forcing sets of $M$ is called the anti-forcing number of $M$, denoted by $af(G, M)$. The minimum (resp. maximum) anti-forcing number $af(G)$ (resp. $Af(G)$) of graph $G$ is the minimum (resp. maximum) value of anti-forcing numbers over all perfect matchings of $G$. The (minimum) anti-forcing number of a graph was first introduced by Vukičević and Trinajstić [32, 33] in 2007-2008. Actually, the hexagonal systems with minimum anti-forcing number 1 had been characterized by Li [21] in 1997, where he called such a hexagonal system has a forcing single edge. Deng [6, 7] obtained the minimum anti-forcing numbers of benzenoid chains and double benzenoid chains. Zhang et al. [44] computed the minimum anti-forcing number of catacondensed phenylene. Yang et al. [36] showed that a fullerene graph has the minimum anti-forcing number at least 4, and characterized the fullerene graphs with minimum anti-forcing number 4.

In 2015, Lei et al. [20] generalized the anti-forcing number to single perfect matching of a graph. By an analogous manner as the forcing number, the anti-forcing spectrum of a graph $G$ was proposed, denoted by $Spec_{af}(G)$, which is the collection of anti-forcing numbers of all perfect matchings of $G$. Further, Hwang et al. [14] introduced the anti-forcing polynomial of a graph, which can enumerate the number of perfect matchings with the same anti-forcing number. Lei et al. [20] proved that the maximum anti-forcing number of a hexagonal system equals its Fries number, which can measure the stability of benzenoid hydrocarbons. Analogous results were obtained on (4,6)-fullerenes [28]. Further more, two tight upper bounds on the maximum anti-forcing numbers of graphs were obtained [10, 29]. The anti-forcing spectra of some types of
hexagonal systems were proved to be continuous, such as monotonic constructable hexagonal systems [8], catacondensed hexagonal systems [9]. Zhao and Zhang [46, 47] computed the anti-forcing polynomials of benzenoid systems with minimum forcing number 1 and some rectangle grids.

In this paper, we will calculate the forcing and anti-forcing polynomials of a pyrene system. In section 2, as a preparation, some basic results on forcing and anti-forcing numbers are introduced, and we characterize the maximum set of disjoint $M$-alternating cycles and the maximum set of compatible $M$-alternating cycles with respect to a perfect matching $M$ of a pyrene system. In section 3, we give a recurrence formula for the forcing polynomial of a pyrene system, and derive the explicit expressions of forcing polynomial and degree of freedom of a pyrene system. As corollaries, the minimum forcing number, maximum forcing number and the forcing spectrum of a pyrene system are determined, and an asymptotic behavior of degree of freedom is revealed. In section 4, we obtain a recurrence formula for the anti-forcing polynomial of a pyrene system, and derive the explicit expressions of anti-forcing polynomial and the sum over the anti-forcing numbers of all perfect matchings of a pyrene system. As consequences, the minimum anti-forcing number, maximum anti-forcing number and the anti-forcing spectrum of a pyrene system are determined, and an asymptotic behavior of the sum over the anti-forcing numbers of all perfect matchings of a pyrene system is obtained.

2 Preliminaries

Let $M$ be a perfect matching of a graph $G$. A cycle $C$ of $G$ is called an $M$-alternating cycle if the edges of $C$ appear alternately in $M$ and $E(G) \setminus M$. If $C$ is an $M$-alternating cycle, then the symmetric difference $M \triangle C$ is the another perfect matching of $G$, here $C$ may be viewed as its edge set. Let $c(M)$ be the maximum number of disjoint $M$-alternating cycles of $G$. Since any forcing set of $M$ has to contain at least one edge of each $M$-alternating cycle, $f(G, M) \geq c(M)$. Pachter and Kim [23] proved the following theorem by using the minimax theorem on feedback set [22].

**Theorem 2.1** [23]. Let $M$ be a perfect matching in a planar bipartite graph $G$. Then $f(G, M) = c(M)$.

A pyrene system with $n$ pyrene fragments is denoted by $H_n$, see Fig. [1(a)]. $H_n$ is a hexagonal system with perfect matchings, by Theorem 2.1 $f(H_n, M) = c(M)$ for any perfect matching $M$ of $H_n$.

**Lemma 2.2** [37, 41]. Let $M$ be a perfect matching of a hexagonal system $H$, $C$ an $M$-alternating cycle in $H$. Then there is an $M$-alternating hexagon in the interior of $C$. 


Fig. 1. Pyrene system $H_n$ with $n$ pyrene (a) and the auxiliary graph $G_n$ (b)

Let $H$ be a hexagonal system with a perfect matching $M$. A set of disjoint $M$-alternating hexagons of $H$ is called an $M$-resonant set, the size of a maximum $M$-resonant set is denote by $h(M)$.

Lemma 2.3. Let $M$ be a perfect matching of the pyrene system $H_n$. Then $f(H_n, M) = h(M)$.

Proof. Let $\mathcal{A}$ be a maximum set of disjoint $M$-alternating cycles containing hexagons as more as possible. By Theorem 2.1, $f(H_n, M) = |\mathcal{A}|$. We claim that $\mathcal{A}$ is an $M$-resonance set, otherwise $\mathcal{A}$ contains a non-hexagonal cycle $C$. By Lemma 2.2, there is an $M$-alternating hexagon $h$ in the interior of $C$. Note that $\mathcal{A}' = (\mathcal{A} \setminus \{C\}) \cup \{h\}$ also is a maximum set of disjoint $M$-alternating cycles, but $\mathcal{A}'$ contains more hexagons than $\mathcal{A}$, a contradiction. We have $|\mathcal{A}| \leq h(M) \leq f(H_n, M) = |\mathcal{A}|$, i.e. $f(H_n, M) = h(M)$.

Let $M$ be a perfect matching of a graph $G$. A set $\mathcal{A}$ of $M$-alternating cycles of $G$ is called a compatible $M$-alternating set if any two cycles of $\mathcal{A}$ either are disjoint or intersect only at edges in $M$. Let $\mathcal{C}'(M)$ denote the maximum cardinality over all compatible $M$-alternating sets of $G$. Since any anti-forcing set of $M$ must contain at least one edge of each $M$-alternating cycle, $af(G, M) \geq \mathcal{C}'(M)$. Lei et al. [20] gave the following minimax theorem.

Theorem 2.4 [20]. Let $G$ be a planar bipartite graph with a perfect matching $M$. Then $af(G, M) = \mathcal{C}'(M)$. 

5
Let $G$ be a plane bipartite graph with a perfect matching $M$. Given a compatible $M$-alternating set $A$, two cycles $C_1$ and $C_2$ of $A$ are crossing if they share an edge $f$ in $M$ and the four edges adjacent to $f$ alternate in $C_1$ and $C_2$ (i.e., $C_1$ enters into $C_2$ from one side and leaves for the other side via $f$). A compatible $M$-alternating set $A$ is called non-crossing if any two cycles of $A$ are non-crossing.

**Lemma 2.5** [10][20]. Let $G$ be a plane bipartite graph with a perfect matching $M$. Then there is a non-crossing compatible $M$-alternating set $A$ such that $|A| = c'(M)$.

A triphenylene is a benzenoid consisting of four hexagons, one hexagon at the center, for the other three disjoint hexagons, each of them has a common edge with the center one. For example, the four hexagons $s_{1,1}, s_{1,2}, h_{1,2}, h_{2,1}$ form a triphenylene, see Fig. 1(a).

**Lemma 2.6.** Let $M$ be a perfect matching of the pyrene system $H_n$. Then there is a maximum non-crossing compatible $M$-alternating set $A$ such that each member of $A$ either is a hexagon or the periphery of a triphenylene.

**Proof.** By Lemma 2.5 there is a maximum non-crossing compatible $M$-alternating set $A$ with $I(A) = \sum_{C \in A} I(C)$ as small as possible, where $I(C)$ denotes the number of hexagons in the interior of $C$. Let $C$ be a member of $A$. Suppose $C$ is not a hexagon, by Lemma 2.2 there is an $M$-alternating hexagon $h$ in the interior of $C$. Note that $C$ and $h$ must be compatible, otherwise $A' = (A \setminus \{C\}) \cup \{h\}$ can be a maximum non-crossing compatible $M$-alternating set such that $I(A') < I(A)$, a contradiction. In fact, $C$ has to be compatible with any $M$-alternating hexagon, which implies that $h := h_{i,j}$, without loss of generality, let $h := h_{i,1}(i \neq 1)$ (see Fig. 1(a)). Then $e_{i,1}, f_{i,1}$ and the right vertical edge of $h_{i,1}$ all belong to $M$. Let $M' = M \triangle h_{i,1}$. Then $s_{i,1}$ and $s_{i,2}$ both are $M'$-alternating hexagons.

**Claim 1.** $h_{i-1,2}$ also is $M'$-alternating.

**Proof.** Suppose $h_{i-1,2}$ is not $M'$-alternating. Then at least one of $p_{i-1,2}$ and $q_{i-1,2}$ does not belong to $M$. If only one of $p_{i-1,2}$ and $q_{i-1,2}$ belongs to $M$, say $p_{i-1,2} \in M$, then $s_{i-1,2}$ is an $M$-alternating hexagon which is not compatible with $C$, a contradiction. Therefore both of $p_{i-1,2}$ and $q_{i-1,2}$ are not in $M$, then $h_{i-1,1}$ is $M$-alternating. If $p_{i-2,2}$ and $q_{i-2,2}$ both belong to $M$, then the four hexagons $h_{i-2,2}, h_{i-1,1}, s_{i-1,1}$, and $s_{i-1,2}$ form a triphenylene whose periphery $T$ is an $M$-alternating cycle. Note that $T$ is compatible with each cycle of $A \setminus \{C\}$, thus $(A \setminus \{C\}) \cup \{T\}$ can be a maximum non-crossing compatible $M$-alternating set with $I((A \setminus \{C\}) \cup \{T\}) < I(A)$, a contradiction. Hence at least one of $p_{i-2,2}$ and $q_{i-2,2}$ does not belong to $M$, by similar discussion as in the previous steps, we can show that $h_{i-2,1}$ is $M$-alternating. Keeping on the process, and finally we will prove that $h_{i,1}$ is $M$-alternating, however $h_{1,1}$ is not compatible with $C$, a contradiction.
According to Claim 1 and the minimality of $I(A)$, $C$ has to be the periphery of the triphenylene consisting of the four hexagons $h_{i-1,2}$, $h_{i,1}$, $s_{i,1}$ and $s_{i,2}$ (see Fig. 1(a)). 

### 3 Forcing polynomial of pyrene system

The forcing polynomial of a graph $G$ is defined as follow [42]:

$$F(G, x) = \sum_{M \in \mathcal{M}(G)} x^{f(G, M)} = \sum_{i=1}^{f(G)} w_i x^i, \quad (3.1)$$

where $\mathcal{M}(G)$ is the collection of all perfect matchings of $G$, $w_i$ is the number of perfect matchings of $G$ with the forcing number $i$.

As a consequence, let $\Phi(G)$ be the number of perfect matchings of a graph $G$, then $\Phi(G) = F(G, 1)$. Recall that the degree of freedom of a graph $G$ is the sum over the forcing numbers of all perfect matchings of $G$, denoted by $IDF(G)$, then $IDF(G) = \frac{d}{dx} F(G, x)|_{x=1}$. $\Phi(G)$ and $IDF(G)$ both are chemically meaningful indices within a resonance theoretic context [17][24]. Note that if $G$ is a null graph or a graph has a unique perfect matching, then $F(G, x) = 1$.

![Fig. 2. Pyrene (a), Phenanthrene (b) and Diphenyl (c)](image)

In the following we want to derive a recurrence formula for forcing polynomial of a pyrene system, as preparations the forcing polynomials of pyrene, phenanthrene and diphenyl are computed: $F(H_1, x) = 4x^2 + 2x$, $F(L, x) = 4x^2 + x$, $F(N, x) = 4x^2$ (see Fig. 2).

**Theorem 3.1.** Let $H_n$ be a pyrene system with $n$ pyrene fragments. Then

$$F(H_n, x) = (4x^2 + 2x)F(H_{n-1}, x) - x^2F(H_{n-2}, x), \quad (3.2)$$

where $n \geq 2$, $F(H_0, x) = 1$ and $F(H_1, x) = 4x^2 + 2x$.

**Proof.** First we introduce an auxiliary graph $G_n$ obtained by deleting the leftmost hexagon $h_{1,1}$ from $H_n$, see Fig. 1(b). We divide $\mathcal{M}(H_n)$ in two subsets: $\mathcal{M}_{j_1,2}(H_n) = \ldots$
\{M \in \mathcal{M}(H_n) \mid e_{1,2}, f_{1,2} \in M\}, \mathcal{M}^{e_{1,2}}_{f_{1,2}}(H_n) = \{M \in \mathcal{M}(H_n) \mid e_{1,2}, f_{1,2} \notin M\}. If M \in \mathcal{M}^{e_{1,2}}_{f_{1,2}}(H_n), then h_{1,2} is a unique M-alternating hexagon in the leftmost pyrene fragment, and M' = M \cap E(G_{n-1}) is a perfect matching of the graph G_{n-1} obtained by deleting vertices of the leftmost pyrene fragment and their incident edges from H_n. By Lemma 2.3, f(H_n, M) = f(G_{n-1}, M') + 1. If M \in \mathcal{M}^{e_{1,2}}_{f_{1,2}}(H_n), then the restriction M_1 of M on the phenanthrene L consisting of three hexagons s_{1,1}, h_{1,1}, s_{1,2} is a perfect matching of L, and M_2 = M \cap E(H_{n-1}) is a perfect matching of the subsystem H_{n-1} obtained by deleting vertices of L and their incident edges from H_n, see Fig. 1(b). According to Lemma 2.3, f(H_n, M) = f(L, M_1) + f(H_{n-1}, M_2). By Eq. (3.1), we have

\begin{align*}
F(H_n, x) &= \sum_{M \in \mathcal{M}(H_n)} x^{f(H_n, M)} \\
&= \sum_{M \in \mathcal{M}^{e_{1,2}}_{f_{1,2}}(H_n)} x^{f(H_n, M)} + \sum_{M \in \mathcal{M}^{e_{1,2}}_{f_{1,2}}(H_n)} x^{f(H_n, M)} \\
&= \sum_{M' \in \mathcal{M}(G_{n-1})} x^{f(G_{n-1}, M') + 1} + \sum_{M \in \mathcal{M}(L), M_2 \in \mathcal{M}(H_{n-1})} x^{f(L, M_1) + f(H_{n-1}, M_2)} \\
&= x \sum_{M' \in \mathcal{M}(G_{n-1})} x^{f(G_{n-1}, M')} + \sum_{M_1 \in \mathcal{M}(L), M_2 \in \mathcal{M}(H_{n-1})} x^{f(L, M_1)} x^{f(H_{n-1}, M_2)} \\
&= x F(G_{n-1}, x) + \left( \sum_{M_1 \in \mathcal{M}(L)} x^{f(L, M_1)} \right) \left( \sum_{M_2 \in \mathcal{M}(H_{n-1})} x^{f(H_{n-1}, M_2)} \right) \\
&= x F(G_{n-1}, x) + (4x^2 + x) F(H_{n-1}, x).
\end{align*}

(3.3)

Now we deduce a recurrence relation for forcing polynomial of the auxiliary graph G_n. We can divide \mathcal{M}(G_n) in two types, one is perfect matchings which containing edges e_{1,2} and f_{1,2}, and another is on the converse. For a perfect matching M \in \mathcal{M}(G_n), if e_{1,2}, f_{1,2} \in M, then h_{1,2} is a unique M-alternating hexagon in the leftmost phenanthrene consisting of three hexagons s_{1,1}, s_{1,2}, h_{1,2}, and the restriction M' of M on the graph G_{n-1} obtained by deleting vertices of the leftmost phenanthrene and their incident edges from G_n is a perfect matching of G_{n-1}. By Lemma 2.3, f(G_n, M) = f(G_{n-1}, M') + 1. On the other hand, if e_{1,2}, f_{1,2} \notin M, then the restriction M_1 of M on the leftmost diphenyl N is a perfect matching of N, and the restriction M_2 of M on the successive subsystem H_{n-1} is a perfect matching of H_{n-1}. Therefore f(G_n, M) = f(N, M_1) + f(H_{n-1}, M_2), see Fig. 1(b). By a similar deducing as Eq. (3.3), we can obtain the following formula

\[ F(G_n, x) = x F(G_{n-1}, x) + 4x^2 F(H_{n-1}). \]

(3.4)
Eq. (3.3) minus Eq. (3.4), we have
\[ F(G_n, x) = F(H_n, x) - xF(H_{n-1}, x), \]
which implies
\[ F(G_{n-1}, x) = F(H_{n-1}, x) - xF(H_{n-2}, x). \]
Substituting this expression into Eq. (3.3), we can obtain Eq. (3.2), the proof is completed.

**Theorem 3.2.** Let \( H_n \) be a pyrene system with \( n \) pyrene fragments. Then
\[ F(H_n, x) = x^n \sum_{j=0}^{n} \sum_{i=\left\lfloor \frac{j+n}{n} \right\rfloor} (-1)^{n-i} 2^{2i+j-n} \binom{i}{n-i} \binom{2i-n}{j} x^j. \]

**Proof.** For convenience, let \( F_n := F(H_n, x) \), then the generating function of sequence \( \{F_n\}_{n=0}^\infty \) is obtained as follow
\[
G(z) = \sum_{n=0}^\infty F_n z^n = 1 + (4x^2 + 2x)z + \sum_{n=2}^\infty F_n z^n \\
= 1 + (4x^2 + 2x)z + \sum_{n=2}^\infty ((4x^2 + 2x)F_{n-1} - x^2 F_{n-2}) z^n \\
= 1 + (4x^2 + 2x)z + (4x^2 + 2x)z(G(z) - 1) - x^2 z^2 G(z) \\
= 1 + (4x^2 + 2x)zG(z) - x^2 z^2 G(z).
\]

Therefore
\[
G(z) = \frac{1}{1 - ((4x^2 + 2x)z - x^2 z^2)} \\
= \sum_{i=0}^\infty ((4x^2 + 2x)z - x^2 z^2)^i \\
= \sum_{i=0}^\infty x^i z^i \sum_{j=0}^i \binom{i}{j} (4x + 2)^{i-j} (-xz)^j \\
= \sum_{n=0}^\infty \sum_{i=\left\lfloor \frac{n}{2} \right\rfloor} (-1)^{n-i} \binom{i}{n-i} (4x + 2)^{2i-n} x^n z^n,
\]
which implies
\[
F_n = x^n \sum_{i=\left\lfloor \frac{n}{2} \right\rfloor} (-1)^{n-i} \binom{i}{n-i} (4x + 2)^{2i-n} \\
= x^n \sum_{i=\left\lfloor \frac{n}{2} \right\rfloor} (-1)^{n-i} \binom{i}{n-i} \sum_{j=0}^{2i-n} 2^{2i+j-n} \binom{2i-n}{j} x^j \\
= x^n \sum_{j=0}^n \sum_{i=\left\lfloor \frac{j+n}{2} \right\rfloor} (-1)^{n-i} 2^{2i+j-n} \binom{i}{n-i} \binom{2i-n}{j} x^j.
\]
The proof is completed. □

As a consequence, the following corollary is immediate.

**Corollary 3.3.** Let $H_n$ be a pyrene system with $n$ pyrene fragments. Then

1. $f(H_n) = n$;
2. $F(H_n) = 2n$;
3. $\text{Spec}_f(H_n) = [n, 2n]$.

In the following we compute the degree of freedom of $H_n$, and discuss its asymptotic behavior. He and He [13] gave the following formula:

$$\Phi(H_n) = 6\Phi(H_{n-1}) - \Phi(H_{n-2}),$$

Further we can obtain an general formula as follow:

$$\Phi(H_n) = \frac{17 - 12\sqrt{2}}{16 - 12\sqrt{2}} (3 - 2\sqrt{2})^n + \frac{17 + 12\sqrt{2}}{16 + 12\sqrt{2}} (3 + 2\sqrt{2})^n. \tag{3.6}$$

**Theorem 3.4.**

$$IDF(H_n) = \frac{\sqrt{2}}{32} (3 - 2\sqrt{2})^n + \frac{7 - 5\sqrt{2}}{8} n(3 - 2\sqrt{2})^n - \frac{\sqrt{2}}{32} (3 + 2\sqrt{2})^n + \frac{7 + 5\sqrt{2}}{8} n(3 + 2\sqrt{2})^n. \tag{3.7}$$

**Proof.** According to Eq. (3.2),

$$\frac{d}{dx} F(H_n, x) = (8x + 2)F(H_{n-1}, x) + (4x^2 + 2x) \frac{d}{dx} F(H_{n-1}, x) - 2xF(H_{n-2}, x) - x^2 \frac{d}{dx} F(H_{n-2}, x).$$

For convenience, let $\Phi_n := \Phi(H_n)$ and $IDF_n := IDF(H_n)$, then we have

$$IDF_n = \frac{d}{dx} F(H_n, x) \bigg|_{x=1} = 6IDF_{n-1} - IDF_{n-2} + 10\Phi_{n-1} - 2\Phi_{n-2}.$$ 

So

$$IDF_{n+1} = 6IDF_n - IDF_{n-1} + 10\Phi_n - 2\Phi_{n-1},$$

$$IDF_{n+2} = 6IDF_{n+1} - IDF_n + 10\Phi_{n+1} - 2\Phi_n.$$
Suppose the general solution of Eq. (3.3), \( \Phi_{n+1} = 6\Phi_n - \Phi_{n-1} \) and \( \Phi_n = 6\Phi_{n-1} - \Phi_{n-2} \), which implies

\[
IDF_{n+2} = 6IDF_{n+1} - IDF_n + 10(6\Phi_n - \Phi_{n-1}) - 2(6\Phi_{n-1} - \Phi_{n-2}) = 6IDF_{n+1} - IDF_n + 6(6IDF_n - IDF_{n-1} + 10\Phi_n - 2\Phi_{n-1}) - 6IDF_{n-1} - 10\Phi_{n-1} + 2\Phi_{n-2} - 36IDF_n + 12IDF_{n-1} - IDF_{n-2} = 12IDF_{n+1} - 38IDF_n + 12IDF_{n-1} - IDF_{n-2}.
\] (3.8)

Therefore the homogeneous characteristics equation of recurrence formula (3.8) is \( x^4 - 12x^3 + 38x^2 - 12x + 1 = 0 \), and its roots are \( x_1 = x_2 = 3 - 2\sqrt{2}, x_3 = x_4 = 3 + 2\sqrt{2} \). Suppose the general solution of Eq. (3.8) is \( IDF_n = \lambda_1(3 - 2\sqrt{2})^n + \lambda_2n(3 - 2\sqrt{2})^n + \lambda_3(3 + 2\sqrt{2})^n + \lambda_4n(3 + 2\sqrt{2})^n \). According to the initial values \( IDF_3 = 1036, IDF_4 = 8068, IDF_5 = 58854 \) and \( IDF_6 = 411978 \), we can obtain \( \lambda_1 = \frac{\sqrt{2}}{8}, \lambda_2 = \frac{7 - 5\sqrt{2}}{8}, \lambda_3 = -\frac{\sqrt{2}}{8} \) and \( \lambda_4 = \frac{7 + 5\sqrt{2}}{8} \), so Eq. (3.7) holds for \( n \geq 3 \). In fact, we can check that Eq. (3.7) also holds for \( n = 0, 1, 2 \), so the proof is completed.

By Eq. (3.6) and Eq. (3.7), the following result is obtained.

**Corollary 3.5.** Let \( H_n \) be a pyrene system with \( n \) pyrene fragments. Then

\[
\lim_{n \to \infty} \frac{IDF(H_n)}{n\Phi(H_n)} = 1 + \frac{\sqrt{2}}{2}.
\]

## 4 Anti-forcing polynomial of pyrene system

The anti-forcing polynomial of a graph \( G \) is defined as follow [14]:

\[
Af(G, x) = \sum_{M \in \mathcal{M}(G)} x^{af(G,M)} = \sum_{i=af(G)} u_i x^i,
\] (4.1)

where \( u_i \) is the number of perfect matchings of \( G \) with the anti-forcing number \( i \).

As a consequence, \( \Phi(G) = Af(G, 1) \), and the sum over the anti-forcing numbers of all perfect matchings of \( G \) equals \( \frac{d}{dx} Af(G, x) \big|_{x=1} \). If \( G \) is a null graph or a graph with unique perfect matching, then \( Af(G, x) = 1 \). Lemma 2.6 provides an approach for calculating the anti-forcing number of a perfect matching of a pyrene system, further we can obtain the following recursive formula.

**Theorem 4.1.** Let \( H_n \) be the pyrene system with \( n \) pyrene fragments. Then

\[
Af(H_n, x) = (2x^3 + 2x^2 + 2x)Af(H_{n-1}, x) - x^2 Af(H_{n-2}, x),
\] (4.2)

where \( n \geq 2 \), \( Af(H_0, x) = 1 \) and \( Af(H_1, x) = 2x^3 + 2x^2 + 2x \).
Recall that the vertices of the leftmost diphenyl of \(G\) consisting of the four hexagons both are \(M\)-alternating, and the four hexagons \(s_1, s_2, h_1, h_2\) form a triphenylene whose perimeter \(T\) is an \(M\)-alternating cycle, and \(\{h_1, s_2, s_2, T\}\) is a non-crossing compatible \(M\)-alternating set. Note that the restriction \(M_1\) of \(M\) on the subsystem \(H_{n-2}\) obtained by the removal of the first two pyrene fragments is a perfect matching of \(H_{n-2}\). Let \(A'\) be a maximum non-crossing compatible \(M'\)-alternating set of \(H_{n-2}\), by Lemma 2.6 then \(\{h_1, s_2, s_2, T\}\) \(\cup\) \(A'\) is a maximum non-crossing compatible \(M\)-alternating set of \(H_n\). By Theorem 2.4, \(af(H_n, M) = 4 + af(H_{n-2}, M')\). Let \(Y_1 = \{M \in \mathcal{M}_{f_{1,2}}^{(1,2)}(H_n) \mid p_{1,2}, q_{1,2} \in M\}\), by Eq. (4.1),

\[
\sum_{M \in Y_1} x^{af(H_n, M)} = \sum_{M' \in \mathcal{M}(H_{n-2})} x^{4+af(H_{n-2}, M')} = x^4 Af(H_n, x) .
\]

**Subcase 1.2.** If one of \(p_{1,2}, q_{1,2}\) does not belong to \(M\), then the perimeter of the triphenylene consisting of the four hexagons \(s_1, s_2, h_1, h_2\) is not \(M\)-alternating. Recall that \(M_1 \subseteq M\) is a perfect matching of the first pyrene fragment, thus \(M_2 = M \setminus M_1\) is a perfect matching of the subgraph \(G_{n-1}\) (see Fig. 1(b)). By Lemma 2.6, \(af(H_n, M) = 1 + af(G_{n-1}, M_2)\). Let \(X\) be a perfect matching of \(G_{n-1}\). Suppose \(X\) contains edges \(p_{1,2}, q_{1,2}\), then \(s_2\) and \(s_2\) both are \(X\)-alternating hexagons, and \(X_1 = X \cap E(H_{n-2})\) is a perfect matching of the subsystem \(H_{n-2}\) obtained by deleting the vertices of the leftmost diphenyl of \(G_{n-1}\) and their incident edges. Note that Lemma 2.6 also holds for the auxiliary graph \(G_n\), and \(h_2\) is not \(X\)-alternating, so \(af(G_{n-1}, X) = 2 + af(H_{n-2}, X_1)\). Let \(\mathcal{M}_{q_{1,2}}^{(2,1)}(G_{n-1}) = \{X \in \mathcal{M}(G_{n-1}) \mid p_{1,2}, q_{1,2} \in X\}\), \(Y_2 = \mathcal{M}_{f_{1,2}}^{(1,2)}(H_n) \setminus Y_1\), then

\[
\sum_{M \in Y_2} x^{af(H_n, M)} = \sum_{M \in \mathcal{M}(G_{n-1}) \setminus \mathcal{M}_{q_{1,2}}^{(2,1)}(G_{n-1})} x^{1+af(G_{n-1}, M_2)}
= \sum_{X \in \mathcal{M}(G_{n-1})} x^{af(G_{n-1}, X)} - \sum_{X \in \mathcal{M}_{q_{1,2}}^{(2,1)}(G_{n-1})} x^{af(G_{n-1}, X)}
= Af(G_{n-1}, x) - \sum_{X_1 \in \mathcal{M}(H_{n-2})} x^{2+af(H_{n-2}, X_1)}
= x Af(G_{n-1}, x) - x^3 Af(H_{n-2}, x).
\]

**Case 2.** Suppose \(e_{1,2}\) and \(f_{1,2}\) both are not in \(M\), then we can divide \(\mathcal{M}_{f_{1,2}}^{(1,2)}(H_n)\) in
two subsets \( Y_3 = \{ M \in \mathcal{M}_{f_{1,2}}(H_n) | e_{2,1}, f_{2,1} \in M \} \) and \( Y_4 = \{ M \in \mathcal{M}_{f_{1,2}}(H_n) | e_{2,1}, f_{2,1} \notin M \} \).

**Subcase 2.1.** Suppose \( M \in Y_3 \), then \( h_{2,1} \) must be an \( M \)-alternating hexagon, and the restrictions \( M_1 \) and \( M_2 \) of \( M \) on the leftmost phenanthrene \( L \) and the rightmost subsystem \( H_{n-2} \) are perfect matchings of \( L \) and \( H_{n-2} \) respectively (see Fig. 1(a)). Let \( \mathcal{A}' \) be a maximum non-crossing compatible \( M_3 \)-alternating set of \( H_{n-2} \). Note that \( M_1 \) contains only five distinct members, we can divide \( Y_3 \) in five subsets: \( Y_{3,1} = \{ M \in Y_3 | p_{1,2}, q_{1,2} \in M \} \), \( Y_{3,2} = \{ M \in Y_3 | p_{1,1}, q_{1,1} \in M \} \), \( Y_{3,3} = \{ M \in Y_3 | e_{1,1}, f_{1,1} \in M \} \), \( Y_{3,4} = \{ M \in Y_3 | p_{1,2} \in M, q_{1,2} \notin M \} \), \( Y_{3,5} = \{ M \in Y_3 | p_{1,2} \notin M, q_{1,2} \in M \} \). If \( M \in Y_{3,1} \), then the four hexagons \( h_{1,2}, h_{2,1}, s_{1,2}, s_{2,2} \) form a triphenylene whose perimeter \( T \) is an \( M \)-alternating cycle, and \( \{s_{1,1}, s_{1,2}, h_{2,1}, T \} \) is a non-crossing compatible \( M \)-alternating set. By Lemma 2.6, \( \{s_{1,1}, s_{1,2}, h_{2,1}, T \} \cup \mathcal{A}' \) is a maximum non-crossing compatible \( M \)-alternating set of \( H_n \). By Theorem 2.4, \( a_f(H_n, M) = 4 + a_f(H_{n-2}, M_2) \), which implies that \( \sum_{M \in Y_{3,1}} x_{a_f(H_n, M)} = x^4 A_f(H_{n-2}, x) \). If \( M \in Y_{3,2}, \) then \( \{s_{1,1}, s_{1,2}, h_{1,1}, h_{2,1}\} \) is a non-crossing compatible \( M \)-alternating set, and \( \{s_{1,1}, s_{1,2}, h_{1,1}, h_{2,1}\} \cup \mathcal{A}' \) is a maximum non-crossing compatible \( M \)-alternating set of \( H_n \). By Theorem 2.4, \( a_f(H_n, M) = 2 + a_f(H_{n-2}, M_2) \), we have \( \sum_{M \in Y_{3,2}} x_{a_f(H_n, M)} = x^2 A_f(H_{n-2}, x) \). If \( M \in Y_{3,3}, \) then \( \{h_{1,1}, h_{2,1}\} \cup \mathcal{A}' \) is a maximum non-crossing compatible \( M \)-alternating set of \( H_n \). By Theorem 2.4, \( a_f(H_n, M) = 3 + a_f(H_{n-2}, M_2) \), thus \( \sum_{M \in Y_{3,3}} x_{a_f(H_n, M)} + \sum_{M \in Y_{3,4}} x_{a_f(H_n, M)} = 2 x^3 A_f(H_{n-2}, x) \). Finally, we have

\[
\sum_{M \in Y_3} x_{a_f(H_n, M)} = \sum_{j=1}^{5} \sum_{M \in Y_{3,j}} x_{a_f(H_n, M)} = (2x^4 + 2x^3 + x^2) A_f(H_{n-2}, x).
\]

**Subcase 2.2.** If \( M \in Y_4 \), then the common vertical edge \( d \) of \( h_{1,2} \) and \( h_{2,1} \) belongs to \( M \), and the restrictions \( M_1 \) and \( M_2 \) of \( M \) on the leftmost pyrene fragment \( H_1 \) and the rightmost subsystem \( H_{n-1} \) are perfect matchings of \( H_1 \) and \( H_{n-1} \) respectively (see Fig. 1(a)). We divide \( \mathcal{M}(H_1) \) in two subsets: \( \mathcal{M}_d(H_1) = \{ M_1 \in \mathcal{M}(H_1) | d \in M_1 \} \), \( \mathcal{M}_d(H_1) = \{ M_1 \in \mathcal{M}(H_1) | d \notin M_1 \} \). Note that \( \mathcal{M}_d(H_1) \) contains only one perfect matching \( M'_1 \) of \( H_1 \), and \( h_{1,2} \) is the unique \( M'_1 \)-alternating hexagon in \( H_1 \), so \( a_f(H_1, M'_1) = 1 \), we have

\[
\sum_{M_1 \in \mathcal{M}_d(H_1)} x_{a_f(H_1, M_1)} = \sum_{M_1 \in \mathcal{M}(H_1)} x_{a_f(H_1, M_1)} - \sum_{M'_1 \in \mathcal{M}_d(H_1)} x_{a_f(H_1, M'_1)} = A_f(H_1, x) - x = 2x^3 + 2x^2 + x.
\]

We also divide \( \mathcal{M}(H_{n-1}) \) in two subsets: \( \mathcal{M}_d(H_{n-1}) = \{ M_2 \in \mathcal{M}(H_{n-1}) | d \in M_2 \} \), \( \mathcal{M}_d(H_{n-1}) = \{ M_2 \in \mathcal{M}(H_{n-1}) | d \notin M_2 \} \). Suppose \( M_2 \in \mathcal{M}_d(H_{n-1}) \), then \( e_{2,1}, f_{2,1} \in \mathcal{M}_d(H_{n-1}) \), then \( e_{2,1}, f_{2,1} \in \mathcal{M}_d(H_{n-1}) \).
$M_2$ and $h_{2,1}$ is an $M_2$-alternating hexagon, and the restriction $M'_2$ of $M_2$ on the rightmost subsystem $H_{n-2}$ is a perfect matching of $H_{n-2}$. Let $A'$ be a maximum non-crossing compatible $M'_2$-alternating set of $H_{n-2}$. Then $A' \cup \{h_{2,1}\}$ is a maximum non-crossing compatible $M_2$-alternating set of $H_{n-1}$. Thus $a_f(H_{n-1,M_2}) = 1 + a_f(H_{n-2,M'_2})$, we have

$$
\sum_{M_2 \in \mathcal{M}_d(H_{n-1})} x^{a_f(H_{n-1},M_2)} = \sum_{M_2 \in \mathcal{M}(H_{n-1})} x^{a_f(H_{n-1},M_2)} - \sum_{M_2 \in \mathcal{M}_d(H_{n-1})} x^{a_f(H_{n-1},M_2)} = A_f(H_{n-1},x) - \sum_{M_2 \in \mathcal{M}(H_{n-2})} x^{1+a_f(H_{n-2},M'_2)} = A_f(H_{n-1},x) - xA_f(H_{n-2},x). (4.7)
$$

Recall that $d$ is the common edge of $h_{1,2}$ and $h_{2,1}$, for any $M \in Y_4$, then $M = M_1 \cup M_2$, where $M_1$ is a perfect matching of the first pyrene fragment $H_1$ and $M_2$ is a perfect matching of the rightmost subsystem $H_{n-1}$, and $\{d\} = M_1 \cap M_2$. By Theorem 2.4 and Lemma 2.6, we have $a_f(H_n,M) = a_f(H_1,M_1) + a_f(H_{n-1},M_2)$. According to Eqs. (4.6) and (4.7), we have

$$
\sum_{M \in Y_4} x^{a_f(H_n,M)} = \sum_{M_1 \in \mathcal{M}_d(H_1), M_2 \in \mathcal{M}_d(H_{n-1})} x^{a_f(H_1,M_1) + a_f(H_{n-1},M_2)} = \left( \sum_{M_1 \in \mathcal{M}_d(H_1)} x^{a_f(H_1,M_1)} \right) \left( \sum_{M_2 \in \mathcal{M}_d(H_{n-1})} x^{a_f(H_{n-1},M_2)} \right) = (2x^3 + 2x^2 + x)(A_f(H_{n-1},x) - xA_f(H_{n-2},x)) = (2x^3 + 2x^2 + x)A_f(H_{n-1},x) - (2x^4 + 2x^3 + x^2)A_f(H_{n-2},x). (4.8)
$$

By Eqs. (4.3), (4.4), (4.5) and (4.8), we obtain a recursive relation as below:

$$
A_f(H_n,x) = \sum_{M \in \mathcal{M}(H_n)} x^{a_f(H_n,M)} = \sum_{M \in Y_1} x^{a_f(H_{n-1},x)} + \sum_{M \in Y_2} x^{a_f(H_{n-1},x)} + \sum_{M \in Y_3} x^{a_f(H_{n-1},x)} + \sum_{M \in Y_4} x^{a_f(H_{n-1},x)} = (2x^3 + 2x^2 + x)A_f(H_{n-1},x) + (x^4 - x^3)A_f(H_{n-2},x) + xA_f(G_{n-1},x). (4.9)
$$

By a similar discussion as above, we can prove the following recursive formula for the auxiliary graph $G_n$ (see Fig. 1(b))

$$
A_f(G_n,x) = (x^3 + 3x^2)A_f(H_{n-1},x) + (x^4 - x^3)A_f(H_{n-2},x) + xA_f(G_{n-1},x). (4.10)
$$

Eq. (4.9) subtracts Eq. (4.10), we have

$$
A_f(G_n,x) = A_f(H_n,x) - (x^3 - x^2 + x)A_f(H_{n-1},x),
$$
so
\[ A_f(G_{n-1}, x) = A_f(H_{n-1}, x) - (x^3 - x^2 + x)A_f(H_{n-2}, x). \]

Substituting this expression into Eq. (4.9), we can obtain the Eq. (4.2), the proof is completed.

By theorem 4.1, we can obtain an explicit expression as below.

**Theorem 4.2.** Let \( H_n \) be the pyrene system with \( n \) pyrene fragments. Then

\[ A_f(H_n, x) = x^n \sum_{l=0}^{2n} \sum_{i=\begin{array}{c}1 \leq j \leq l \end{array}}^{n} (-1)^{n-i} 2^{i-n} \left( \binom{i}{2i-n} \right) \left( \binom{j}{l-j} \right) x^l. \quad (4.11) \]

**Proof.** Let \( A_n := A_f(H_n, x) \), then the generating function of sequence \( \{A_n\}_{n=0}^{\infty} \) is

\[ G(t) = \sum_{n=0}^{\infty} A_n t^n = 1 + (2x^3 + 2x^2 + 2x)t \sum_{n=2}^{\infty} A_n t^n \]

\[ = 1 + (2x^3 + 2x^2 + 2x)t \sum_{n=2}^{\infty} ((2x^3 + 2x^2 + 2x)A_{n-1} - x^2A_{n-2})t^n \]

\[ = 1 + (2x^3 + 2x^2 + 2x)t \sum_{n=0}^{\infty} A_n t^n - x^2t^2 \sum_{n=0}^{\infty} A_n t^n \]

\[ = 1 + (2x^3 + 2x^2 + 2x)tG(t) - x^2t^2G(t). \]

So

\[ G(t) = \frac{1}{1 - ((2x^3 + 2x^2 + 2x)t - x^2t^2)} \]

\[ = \sum_{i=0}^{\infty} ((2x^3 + 2x^2 + 2x)t - x^2t^2)^i \]

\[ = \sum_{i=0}^{\infty} \sum_{j=0}^{i} \binom{i}{j} (2x^3 + 2x^2 + 2x)^j t^i (-x^2t^2)^{i-j} \]

\[ = \sum_{i=0}^{\infty} \sum_{n=i}^{2i} (-1)^{n-i} 2^{i-n} \binom{i}{2i-n} (x^2 + x + 1)^{2i-n} x^n t^n \]

\[ = \sum_{n=0}^{\infty} \sum_{i=\begin{array}{c}n \leq i \leq \frac{n}{2} \end{array}} (-1)^{n-i} 2^{i-n} \binom{i}{2i-n} (x^2 + x + 1)^{2i-n} x^n t^n, \]

15
we have

\[
Af(H_n, x) = \sum_{i=\lceil \frac{n}{2} \rceil}^{n} (-1)^{n-i} 2^{2i-n} \left( \binom{i}{2i-n} \right) (x^2 + x + 1)^{2i-n}
\]

\[
= \sum_{i=\lceil \frac{n}{2} \rceil}^{n} (-1)^{n-i} 2^{2i-n} \binom{i}{2i-n} \sum_{j=0}^{\frac{i}{2}-n} \binom{j}{2i-n} \sum_{k=0}^{j} \binom{j}{k} x^k
\]

\[
= \sum_{i=\lceil \frac{n}{2} \rceil}^{n} (-1)^{n-i} 2^{2i-n} \binom{i}{2i-n} \sum_{l=j}^{\frac{i}{2}} \binom{j}{2i-n} \binom{j}{l-j} x^l
\]

\[
= \sum_{i=\lceil \frac{n}{2} \rceil}^{n} \sum_{l=0}^{\frac{n}{2}} \sum_{j=\frac{l}{4}}^{\frac{n}{4}} (-1)^{n-i} 2^{2i-n} \binom{i}{2i-n} \binom{j}{2i-n} \binom{j}{l-j} x^l.
\]

\[\square\]

According to Theorem 4.2, the following corollary is immediate.

**Corollary 4.3.** Let \( H_n \) be a pyrene system with \( n \) pyrene fragments. Then

1. \( af(H_n) = n \);
2. \( A\varepsilon f(H_n) = 3n \);
3. \( \text{Spec}_{af}(H_n) = [n, 3n] \).

In the following, we will calculate the sum over the anti-forcing numbers of all perfect matchings of \( H_n \), and investigate its asymptotic behavior.

**Theorem 4.4.** The sum over the anti-forcing numbers of all perfect matchings of \( H_n \) is

\[
\frac{d}{dx}Af(H_n, x) \bigg|_{x=1} = \frac{3\sqrt{2}}{64} (3 - 2\sqrt{2})^n + \frac{17 - 12\sqrt{2}}{16} n(3 - 2\sqrt{2})^n - \frac{3\sqrt{2}}{64} (3 + 2\sqrt{2})^n
\]

\[ + \frac{17 + 12\sqrt{2}}{16} n(3 + 2\sqrt{2})^n. \]

\[ (4.12) \]

**Proof.** By Theorem 4.1,

\[
\frac{d}{dx}Af(H_n, x) = (6x^2 + 4x + 2)Af(H_{n-1}, x) + (2x^3 + 2x^2 + 2x) \frac{d}{dx}Af(H_{n-1}, x)
\]

\[ - 2x Af(H_{n-2}, x) - x^2 \frac{d}{dx}Af(H_{n-2}, x). \]

\[ (4.13) \]

For convenience, let \( \Phi_n := \Phi(H_n) \) and \( AF_n := \frac{d}{dx}Af(H_n, x) \bigg|_{x=1} \), by Eq. \[ (4.13) \], we have

\[
AF_n = 6AF_{n-1} - AF_{n-2} + 12\Phi_{n-1} - 2\Phi_{n-2}.
\]

\[ (4.14) \]
By Eq. (3.5), $\Phi_n = 6\Phi_{n-1} - \Phi_{n-2}$, so $AF_n = 6AF_{n-1} - AF_{n-2} + 2\Phi_n$, which implies $2\Phi_n = AF_n - 6AF_{n-1} + AF_{n-2}$. Therefore $2\Phi_{n-1} = AF_{n-1} - 6AF_{n-2} + AF_{n-3}$ and $2\Phi_{n-2} = AF_{n-2} - 6AF_{n-3} + AF_{n-4}$, substituting them into Eq. (4.14), we obtain the following recurrence formula

$$AF_n = 12AF_{n-1} - 38AF_{n-2} + 12AF_{n-3} - AF_{n-4}.$$  \hspace{1cm} (4.15)

Note that recurrence formulas (3.8) and (4.15) have the same homogeneous characteristics equation, so the general solution of Eq. (4.15) is $AF_n = \lambda_1(3 - 2\sqrt{2})^n + \lambda_2n(3 - 2\sqrt{2})^n + \lambda_3(3 + 2\sqrt{2})^n + \lambda_4n(3 + 2\sqrt{2})^n$. By the initial values $AF_5 = 70956$, $AF_7 = 496794$, $AF_9 = 22531256$, we have $\lambda_1 = \frac{3\sqrt{2}}{64}$, $\lambda_2 = \frac{17-12\sqrt{2}}{16}$, $\lambda_3 = -\frac{3\sqrt{2}}{64}$ and $\lambda_4 = \frac{17+12\sqrt{2}}{16}$, so Eq. (4.12) holds for $n \geq 5$. We can check that Eq. (4.12) also holds for $n = 0, 1, 2, 3, 4$, the proof is completed. \hfill \Box

By Eq. (3.6) and Eq. (4.12), we can prove the following corollary.

**Corollary 4.5.** Let $H_n$ be a pyrene system with $n$ pyrene fragments. Then

$$\lim_{n \to \infty} \frac{AF_n}{n\Phi_n} = 1 + \frac{3\sqrt{2}}{4}.$$  

\[\]

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