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Transfer-matrix Calculation of the Clar Covering Polynomial of Hexagonal Systems*

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Abstract

In the paper, a transfer-matrix expression of the Clar covering polynomial of some hexagonal systems is given. As examples, we present the explicit expressions of the Clar covering polynomials of several types of hexagonal systems. Consequently, a series of topological indices such as Clar number, Kekulé structure count and the first Herndon number are obtained. For any unbranched catacondensed hexagonal system, a method for determining its Clar covering polynomial is also presented.

1 Introduction

Transfer-matrix method is widely used in statistical mechanics and mathematical chemistry. There are many investigations about the enumeration of matchings by using this tool [1, 3, 8, 9, 11]. Babić et al. [2] determined the matching polynomial of a polygraph. Randić et al. [12] gave an algorithm for obtaining the matching polynomial of an unbranched catacondensed hexagonal system.

A hexagonal system is a finite 2-connected plane graph in which every interior face is bounded by a regular hexagon. Its subgraph is called a generalized hexagonal system. The Clar covering polynomial of a (generalized) hexagonal system was first introduced by H. Zhang and F. Zhang [15], and thus called Zhang-Zhang polynomial [4]. It unifies many

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useful topological indices such as Clar number, the number of Kekulé structures and the first Herndon number. Gutman et al. [5, 6] showed that the Clar covering polynomial is related to resonance energy, and some basic properties of $P(G;1)$ were established. The Clar covering polynomial of a hexagonal system can be used to estimate the resonance energy of a hexagonal system [13] and to deal with the comparison of topological properties of some S, T-isomers [14]. Gutman et al. [4] gave an explicit combinatorial expression of the Clar covering polynomial of a large class of pericondensed benzenoid systems, the multiple linear hexagonal chains $M_{n,m}$. C. Lin and G. Fan [10] showed a compute method for calculating the Clar covering polynomial. In this paper, a transfer-matrix expression of the Clar covering polynomial of a sort of hexagonal systems is given. As examples, the explicit formulae of the Clar covering polynomials of several hexagonal systems are presented. The sextet polynomials of these hexagonal systems are also given here. For any unbranched catacondensed hexagonal system, a method for determining its Clar covering polynomial can be obtained.

2 Preliminary

For convenience, the hexagonal systems we considered are generalized hexagonal systems.

Let G be a generalized hexagonal system. A subgraph H of G is called a Clar cover if it is the union of some mutually disjoint hexagons and independent edges and it covers every vertex of G. When the number of hexagons in H is k, we call H a k-Clar cover. A Kekulé structure (perfect matching) is a Clar cover which is composed of independent edges. Denote the number of Kekulé structures of G by $K(G)$. A subgraph H of G is said to be a nice subgraph of G if $G-H$ has a perfect matching. All the hexagons in a Clar cover form a sextet pattern. A sextet pattern is said to be a Clar formula if it has the maximum number of hexagons. The number of hexagons in a Clar formula of G is called the Clar number of G and denoted by $C(G)$. The Clar covering polynomial of G is defined as follows:

$$P(G;x) = \sum_{k=0}^{C(G)} c(G;k)x^k,$$

where $c(G;k)$ is the number of k-Clar covers of G.

The following theorem shows that many useful topological indices can be got from the Clar covering polynomial of a hexagonal system.

Theorem 1 *[15] Let G be a hexagonal system. Then we have the following properties for the Clar covering polynomial of G:*

(1) $K(G) = c(G;0)$,

(2) the degree of the polynomial $P(G;x)$ is $C(G)$, the Clar number of G,

(3) the coefficient of the highest degree term, $c(G; C(G))$ equals the number of Clar formulas of G,

(4) $h_1(G) = c(G; 1)$, where $h_1(G)$ is the first Herndon number.

In 1975, Hosoya and Yamaguchi[7] proposed the concept of sextet polynomial of a hexagonal system :

$$\sigma(G; x) = \sum_{k=0}^{C(G)} s(G; k)x^k,$$

where $s(G; k)$ is the number of all sextet patterns with k hexagons in G.

The correlation between Clar covering polynomial and sextet polynomial of a class of hexagonal system is given as follows.

Theorem 2 *[16] Let G be a hexagonal system with a perfect matching. Then*

(1) the Clar covering polynomial $P(G; x)$ of G can be expressed in the following form:

$$P(G; x) = \sum_{i=0}^{C(G)} c(G; i)x^i = \sum_{i=0}^{C(G)} a(G; i)(x + 1)^i,$$

(2) $\sum_{i=0}^{C(G)} a(G; i)x^i$ is the sextet polynomial of G if and only if G has no coronene (see Figure 1) as its nice subgraph.

Figure 1: coronene

By the above theorem, we know that if G is a hexagonal system with a perfect matching and has no coronene as its nice subgraph, then the following equation holds:

$$P(G; x) = \sum_{i=0}^{C(G)} c(G; i)x^i = \sum_{i=0}^{C(G)} a(G; i)(x + 1)^i = \sum_{i=0}^{C(G)} s(G; i)(x + 1)^i = \sigma(G; x + 1). \quad (2.1)$$

3 Transfer-matrix method

In this section, we give a transfer-matrix expression of the Clar covering polynomial of a sort of hexagonal systems.

Let G_1 and G_2 be two generalized hexagonal systems and they are connected by two disjoint edges e and e' which lie in a common hexagon, say C. As we see in Figure 2.

Let $G = G_1 \cup G_2 \cup \{e, e'\}$ and $X = \{e, e'\}$. Let $W_1^X = \emptyset, W_2^X = \{e\}, W_3^X = \{e'\}, W_4^X = \{e, e'\}, W_5^X = C$. $c(G(W_i^X); k)$ is the number of k-Clar covers H of G such that $H \cap X = W_i^X$, $i = 1, 2, 3, 4$. $c(G(W_5^X); k)$ is the number of k-Clar covers H of G such that $C \in H$. Let $c(G_m(W_i^X); k)$ be the number of k-Clar covers H of the generalized hexagonal system $G_m - W_i^X$, where $G_m - W_i^X$ is obtained from G_m by deleting all the vertices that are incident with edges in W_i^X, $i = 1, \cdots, 5$, $m = 1, 2$. Then we have

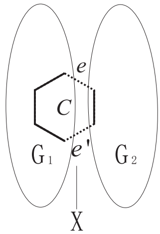


Figure 2: G, G_1, G_2 and X.

$$c(G(W_i^X); k) = \sum_{j=0}^{k} c(G_1(W_i^X); j)c(G_2(W_i^X); k-j), \ i = 1, \cdots, 4,$$

$$c(G(W_5^X); k) = \sum_{j=0}^{k-1} c(G_1(W_5^X); j)c(G_2(W_5^X); k-1-j).$$

Lemma 3

$$\sum_k c(G(W_i^X); k)x^k = (\sum_k c(G_1(W_i^X); k)x^k)(\sum_k c(G_2(W_i^X); k)x^k), \ i = 1, \cdots, 4,$$

$$\sum_k c(G(W_5^X); k)x^k = (\sum_k c(G_1(W_5^X); k)x^{k+\frac{1}{2}})(\sum_k c(G_2(W_5^X); k)x^{k+\frac{1}{2}}).$$

□

Let $P^*(G_m^{i(X)}; x) = \sum_k c(G_m(W_i^X); k)x^k$, $i = 1, \cdots, 4$, and
$P^*(G_m^{5(X)}; x) = \sum_k c(G_m(W_5^X); k)x^{k+\frac{1}{2}}$, $m = 1, 2$. Then lemma 3 can be rewritten as:

$$\sum_k c(G(W_i^X); k)x^k = P^*(G_1^{i(X)}; x)P^*(G_2^{i(X)}; x), \ i = 1, \cdots, 5. \tag{3.1}$$

Lemma 4 *$P(G; x) = L_1^X (L_2^X)^T$, where L_m^X is a vector of dimension 5 with the i-th element $(L_m^X)_i = P^*(G_m^{i(X)}; x)$, $1 \le i \le 5$, $m = 1, 2$.*

Proof:

$$\begin{aligned} P(G;x) &= \sum_k c(G;k)x^k = \sum_k (\sum_{i=1}^{5} c(G(W_i^X);k))x^k = \sum_{i=1}^{5}(\sum_k c(G(W_i^X);k)x^k) \\ &\overset{(3.1)}{=} \sum_{i=1}^{5} P^*(G_1^{i(X)};x)P^*(G_2^{i(X)};x) = L_1^X(L_2^X)^T. \end{aligned}$$ □

Consider a generalized hexagonal system $G(n) = G_1 \cup X_1 \cup G_2 \cdots \cup X_{n-1} \cup G_n$, which is illustrated in Figure 3. Before approaching to the main theorem, we give some notations here. Denote $c(G_m(W_i^{X_p}, W_j^{X_q});k)$ the number of k-Clar covers of the generalized hexagonal system $G_m - (W_i^{X_p} \cup W_j^{X_q}),\ m = 1, \cdots, n$.

$X_i = \{e_i, e_i'\}$, $W_1^{X_i} = \emptyset, W_2^{X_i} = \{e_i\}, W_3^{X_i} = \{e_i'\}, W_4^{X_i} = \{e_i, e_i'\}, W_5^{X_i} = C_i$.

$G_{i,(i+1),\cdots,j} = G_i \cup X_i \cup G_{i+1} \cdots \cup X_{j-1} \cup G_j$.

$P^*(G_m^{i,j(X_p,X_q)};x) = \sum_k c(G_m(W_i^{X_p}, W_j^{X_q});k)x^k,\ i \neq 5$ and $j \neq 5$.

$P^*(G_m^{i,j(X_p,X_q)};x) = \sum_k c(G_m(W_i^{X_p}, W_j^{X_q});k)x^{k+\frac{1}{2}},\ i = 5, j \neq 5$ or $i \neq 5, j = 5$.

$P^*(G_m^{i,j(X_p,X_q)};x) = \sum_k c(G_m(W_i^{X_p}, W_j^{X_q});k)x^{k+1},\ i = 5$ and $j = 5$.

$P^*(G_m(W_i^{X_p}, W_j^{X_q});x) = \sum_k c(G_m(W_i^{X_p}, W_j^{X_q});k)x^k,\ i = 1, \cdots, 4$.

$P^*(G_m(W_i^{X_p}, W_j^{X_q});x) = \sum_k c(G_m(W_i^{X_p}, W_j^{X_q});k)x^{k+\frac{1}{2}},\ i = 5$.

Obviously,

$P^*(G_m^{i,j(X_p,X_q)};x) = P^*(G_m(W_i^{X_p}, W_j^{X_q});x),\ j \neq 5$.

$P^*(G_m^{i,j(X_p,X_q)};x) = P^*(G_m(W_i^{X_p}, W_j^{X_q});x)x^{\frac{1}{2}},\ j = 5$.

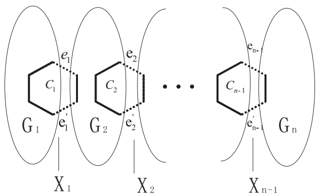


Figure 3: $G(n)$

Theorem 5 *For any* $n \geq 2$,

$$P(G(n);x) = L_1^{X_1} \prod_{i=1}^{n-2} T_{i(i+1)}(L_n^{X_{n-1}})^T,$$

where $L_1^{X_1}$ and $L_n^{X_{n-1}}$ are two vectors of dimension 5, $(L_1^{X_1})_i = P^*(G_1^{i(X_1)};x)$, $(L_n^{X_{n-1}})_i = P^*(G_n^{i(X_{n-1})};x)$, $i = 1, \cdots, 5$. Transfer-matrix $T_{i(i+1)}$ is a 5×5 matrix with $[T_{i(i+1)}]_{lm} = P^*(G_{i+1}^{l,m(X_i,X_{i+1})};x)$, $1 \leq l \leq 5$, $1 \leq m \leq 5$.

Proof: We apply induction on n ($n \geq 2$). For $n = 2$, the assertion is true by Lemma 4. Assume it states for $n-1$, consider $G(n)$ ($n > 2$). By Lemma 4,

$$P(G(n); x) \;=\; (P^*(G^{1(X_{n-1})}_{1,\cdots,n-1}; x), \cdots, P^*(G^{5(X_{n-1})}_{1,\cdots,n-1}; x))$$
$$(P^*(G^{1(X_{n-1})}_{n}; x), \cdots, P^*(G^{5(X_{n-1})}_{n}; x))^T, (3.2)$$

where, $G^{i(X_{n-1})}_{1,\cdots,n-1} = G_{1,\cdots,n-1} - W_i^{X_{n-1}}$ Then by induction hypothesis, for $i = 1, \cdots, 4$,
$P^*(G^{i(X_{n-1})}_{1,\cdots,n-1}; x) = \sum_k c(G_{1,\cdots,n-1}(W_i^{X_{n-1}}); k)x^k$

$$= L_1^{X_1} \prod_{i=1}^{n-3} T_{i(i+1)}(P^*(G_{n-1}(W_1^{X_{n-2}}, W_i^{X_{n-1}}); x), \cdots, P^*(G_{n-1}(W_5^{X_{n-2}}, W_i^{X_{n-1}}); x))^T,$$

and
$P^*(G^{5(X_{n-1})}_{1,\cdots,n-1}; x) = \sum_k c(G_{1,\cdots,n-1}(W_5^{X_{n-1}}); k)x^{k+\frac{1}{2}}$
$= (\sum_k c(G_{1,\cdots,n-1}(W_5^{X_{n-1}}); k)x^k)x^{\frac{1}{2}}$
$= L_1^{X_1} \prod_{i=1}^{n-3} T_{i(i+1)}(P^*(G_{n-1}(W_1^{X_{n-2}}, W_5^{X_{n-1}}); x), \cdots, P^*(G_{n-1}(W_5^{X_{n-2}}, W_5^{X_{n-1}}); x))^T x^{\frac{1}{2}}.$

That is, for $i = 1, \cdots, 5$,

$$P^*(G^{i(X_{n-1})}_{1,\cdots,n-1}; x) = L_1^{X_1} \prod_{i=1}^{n-3} T_{i(i+1)}(P^*(G^{1,i(X_{n-2},X_{n-1})}_{n-1}; x), \cdots, P^*(G^{5,i(X_{n-2},X_{n-1})}_{n-1}; x))^T,$$

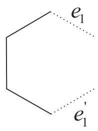
Then
$(P^*(G^{1(X_{n-1})}_{1,\cdots,n-1}; x), \cdots, P^*(G^{5(X_{n-1})}_{1,\cdots,n-1}; x)) = L_1^{X_1} \prod_{i=1}^{n-3} T_{i(i+1)} \cdot T_{(n-2)(n-1)},$

By (3.2), we have that
$P(G(n); x) = L_1^{X_1} \prod_{i=1}^{n-2} T_{i(i+1)}(L_n^{X_{n-1}})^T.$

□

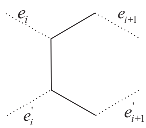
4 Applications of Theorem 5

In [15], the recurrence for the Clar covering polynomial of unbranched catacondensed hexagonal system (also called hexagonal chain) is given. As a conclusion of Theorem 5, the Clar covering polynomial of unbranched catacondensed can be presented as the multiplication of some matrices. The patterns of fusions determine the sequences of matrices. For unbranched catacondensed hexagonal system:

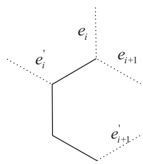


$$L_1^{X_1} = L = (1, 0, 0, 1, x^{\frac{1}{2}}),$$

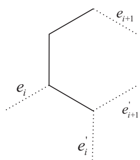
$$L_n^{X_{n-1}} = R = (1, 0, 0, 1, x^{\frac{1}{2}})^T,$$



$$T_{i(i+1)} = I = \begin{pmatrix} 1 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & x^{\frac{1}{2}} & 0 \end{pmatrix},$$



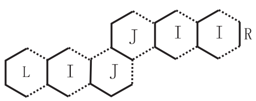
$$T_{i(i+1)} = J = \begin{pmatrix} 1 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ x^{\frac{1}{2}} & 0 & 0 & 0 & 0 \end{pmatrix},$$



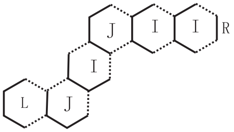
$$T_{i(i+1)} = K = \begin{pmatrix} 1 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ x^{\frac{1}{2}} & 0 & 0 & 0 & 0 \end{pmatrix}.$$

It is easy to see that $L = R$ and $J = K$.

We calculate the Clar covering polynomials of two small unbranched catacondensed hexagonal systems to illustrate how we work with this method.



$$P(G; x) = LIJ^2I^2R = 15 + 22x + 8x^2.$$



$$P(G;x) = LJIJI^2R = 17 + 28x + 14x^2 + 2x^3.$$

In the following, we get the explicit formulae of the Clar covering polynomials of some hexagonal systems. Combine the facts shown in Section 2, we also give the sextet polynomials and some topological indices of these hexagonal systems.

As before, let $W_1^{X_i} = \emptyset$, $W_2^{X_i} = \{e_i\}$, $W_3^{X_i} = \{e_i'\}$, $W_4^{X_i} = \{e_i, e_i'\}$, $W_5^{X_i} = C_i$.
Example 1. Let $F(n)$ be a hexagonal system (see Figure 4), $n \geq 2$. Then

$L_1^{X_1} = (x^2 + 5x + 5, 0, 0, 1, x^{\frac{1}{2}})$,

$L_n^{X_{n-1}} = (1, 0, 0, 1, x^{\frac{1}{2}})$,

$T_{i(i+1)} = T, \quad \forall\, i \in \{1, \cdots, n-2\}$.

$P(F(n);x) = (x^2 + 5x + 5, 0, 0, 1, x^{\frac{1}{2}})T^{n-2}(1, 0, 0, 1, x^{\frac{1}{2}})^T$.

where

$$T = \begin{pmatrix} x^2+5x+5 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ x^2+4x+4 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ x^{\frac{1}{2}}(x^2+4x+4) & 0 & 0 & x^{\frac{1}{2}} & x \end{pmatrix}$$

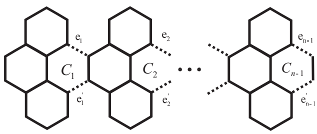


Figure 4: The hexagonal system $F(n)$

Now we put the concrete expressions of vectors and formula of $P(F(n);x)$ into the software *Mathematica* and run: *L.MatrixPower[T, n-2].R*. We get the explicit expression of the Clar polynomial of $F(n)$ and also the expression of the number of Kekulé structures when we put $x = 0$ in $P(F(n);x)$. Note that we get all the expressions in the following examples with the same way.

The Clar covering polynomials of $F(n)$ is

$$P(F(n);x) = \frac{1}{2^n(2+x)\sqrt{8+8x+8x^2}}\Bigg(\Big(6+6x+x^2+(2+x)\sqrt{8+8x+x^2}\Big)^n - \Big(6+6x+x^2-(2+x)\sqrt{8+8x+8x^2}\Big)^n\Bigg) \qquad (4.1).$$

In Appendix, we give the Clar covering polynomials of $F(n)$ for small n, see Table 1. Let $x = 0$ in $P(F(n);x)$ then we obtain the number of Kekulé structures of $F(n)$:

$$K(F(n)) = \frac{(3+2\sqrt{2})^n - (3-2\sqrt{2})^n}{4\sqrt{2}} = \frac{(\sqrt{2}+1)^{2n} - (\sqrt{2}-1)^{2n}}{4\sqrt{2}}.$$

It is clear that $C(F(G)) = 2(n-1)$.
Let $x = 0$ in $P'(F(n);x)$ then we obtain the first Herndon number of $F(n)$:

$$h_1(F(n)) = \frac{n-1}{4\sqrt{2}}\Big((3+2\sqrt{2})^n - (3-2\sqrt{2})^n\Big) = (n-1)K(F(n)).$$

It is easy to see that $F(n)$ has no coronene as its nice subgraphs, as in (2.1), we can get the sextet polynomials of $F(n)$ immediately:

$$\begin{aligned}\sigma(F(n);x) &= P(F(n);x-1)\\ &= \frac{1}{2^n\,(1+x)\,\sqrt{1+6x+x^2}}\Bigg(\Big(1+4x+x^2+(1+x)\sqrt{1+6x+x^2}\Big)^n - \Big(1+4x+x^2-(1+x)\sqrt{1+6x+x^2}\Big)^n\Bigg).\end{aligned}$$

Example 2. Let $L(n)$ be a hexagonal system (see Figure 5), $n \geq 2$.

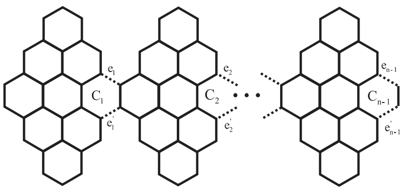


Figure 5: The hexagonal system $L(n)$

$$P(L(n);x) = (x^3+12x^2+29x+19, 0, 0, 1, x^{\frac{1}{2}})T^{n-2}(1, 0, 0, 1, x^{\frac{1}{2}})^T.$$

where

$$T=\begin{pmatrix} x^3+12x^2+29x+19 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ x^3+12x^2+28x+18 & 0 & 0 & 1 & x^{\frac{1}{2}} \\ x^{\frac{1}{2}}(x^3+12x^2+28x+18) & 0 & 0 & x^{\frac{1}{2}} & x \end{pmatrix}.$$

$$P(L(n);x)=\frac{1}{2^n\cdot\sqrt{396+1192x+1376x^2+760x^3+204x^4+24x^5+x^6}}$$
$$\cdot\Big(\Big(20+30x+12x^2+x^3+\sqrt{396+1192x+1376x^2+760x^3+204x^4+24x^5+x^6}\Big)^n$$
$$-\Big(20+30x+12x^2+x^3-\sqrt{396+1192x+1376x^2+760x^3+204x^4+24x^5+x^6}\Big)^n\Big) \quad (4.2).$$

In Appendix, we also give the Clar covering polynomials of $L(n)$ for small n, see Table 2. Similarly, we obtain the $C(L(n)), K(L(n))$ and $h_1(L(n))$:

$$\begin{aligned} C(L(n)) &= 3(n-1), \\ K(L(n)) &= \frac{(10+3\sqrt{11})^n-(10-3\sqrt{11})^n}{6\sqrt{11}}, \\ h_1(L(n)) &= \frac{1}{6534}\Big(\Big(99\sqrt{11}n+165n-149\sqrt{11}\Big)\Big(10+3\sqrt{11}\Big)^n \\ &\quad -\Big(99\sqrt{11}n-165n-149\sqrt{11}\Big)\Big(10-3\sqrt{11}\Big)^n\Big). \end{aligned}$$

Also we can get the sextet polynomials of $L(n)$ immediately, since $L(n)$ has no coronene as its nice subgraphs:

$$\sigma(L(n);x)=\frac{1}{2^n\cdot\sqrt{1+18x+95x^2+164x^3+99x^4+18x^5+x^6}}$$
$$\cdot\Big(\Big(1+9x+9x^2+x^3+\sqrt{1+18x+95x^2+164x^3+99x^4+18x^5+x^6}\Big)^n$$
$$-\Big(1+9x+9x^2+x^3-\sqrt{1+18x+95x^2+164x^3+99x^4+18x^5+x^6}\Big)^n\Big).$$

5 Further example

Let $G(n)$ be a hexagonal system shown in Figure 6, $n\geq 2$.

By Theorem 5, we obtain

$$P(G(n);x)=(x^3+9x^2+21x+14,0,0,x^2+6x+6,x^{\frac{1}{2}}(x^2+5x+5))T^{n-2}(1,0,0,1,x^{\frac{1}{2}})^T.$$

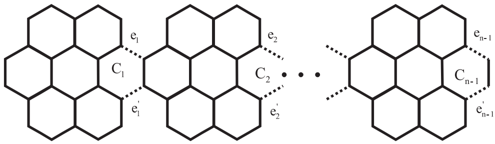


Figure 6: The hexagonal system $G(n)$

where

$$T = \begin{pmatrix} x^3+9x^2+21x+14 & 0 & 0 & x^2+6x+6 & x^{\frac{1}{2}}(x^2+5x+5) \\ 0 & 3x+4 & 0 & 0 & 0 \\ 0 & 0 & 3x+4 & 0 & 0 \\ 4x^2+12x+9 & 0 & 0 & x^2+5x+5 & x^{\frac{1}{2}}(x^2+4x+4) \\ x^{\frac{1}{2}}(4x^2+12x+9) & 0 & 0 & x^{\frac{1}{2}}(x^2+5x+5) & x(x^2+4x+4) \end{pmatrix}.$$

If we denote

$$\begin{cases} \alpha = & 2x^3+14x^2+30x+19, \\ \beta = & (2x+3)\sqrt{4x^3+28x^2+56x+33}, \\ \gamma = & 2x^4+18x^3+58x^2+86x+51, \end{cases}$$

then

$$\begin{aligned} P(G(n);x) = & \frac{(\gamma-\beta)(\alpha+\beta)^n-(\gamma+\beta)(\alpha-\beta)^n}{2^n(\gamma-\alpha)\beta} \\ = & \frac{1}{2^{n+1}(x+2)(x+4)(2x+3)\,(x^2+2x+2)\,\sqrt{4x^3+28x^2+56x+33}} \\ & \cdot\Bigg(\Big(2x^4+18x^3+58x^2+86x+51-(2x+3)\sqrt{4x^3+28x^2+56x+33}\Big) \\ & \cdot\Big(2x^3+14x^2+30x+19+(2x+3)\sqrt{4x^3+28x^2+56x+33}\Big)^n \\ & -\Big(2x^4+18x^3+58x^2+86x+51+(2x+3)\sqrt{4x^3+28x^2+56x+33}\Big) \\ & \cdot\Big(2x^3+14x^2+30x+19-(2x+3)\sqrt{4x^3+28x^2+56x+33}\Big)^n\Bigg) \quad (5.1). \end{aligned}$$

In Appendix, we also give the Clar covering polynomials of $G(n)$ for small n, see Table 3. Similarly, we obtain the $K(G(n))$ and $h_1(G(n))$:

$$
\begin{aligned}
C(L(n)) &= 3(n-1),\\
K(G(n)) &= \frac{1}{32\sqrt{33}}\left((17-\sqrt{33})\Big(\frac{19+3\sqrt{33}}{2}\Big)^n-(17+\sqrt{33})\Big(\frac{19-3\sqrt{33}}{2}\Big)^n\right),\\
h_1(G(n)) &= P'(G(n);0)\\
&= \frac{1}{46464}\bigg(\big(2541-4125n-1181\sqrt{33}+1485\sqrt{33}n\big)\Big(\frac{19+3\sqrt{33}}{2}\Big)^n\\
&\quad -\big(2541-4125n+1181\sqrt{33}-1485\sqrt{33}n\big)\Big(\frac{19-3\sqrt{33}}{2}\Big)^n\bigg).
\end{aligned}
$$

A hexagonal system G is said to be k-resonant ($k \geq 1$) if, for any $i(1 \leq i \leq k)$ disjoint hexagons $h_1, \cdots, h_i$ of G, $G - \bigcup_{j=1}^{k} h_j$ has a perfect matching. M. Zheng showed that a hexagonal system is 3-resonant if and only if it's k-resonant ($k \geq 3$) [17], and gave the construction of any 3-resonant hexagonal system in [18]. From the construction in [17], we know $G(n)$ in Figure 6 is 3-resonant, so it is k-resonant. Then any k mutually disjoint hexagons in $G(n)$ form a sextet pattern. Hence, it is not hard to see that $C(G(n)) = 3(n-1)$ and the coefficient of the highest term of $P(G(n))$ is n. Of course, this can also be obtained from $P(G(n))$ directly as above. As $G(n)$ contains coronene as its nice subgraph, equation (2.1) can not be used. But since any k mutually disjoint hexagons form a sextet pattern in $G(n)$, the transfer-matrix can be easily used here to determine its sextet polynomial, details are omitted. The order of the transfer-matrix is 2:

$$
\begin{aligned}
\sigma(G(n);x) &= \Big(1+6x+6x^2+x^3,\, x^{\frac12}(1+3x+x^2)\Big)\\
&\quad\cdot\begin{pmatrix} 1+6x+6x^2+x^3 & x^{\frac12}(1+3x+x^2)\\ x^{\frac12}(1+2x)^2 & x(1+x)^2\end{pmatrix}^{n-2}\cdot\begin{pmatrix}1\\ x^{\frac12}\end{pmatrix}\\
&= \frac{1}{2^{n+1}\left(x^4+4x^3+3x^2+2x+1\right)\sqrt{16x^5+80x^4+108x^3+61x^2+14x+1}}\\
&\quad\cdot\bigg(\Big(2x^4+10x^3+14x^2+11x+3-\sqrt{16x^5+80x^4+108x^3+61x^2+14x+1}\Big)\\
&\quad\cdot\Big(2x^3+8x^2+7x+1+\sqrt{16x^5+80x^4+108x^3+61x^2+14x+1}\Big)^n\\
&\quad-\Big(2x^4+10x^3+14x^2+11x+3+\sqrt{16x^5+80x^4+108x^3+61x^2+14x+1}\Big)\\
&\quad\cdot\Big(2x^3+8x^2+7x+1-\sqrt{16x^5+80x^4+108x^3+61x^2+14x+1}\Big)^n\bigg).
\end{aligned}
$$

Some enumeration results are illustrated in Appendix. They are all obtained in Mathematica by putting $n = 2, 3, \cdots$.

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Appendix

Table 1. Clar covering polynomial of $F(n)$:

n	Clar covering polynomial $P(F(n);x)$
2	x^2+6x+6
3	$x^4+12x^3+47x^2+70x+35$
4	$x^6+18x^5+124x^4+416x^3+718x^2+612x+204$
5	$x^8+24x^7+237x^6+1254x^5+3886x^4+7240x^3+7962x^2+4756x+1189$
6	$x^{10}+30x^9+386x^8+2800x^7+12671x^6+37398x^5+73044x^4+93504x^3+75351x^2+34650x+6930$
7	$x^{12}+36x^{11}+571x^{10}+5270x^9+31501x^8+128472x^7+366827x^6+739890x^5+1048311x^4$ $+1019860x^3+648273x^2+242346x+40391$
8	$x^{14}+42x^{13}+792x^{12}+8880x^{11}+66100x^{10}+345496x^9+1308008x^8+3646144x^7+7528102x^6$ $+11472076x^5+12721896x^4+9972288x^3+5232524x^2+1647912x+235416$
9	$x^{16}+48x^{15}+1049x^{14}+13846x^{13}+123488x^{12}+788928x^{11}+3734972x^{10}+13370424x^9$ $+36597742x^8+76915536x^7+123828046x^6+151279748x^5+137661324x^4+90318032x^3$ $+40344676x^2+10976840x+1372105$
10	$x^{18}+54x^{17}+1342x^{16}+20384x^{15}+211981x^{14}+1602426x^{13}+9124816x^{12}+40027248x^{11}$ $+137165018x^{10}+370116876x^9+788779316x^8+1325566816x^7+1745113938x^6+1777076308x^5$ $+1370321816x^4+772867840x^3+300537437x^2+71974926x+7997214.$

Table 2. Clar covering polynomial of $L(n)$:

n	Clar covering polynomial $P(L(n);x)$
2	$x^3+12x^2+30x+20$
3	$x^6+24x^5+204x^4+760x^3+1379x^2+1198x+399$
4	$x^9+36x^8+522x^7+3948x^6+17098x^5+44612x^4+71290x^3+68216x^2+35860x+7960$
5	$x^{12}+48x^{11}+984x^{10}+11312x^9+80853x^8+378642x^7+1198281x^6+2602824x^5+3882289x^4$ $+3905844x^3+2531466x^2+954004x+158801$
6	$x^{15}+60x^{14}+1590x^{13}+24580x^{12}+247076x^{11}+1707880x^{10}+8393220x^9+29953488x^8$ $+78611931x^7+152460896x^6+217749132x^5+225897288x^4+165424127x^3+81007156x^2$ $+23792330x+3168060$
7	$x^{18}+72x^{17}+2340x^{16}+45480x^{15}+590935x^{14}+5441942x^{13}+36790579x^{12}+186836720x^{11}$ $+723903526x^{10}+2161721448x^9+5002671156x^8+8979574344x^7+12447597245x^6$ $+13183724714x^5+10462322329x^4+6017450460x^3+2367331465x^2+569616794x+63202399$
8	$x^{21}+84x^{20}+3234x^{19}+75740x^{18}+1208334x^{17}+13944300x^{16}+120729822x^{15}+803372808x^{14}$ $+4178202550x^{13}+17187250328x^{12}+56385112656x^{11}+148292894368x^{10}+313370140886x^9$ $+531655906848x^8+721085140272x^7+775215148280x^6+651285933300x^5+418109802056x^4$ $+197916326308x^3+65061802032x^2+13258279400x+1260879920$

Table 3. Clar covering polynomial of $G(n)$:

n	Clar covering polynomial $P(G(n);x)$
2	$2x^3+15x^2+32x+20$
3	$3x^6+48x^5+295x^4+896x^3+1431x^2+1148x+364$
4	$4x^9+103x^8+1092x^7+6334x^6+22332x^5+49945x^4+71214x^3+62685x^2+31020x+6596$
5	$5x^{12}+184x^{11}+2854x^{10}+25164x^9+142039x^8+544612x^7+1461973x^6+2779440x^5$ $+3725975x^4+3443860x^3+2087967x^2+747052x+119500$
6	$6x^{15}+295x^{14}+6156x^{13}+74308x^{12}+588614x^{11}+3269343x^{10}+13230576x^9+39891799x^8$ $+90643392x^7+155617332x^6+200639916x^5+191131773x^4+130425994x^3+60271749x^2$ $+16886908x+2164964$
7	$7x^{18}+440x^{17}+11733x^{16}+182484x^{15}+1887650x^{14}+13933172x^{13}+76562096x^{12}+321733860x^{11}$ $+1051793315x^{10}+2702198964x^9+5480598823x^8+8770251984x^7+11007694447x^6$ $+10703499240x^5+7894921051x^4+4266830328x^3+1592616375x^2+366677340x+39222316$
8	$8x^{21}+623x^{20}+20496x^{19}+394710x^{18}+5094484x^{17}+47416826x^{16}+332864244x^{15}$ $+1815047486x^{14}+7842465840x^{13}+27216098459x^{12}+76526223940x^{11}+175204878000x^{10}$ $+327116898664x^9+497178892267x^8+611860206268x^7+603863356354x^6+470694806988x^5$ $+283053795089x^4+126596507558x^3+39628074669x^2+7743450572x+710584580$