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A Relation between Clar Covering Polynomial and Cube Polynomial*

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Abstract

The Clar covering polynomial (Zhang-Zhang polynomial) of a hexagonal system is a counting polynomial of resonant structures called Clar covers, which can be used to determine the Kekulé count, the first Herndon number and Clar number. In this paper we prove that the Clar covering polynomial of a hexagonal system H coincides with the cube polynomial of its resonance graph $R(H)$ by establishing a bijection between the Clar covers of H and the hypercubes in $R(H)$. Moreover, some important applications of this relation are presented.

1 Introduction

A hexagonal or benzenoid system is a 2-connected finite plane graph such that every interior face is a regular hexagon of side length one. It can also be formed by a cycle with its interior in the infinite hexagonal lattice on the plane (graphene). A hexagonal system with a Kekulé structure (or perfect matching in graph theory) is called Kekuléan and is viewed as the carbon–skeleton of a benzenoid hydrocarbon. Based on the Kekulé structures, there are several classical models of benzenoid molecules relating with resonance

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energy (extra stability) such as Clar's aromatic sextet theory [7] and Randić conjugated circuit model [24].

In 1996, Zhang and Zhang [36] formally introduced the Clar covering polynomial (Zhang-Zhang polynomial) of a hexagonal system, which unifies some topological indices such as the Clar number, the Kekulé count and the first Herndon number. Moreover, it is closely related to [37] sextet polynomial introduced by Hosoya and Yamaguchi [16].

A *generalized hexagonal system* H is a subgraph of a hexagonal system and a *Clar cover* is a spanning subgraph of H such that every component of it is either a hexagon or an edge. The set of hexagons in a Clar cover of H is called a *sextet pattern* or *resonant set* and a *Clar formula* is a maximum sextet pattern of H. Moreover, the *Clar number* $Cl(H)$ of H is the size of a *Clar formula* of H. The *Clar covering polynomial* of H is defined as follows:

$$\zeta(H,x) = \zeta(H) = \sum_{k=0}^{Cl(H)} z(H,k)x^k, \tag{1}$$

where $z(H,k)$ is the number of Clar covers with k hexagons of H.

The dependence of the topological resonance energy on $\zeta(H,x)$ for some values of x was examined in a series of papers due to Gutman et al. [9, 12, 14]. A recent survey [31] and some articles [3–6, 10, 11, 34] established basic properties of Clar covering polynomial and some methods to compute it. In particular, Chou et al. [4, 5] recently carried out an automatic computation program for the Clar covering polynomials of benzenoids and obtained many fruitful results.

The resonance graph $R(H)$ (also called Z-transformation graph) of a hexagonal system H was introduced independently by Gründler [8], Zhang et al. [29, 30] and Randić [24, 25]. It originates from Herndon's resonance theory [15] to reflect an interaction between Kekulé structure of benzenoid hydrocarbons. The vertex set of $R(H)$ is the set of perfect matchings of H. Two vertices are adjacent if their symmetric difference forms a hexagon of H. It is evident that $z(H,0)$ equals the number of the vertices of $R(H)$ and $z(H,1)$, the first Herndon number, equals the number of edges of $R(H)$. The resonance graph was later extended [38] to bipartite plane graphs and Ref. [33] gives a survey on it recently.

The n-dimensional hypercube Q_n (or simply n-cube) is the graph whose vertices are all binary strings of length n and two vertices are adjacent if their strings differ exactly in one position. Brešar, Klavžar and Škrekovski [1] introduced a counting polynomial of hypercubes of a graph G, called the *cube polynomial*, as follows:

$$C(G,x) = \sum_{i\geq 0} \alpha_i(G)x^i \tag{2}$$

where $\alpha_i(G)$ denotes the number of induced subgraphs of G that is isomorphic to the i-cube Q_i.

An important new role of hypercubes of resonance graph was considered in [22,26,28]. Klavžar et al. [21] proved that the Clar number $Cl(H)$ of H is equal to the largest i such that Q_i is a subgraph of $R(H)$. Zhang and Zhang [36] showed that $z(H, Cl(H))$ equals the number of Clar formulas of H; and Salem et al. [27] established a bijection between the Clar formulas of H and the number of the largest hypercubes in $R(H)$. These two results together imply that $z(H, Cl(H))$ is equal to the number of largest hypercubes in $R(H)$.

More generally, in this paper we show that the Clar covering polynomial of a hexagonal system H coincides with the cube polynomial of its resonance graph $R(H)$, that is

$$\zeta(H,x) = C(R(H),x)) \ . \tag{3}$$

Hence the corresponding coefficients of these two polynomials must coincide, i.e. $z(H,i) = \alpha_i(R(H))$ for each $i \geq 0$. The proof is accomplished by establishing a one–to–one correspondence between the Clar covers of H and the hypercubes in $R(H)$. For example, the Clar covering polynomial of a fibonacene with n hexagons is equal to the cube polynomial of Fibonacci cube of order n. This correspondence also derives an isomorphism between the partial orderings on the Clar covers of H and the hypercubes of $R(H)$.

Finally, some further applications of Equation (3) are presented. The derivatives and properties of real roots of the Clar covering polynomial are determined. Also, we derive a novel expression of cube polynomial of a median graph in terms of $(x + 1)$.

2 Equality of two polynomials

The objective of this section is to prove Equation (3) and the following definitions can simplify our proof.

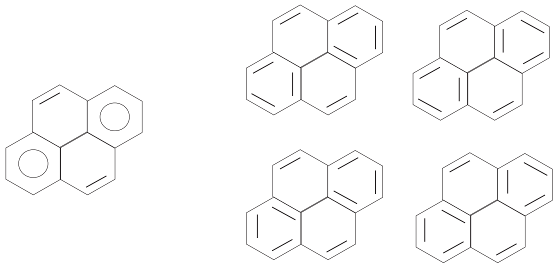
We first recall two important definitions from set theory and graph theory. The *symmetry difference* $A \oplus B$ of two sets A and B is equal to $(A \setminus B) \cup (B \setminus A)$. Let G be a graph with a perfect matching M, a cycle of G is M*-alternating* if its edges belong alternately to M and not to M. Also, the edge set of G is denoted by $E(G)$.

Given any Kekuléan hexagonal system H, let $\mathbb{Z}(H,n)$ be the set of Clar covers of H with exactly n hexagons. On the other hand, consider a graph G. The set of induced subgraphs of G that are isomorphic to n-cube Q_n is denoted by $\mathbb{Q}_n(G)$. Combining these definitions from those in the previous section, we have $z(H,n) = |\mathbb{Z}(H,n)|$ and $\alpha_n(G) = |\mathbb{Q}_n(G)|$.

To prove Equation (3), it is sufficient to establish a bijection between $\mathbb{Z}(H,n)$ and $\mathbb{Q}_n(R(H))$ for each integer $n \geq 0$. To achieve our goal, let

$$f : \mathbb{Z}(H,n) \to \mathbb{Q}_n(R(H)) \tag{4}$$

be the mapping defined as follows: For each Clar cover $C \in \mathbb{Z}(H,n)$, consider those perfect matchings $M_1, M_2, \ldots, M_i$ in H such that each hexagon in C is M_j-alternating and each isolated edge in C is in M_j for all $1 \leq j \leq i$. Define $f(C)$ as the induced subgraph of $R(H)$ with vertices $M_1, M_2, \ldots, M_i$.



(a) (b)

Figure 1. (a) A Clar cover C of pyrene, (b) The four perfect matchings in the image $f(C)$ which induces a square in the resonance graph.

It is not difficult to show that $M_j \oplus E(C)$ only consists of perfect matchings of the hexagons in C. Since each hexagon in C has two perfect matchings, $f(C)$ has exactly 2^n vertices. An example illustrating the definition of f is given in Figure 1; the hexagons with a circle inside represent the hexagons of C and a double bond represents an isolated edge of C.

To facilitate the proof that follows, we orientate the plane graph H such that some edges are vertical. For a perfect matching M of H, an M-alternating hexagon s is called a *proper* (*resp. improper*) *sextet* if the vertical double edge lies on the right (resp. left) (see Figure 2).

The following lemma shows that f is a well-defined mapping.

Lemma 2.1. *For each Clar cover $C \in \mathbb{Z}(H,n)$, we have $f(C) \in \mathbb{Q}_n(R(H))$.*

Proof. It is sufficient to show that $f(C)$ is isomorphic to the n-cube Q_n. Let $h_1,\dots,h_n$ be the hexagons of C. For any vertex M of $f(C)$ (M is also a perfect matching of H), let $b(M) = b_1b_2\cdots b_n$, where $b_i = 1$ or 0 according to whether h_i is a proper or improper M-alternating hexagon for $i = 1,\dots,n$. It is obvious that $b : V(f(C)) \to V(Q_n)$ is a bijection. For $M' \in V(f(C))$, let $b(M') = b'_1b'_2\cdots b'_n$. If M and M' are adjacent in $f(C)$, which means they adjacent in $R(H)$, then $M \oplus M' = h_i$ for some $1 \le i \le n$. Therefore, $b_j = b'_j$ for each $j \ne i$ and $b_i \ne b'_i$, which implies $b_1b_2\cdots b_n$ and $b'_1b'_2\cdots b'_n$ are adjacent in Q_n. Conversely, if $b_1b_2\cdots b_n$ and $b'_1b'_2\cdots b'_n$ are adjacent in Q_n, then it follows that M and M' are adjacent in $f(C)$. Hence b is an isomorphism between $f(C)$ and Q_n. $\square$

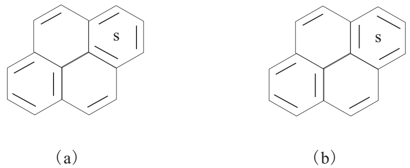


Figure 2. (a) A proper sextet s, (b) An improper sextet s.

Lemma 2.2. *The mapping $f : \mathbb{Z}(H,n) \to \mathbb{Q}_n(R(H))$ is injective for each nonnegative integer n.*

Proof. Given any distinct Clar covers C and C' in $\mathbb{Z}(H,n)$. If C and C' contain the same set of hexagons, then the isolated edges of C and C' are distinct. Therefore, $f(C)$ and $f(C')$ are disjoint induced subgraphs of $R(H)$ and thus $f(C) \ne f(C')$. Suppose C and C' contain different sets of hexagons and let h be a hexagon in $C \setminus C'$. Hence there is at least one edge e of h not belonging to $E(C')$. From the definition of mapping f, e is thus unsaturated by those perfect matchings that correspond to the vertices in $f(C')$. However, there exist vertices M_1 and M_2 of $f(C)$ (M_1 and M_2 are perfect matchings of H) such that $M_1 \oplus M_2 = E(h)$ because h is a hexagon in C. Hence e is saturated by one of M_1 and M_2, say M_1. As a result, $M_1 \notin V(f(C'))$ and $f(C) \ne f(C')$. $\square$

The following lemma is an obvious and known result.

Lemma 2.3. *For a perfect matching M of H, the proper (resp. improper) M-alternating hexagons are pairwise disjoint.*

Lemma 2.4 ([26]). *If the resonance graph $R(H)$ contains a 4-cycle $M_1M_2M_3M_4M_1$, then $h := M_1 \oplus M_2$ and $h' := M_1 \oplus M_4$ are disjoint hexagons. Also, we have $h = M_3 \oplus M_4$ and $h' = M_2 \oplus M_3$.*

Proof. Since $M_1M_2M_3M_4M_1$ is a 4-cycle, the $h_i := M_i \oplus M_{i+1}$, where the subscripts are module 4, are hexagons of H and $h_i \neq h_{i+1}$ for each i. Moreover, the set $h_0 \oplus h_1 \oplus h_2 \oplus h_3 = \varnothing$ because symmetric difference is commutative and associative. It is known that any two distinct hexagons in H are either disjoint or having exactly one edge in common. If $h_0 \neq h_2$, then h_0 has at most three edges in $E(h_1) \cup E(h_2) \cup E(h_3)$ and all other edges are contained in the above symmetry difference, which leads to a contradiction. Hence $h_2 = h_0$ and using similar arguments, we have $h_1 = h_3$ as well as h_0 and h_1 are disjoint. □

We now define the oriented resonance graph $\vec{R}(H)$: an edge MM' is oriented from M to M' if $M \oplus M'$ is a proper sextet with respect to M and an improper sextet with respect to M'. In fact $\vec{R}(H)$ is the Hasse diagram of a distributive lattice on the set of perfect matchings of H [33].

Lemma 2.5 ([33,35]). *The directed resonance graph $\vec{R}(H)$ has no directed cycles.*

Lemma 2.6. *The mapping $f : \mathbb{Z}(H,n) \to \mathbb{Q}_n(R(H))$ is surjective for each nonnegative integer n.*

Proof. For any graph $G_n \in \mathbb{Q}_n(R(H))$, which is isomorphic to the n-cube Q_n, the corresponding oriented subgraph $\vec{G}_n$ in $\vec{R}(H)$ has no directed cycle by Lemma 2.5. Hence $\vec{G}_n$ contains a vertex M_0 (a source) with in-degree 0 and out-degree n, that is, $\vec{G}_n$ has n directed edges from M_0 to $M_1, M_2, \ldots,$ and M_n. Let $h_i = M_0 \oplus M_i$ for $i = 1, \ldots, n$, the directed edges M_0M_i implies that all h_i are proper M_0-alternating hexagons. Moreover, Lemma 2.3 guarantees that all h_i are pairwise disjoint. Therefore, we can obtain a Clar cover C in $\mathbb{Z}(H,n)$ by regarding the M_0-alternating hexagons $h_1, \ldots, h_n$ as components and all others edges of M_0 as isolated edge components. It suffices to prove $f(C) = G_n$.

Let $[\boldsymbol{n}] = \{1, \ldots, n\}$ and for any $I \subseteq [\boldsymbol{n}]$, let $M_I := M_0 \oplus (\bigcup_{i \in I} h_i)$. Then $V(f(C)) = \{M_I : I \subseteq [\boldsymbol{n}]\}$. In particular, $M_0 = M_\varnothing$ as well as $M_i = M_{\{i\}}$ for all i, and all of them belong to both G_n and $f(C)$. On the other hand, since G_n is isomorphic to the n-cube Q_n, every vertex F of G_n can be labeled with binary strings $b(F) = b_1b_2 \cdots b_n$ such that $b(M_0) = 00 \cdots 0$ and for each $b(M_i)$, the i-th coordinate is 1 and the other coordinates are all zeros, and F and F' are adjacent in G_n if and only if $b(F)$ and $b(F')$ are adjacent in Q_n.

For any $F \in V(G_n)$, let $I_F = \{i \in [\boldsymbol{n}] : b_i = 1\}$. We will show that $F = M_{I_F} \in V(f(C))$ by induction on the distance $|I_F|$ between M_0 and F in G_n. If $|I_F| = 0$ or 1, then $F \in \{M_0, M_1, \ldots, M_n\}$. Now suppose $|I_F| \geq 2$, there exist $i, j \in I_F$ with $i \neq j$. Thus, there are vertices F_0, F_1, F_2 of G_n such that $I_{F_0} = I_F \setminus \{i, j\}$, $I_{F_1} = I_F \setminus \{i\}$, and $I_{F_2} = I_F \setminus \{j\}$. By the induction hypothesis, we have $F_k = M_{I_{F_k}}$ for $k = 0, 1$ and 2. Therefore, $F_1 \oplus F_0 = M_{I_{F_1}} \oplus M_{I_{F_0}} = h_j$ and $F_2 \oplus F_0 = M_{I_{F_2}} \oplus M_{I_{F_0}} = h_i$. Since $F_0F_1FF_2F_0$ is a 4-cycle of G_n, it follows from Lemma 2.4 that $F \oplus F_1 = F_2 \oplus F_0 = h_i$. As a result, $F = F_1 \oplus h_i = (M_0 \oplus (\bigcup_{k \in I_{F_1}} h_k)) \oplus h_i = M_0 \oplus (\bigcup_{k \in I_F} h_i) = M_{I_F}$ and this implies that $V(f(C)) = V(G_n)$ and hence $f(C) = G_n$. $\square$

Combining Lemmas 2.1, 2.2 and 2.6, we have the following corollary immediately.

Corollary 2.7. *The mapping $f : \mathbb{Z}(H, n) \to \mathbb{Q}_n(R(H))$ is a bijection for every nonnegative integer n.*

Hence, we obtain the main result of this article as follows:

Theorem 2.8. *For any Kekuléan hexagonal system H, we have $\zeta(H, x) = C(R(H), x)$.*

Corollary 2.7 also implies the following result.

Corollary 2.9 ([26])**.** *Let H be a Kekuléan hexagonal system. For any non–negative integer k, there exists a surjective mapping from the set of k-cubes of $R(H)$ to the set of resonant sets with k hexagons.*

3 Maximal hypercubes

We now consider maximal hypercubes in resonance graphs by establishing ordering relations on the hypercubes and the Clar covers.

For a Kekuléan hexagonal system H, let $\mathbb{Q}$ be the set of induced subgraphs of $R(H)$ that are hypercubes. Thus $\mathbb{Q} = \bigcup_{n \geq 0} \mathbb{Q}_n(R(H))$. We define an ordering $\leq$ on $\mathbb{Q}$ as follows: For any graphs $Q, Q' \in \mathbb{Q}$, we have $Q \leq Q'$ if Q is a subgraph of Q'. Hence $(\mathbb{Q}, \leq)$ is a poset and the maximal hypercubes of $R(H)$ are the maximal elements of the poset $(\mathbb{Q}, \leq)$.

Let $\mathbb{C}$ denote the set of all Clar covers of H. Thus $\mathbb{C} = \bigcup_{n\geq 0} \mathbb{Z}(H,n)$. For any Clar covers $C, C' \in \mathbb{C}$, we set $C \leq C'$ if $f(C) \subseteq f(C')$. The reflexivity and transitivity of this binary relation are obvious and its antisymmetry follows from the bijection f (Corollary 2.7). As a result, $(\mathbb{C}, \leq)$ is also a poset.

Moreover, the bijection f from $(\mathbb{C}, \leq)$ to $(\mathbb{Q}, \leq)$ preserves the ordering relations and we obtain the following result.

Theorem 3.1. *The posets* $(\mathbb{C}, \leq)$ *and* $(\mathbb{Q}, \leq)$ *are isomorphic.*

We now give an explicit description for the partial ordering on the Clar covers of H.

Theorem 3.2. *For any Clar covers* $C, C' \in \mathbb{C}$, $C \leq C'$ *if and only if the hexagons of* C *belong to* C' *as well as* C *and* C' *coincide on the edges apart from those in the hexagons of* C'.

Proof. If the hexagons of C belong to C' as well as C and C' coincide on the edges apart from those in the hexagons of C', then the hexagons in $C' \setminus C$ are alternating in C. Hence $V(f(C)) \subseteq V(f(C'))$ and $f(C) \subseteq f(C')$, that is $C \leq C'$. Conversely, suppose $f(C) \subseteq f(C')$. For any hexagon h in C, there are two perfect matchings M and M' of H in $f(C)$ such that $h = M \oplus M'$. Since M and M' are in $f(C')$, h is also in C'. Moreover, it is obvious that C and C' coincide on the edges apart from those in the hexagons of C'. $\square$

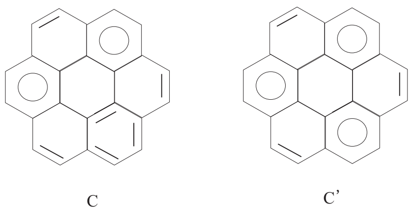


Figure 3. Two Clar covers of coronene: $C \leq C'$.

The theorem shows that a Clar cover C of H is *maximal* if and only if C has no alternating hexagons in H. Accordingly, the isomorphism f between $(\mathbb{C}, \leq)$ and $(\mathbb{Q}, \leq)$ implies the following corollary.

Corollary 3.3. *There is a one-to-one correspondence between the maximal hypercubes of* $R(H)$ *and the Clar covers of* H *that without alternating hexagons.*

Relations between Clar structures and Clar covers without alternating hexagons have already been discussed in [39].

4 Some applications

The Clar covering polynomial and cube polynomial were studied independently in the past. The Clar covering polynomials of many types of hexagonal systems have been obtained explicitly via various approaches [3–6, 10, 11, 34, 36]. Hence, the cube polynomial of their resonance graphs can be obtained by Theorem 2.8. For example,

$$\zeta(\text{pyrene}, x) = C(R(\text{pyrene}), x) = x^2 + 6x + 6 = (x+1)^2 + 4(x+1) + 1$$

and

$$\begin{aligned}\zeta(\text{coronene}, x) = C(R(\text{coronene}), x) &= 2x^3 + 15x^2 + 32x + 20 \\ &= 2(x+1)^3 + 9(x+1)^2 + 8(x+1) + 1\end{aligned}$$

where the resonance graph $R(\text{coronene})$ is illustrated in [35].

In the following subsections we will present some interesting applications of Theorem 2.8.

Although the cube polynomial was defined for any graph, its discussions have been concentrated on median graphs where hypercubes play an important role. A median of a triple of vertices u, v and w of a graph is a vertex that lies on a shortest (u, v)-path, a shortest (u, w)-path and a shortest (v, w)-path simultaneously. A graph is called a *median graph* if every triple of its vertices has a unique median. Zhang et al. [35] proved that the resonance graph of a (weakly) elementary plane bipartite graph is a median graph, which is done by considering a distributive lattice structure on the set of its perfect matchings. A median graph, however, is not necessarily a resonance graph.

4.1 Fibonacci cube

A fibonacene is a hexagonal chain in which no hexagons are linearly attached. Klavžar and Žigert [20] showed that the resonance graph of a fibonacene with n hexagons Z_n is isomorphic to the Fibonacci cube Γ_n, which is the subgraph of the n-cube Q_n induced by all binary strings of length n that contain no two consecutive 1s. The Fibonacci cubes were introduced [17] as a model for interconnection networks and Klavžar [18] gave an extensive survey on it. Also, the chemical graph theory of fibonacenes was studied in [13].

The Clar covering polynomial of a fibonacene Z_n was expressed [32] in terms of binomial coefficients by matching polynomial of a path with $n+1$ vertices; the cube polynomial of Γ_n was derived from generating functions with double variables [19]. Indeed, they have the same expression:

$$\zeta(Z_n,x) = C(\Gamma_n,x) = \sum_{k=0}^{\lfloor\frac{n+1}{2}\rfloor} \binom{n-k}{k}(x+1)^k \ . \tag{5}$$

Besides, the sextet polynomial of Z_n is

$$B(Z_n,x) = \sum_{k=0}^{\lfloor\frac{n+1}{2}\rfloor} \binom{n-k}{k}x^k \ .$$

4.2 Derivatives of Clar covering polynomials

Brešar et al. [1] studied the derivatives of cube polynomials of median graphs, which can be expressed as the cube polynomial of the disjoint union of some subgraphs with median property. Motivated by this, we consider the derivative of the Clar covering polynomial of hexagonal systems directly.

Theorem 4.1. *If H is a generalized hexagonal system, then $\zeta'(H,x) = \sum_h \zeta(H-h,x)$, where the summation goes over all hexagons h of H.*

Proof. We count the ordered pairs (C,h), where C is a Clar cover of H with k hexagons and h is a hexagon of C, in two different ways. Since each Clar cover C is counted k times, we obtain the number $kz(H,k)$ of ordered pairs. On the other hand, when h is fixed, the number of covers C containing h equals to $z(H-h,k-1)$. Hence, the total amount is $\sum_h z(H-h,k-1)$. Therefore, $kz(H,k) = \sum_h z(H-h,k-1)$ for each positive integer k and the result follows. $\square$

The theorem can be applied repeatedly and we obtain the following corollary about high derivatives of Clar covering polynomials of hexagonal systems.

Corollary 4.2. *If H is a hexagonal system, then $\zeta^{(s)}(H,x) = \sum_{\mathcal{R}_s} \zeta(H-\mathcal{R}_s,x)$, where the summation goes over all sextet patterns $\mathcal{R}_s$ with s hexagons.*

4.3 Roots of Clar covering polynomials

Gutman et al. [12] found good linear correlations between topological resonance energy and $\ln \zeta(H,x)$ for fixed values of x lying in the interval [0, 2]. Gojak et al. [9] further implemented a model relating resonance energy with $\sqrt{\zeta(H,x)}$ for suitable values of x. Hence the real roots of Clar covering polynomial facilitate such researches.

Brešar et al. [2] obtained some important properties of the real roots of cube polynomials of median graphs as follows:

Theorem 4.3 ([2]). *If G is a median graph, then $C(G,x)$ has no roots in $[-1,+\infty)$.*

Theorem 4.4 ([2]). *Let G be a median graph. If $C(G,r)=0$ for a rational number r, then $r=-\dfrac{t+1}{t}$ for some integer $t\geq 1$.*

Theorem 4.5 ([2]). *If G is a nontrivial median graph, then $C(G,x)$ has a real root in the interval $[-2,-1)$.*

Theorem 2.8 together with Theorems 4.3 to 4.5 lead to the following results about the real roots of Clar covering polynomials immediately.

Corollary 4.6. *Let H be a Kekuléan hexagonal system. If a rational number r is a root of $\zeta(H,x)$, then $r=-\dfrac{t+1}{t}$ for some integer $t\geq 1$.*

Corollary 4.7. *If H is a Kekuléan hexagonal system, then $\zeta(H,x)$ has no roots in $[-1,+\infty)$ but having a real root in the interval $[-2,-1)$.*

4.4 A transformation of cube polynomials

The Clar covering polynomial of a hexagonal system can be expressed in terms of $(x+1)$ such that all coefficients are nonnegative.

Theorem 4.8 ([37]). *Let H be a Kekuléan hexagonal system. We have*

$$\zeta(H,x)=\sum_{i=0}^{Cl(H)} z(H,i)x^i=\sum_{i=0}^{Cl(H)} a(H,i)(x+1)^i$$

where $a(H,i)$ denotes the number of perfect matchings of H with exactly i proper sextets.

This result together with Theorem 2.8 allow us to conclude that the cube polynomial of resonance graph have the same property. So a question naturally arises: does the cube polynomial of a general median graph have such an expression? We will give an affirmative answer in this subsection.

We first introduce a convex expansion of median graphs. A pair of induced subgraphs $\{G_1, G_2\}$ of a graph G is called a *cubical cover* if $G = G_1 \cup G_2$ and each induced hypercube of G is contained in at least one of the G_1 and G_2. Let G_i^* be an isomorphic copy of G_i for $i = 1, 2$. For every vertex u of $G_0 = G_1 \cap G_2$, let u_i be the corresponding vertex in G_i^*. The *expansion* G^* of G with respect to the cubical cover $\{G_1, G_2\}$ of G is the graph obtained from the disjoint union G_1^* and G_2^* by adding an edge between the corresponding vertices u_1 and u_2 for each vertex $u \in G_0$.

Proposition 4.9 ([1]). *Let G^* be a graph constructed by the expansion with respect to the cubical cover $\{G_1, G_2\}$ with $G_0 = G_1 \cap G_2$. Then*

$$C(G^*, x) = C(G_1, x) + C(G_2, x) + xC(G_0, x) .$$

A subgraph G_1 of a graph G_2 is *convex* if for any pair of vertices u and v in G_1, all shortest (u, v)-paths in G_2 lie completely in G_1. An expansion with respect to $\{G_1, G_2\}$ is called a *peripheral convex expansion* if G_1 is a convex subgraph of G_2. The following result gives a construction of median graphs via a peripheral convex expansion.

Theorem 4.10 ([23]). *Let G be a connected graph. Then G is a median graph if and only if G can be constructed by a sequence of peripheral convex expansions from the single-vertex graph.*

Theorem 4.11. *Let G be a median graph and m be the dimension of the largest hypercube contained in G. Then $C(G, x) = \sum_{i=0}^{m} b_i(G)(x+1)^i$, where $b_0(G) = 1$ and $b_i(G)$ is a positive integer for each i with $0 \le i \le m$.*

Proof. We proceed by induction on the number of vertices of the median graph G. Obviously, $C(K_1, x) = 1$ and $C(K_2, x) = 2 + x = 1 + (x + 1)$, which satisfy the basic step of induction. Suppose G is a median graph with $|V(G)| > 2$. By Theorem 4.10, G can be constructed from a median graph G' by a peripheral convex expansion with respect to $\{G_0, G'\}$. Hence, by Proposition 4.9, we have

$$C(G, x) = C(G', x) + (x + 1)C(G_0, x) .$$

Since G' and G_0 are median graphs that are smaller than G, by induction hypothesis we have $C(G', x) = \sum_{i\ge0} b_i(G')(x + 1)^i$ and $C(G_0, x) = \sum_{i\ge0} b_i(G_0)(x + 1)^i$, which satisfy the conditions of the theorem. Thus $C(G,x) = \sum_{i\geq 1}(b_i(G') + b_{i-1}(G_0))(x+1)^i + b_0(G')$. As a result, $b_0(G) = b_0(G') = 1$ and $b_i(G) = b_i(G') + b_{i-1}(G_0)$, which is a positive integer for each $i \leq m$ and hence the induction step completes. □

Moreover, we will determine the coefficients $b_i(G)$ and reveal their combinatorial meaning.

For a median graph G, Theorem 4.11 implies the following inversion formulas.

Corollary 4.12. *Let G be a median graph, we have*

(i) $\alpha_i(G) = \sum_{k=0}^{m} b_k(G)\binom{k}{i}$ *for* $i = 0, 1, \ldots, m$, *and*

(ii) $b_j(G) = \sum_{k=0}^{m}(-1)^{k-j}\binom{k}{j}\alpha_k(G)$ *for* $j = 0, 1, \ldots, m$.

On the other hand, Brešar et al. [1] introduced the high derivative graph $\partial^k G$ of a median graph G and proved that $C^{(k)}(G,x) = C(\partial^k G, x)$. Let $\theta_i(G)$ be the number of components in $\partial^i(G)$ with $i \geq 0$. Corollary 10 of [1] showed that $\theta_i(G)$ can be expressed as

$$\theta_i(G) = i!\sum_{k\geq 0}(-1)^{k-i}\binom{k}{i}\alpha_k(G)$$

for each $i \geq 0$. Comparing the above equation with Equation (ii) in Corollary 4.12, we conclude that $b_i(G) = \theta_i/i!$ and hence obtain the following results.

Corollary 4.13. *If G is a median graph, then* $C(G,x) = \sum_{i\geq 0}\frac{\theta_i}{i!}(x+1)^i$.

Corollary 4.14. *For a Kekuléan hexagonal system H, we have*

$$i!a(H,i) = \theta_i(R(H)) \tag{6}$$

for $i \geq 0$.

One of the applications of Theorem 4.11 is that it facilitates the studying of the coefficients $\alpha_i(G)$ of cube polynomial. Firstly, Corollary 4.12(ii) together with $b_0(G) = 1$ immediately implies the following well-known result.

Corollary 4.15 ([1])**.** *Let G be a median graph. We have* $\sum_{i\geq 0}(-1)^i\alpha_i(G) = 1$.

Similar to the argument in [37], Corollary 4.12(i) implies a monotonic subsequence of coefficients of cube polynomials.

Corollary 4.16. *Let G be a median graph. We have*

$$\alpha_m(G) < \alpha_{m-1}(G) < \cdots < \alpha_{\lceil \frac{m-1}{2} \rceil}(G) \; .$$

Finally we propose a general conjecture for median graphs.

Conjecture 4.17. *Let G be a median graph and $C(G, x)$ be its cube polynomial. Then the sequence of coefficients of $C(G, x)$ is unimodal.*

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