MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **95** (2026) 487–508
ISSN: 0340–6253
doi: 10.46793/match.95-2.12125

Relations between Polynomials Based on Perfect Matchings and Independent Sets of CERS

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(Received May 20, 2025)

Abstract

In this paper, we firstly focus on catacondensed even ring systems (shortly CERS) without any linearly connected adjacent triple of finite faces. For such a graph G, we describe a bijection between the set of all perfect matchings (Kekulé structures) of G and the set of all independent sets of the inner dual of G, which enables us to prove the equality between three polynomials: the sextet polynomial of G, the independence polynomial of the inner dual of G, and the newly introduced link polynomial of G. These equalities imply that the number of perfect matchings of G equals the number of resonant sets of G and also the number of independent sets of the inner dual of G. Moreover, we show that the number of edges of the resonance graph of G coincides with the derivative of the mentioned polynomials evaluated at $x = 1$. Finally, we provide the generalization of the results to all peripherally 2-colorable graphs.

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1 Introduction

Kekulé structures of aromatic hydrocarbons represent specific arrangements of double bonds within a molecule [6]. In graph-theoretical terms, these structures correspond to perfect matchings of the associated molecular graph. The interplay among different Kekulé structures is captured by resonance graphs, which were introduced independently by chemists El-Basil [7, 8] and Gründler [9] as well as by mathematicians Zhang, Guo, and Chen [18], who referred to them as Z-transformation graphs. Firstly, the research focused on the properties of resonance graphs in hexagonal systems [18]. Subsequently, the concept was generalized to catacondensed even ring systems, shortly CERS [16], and to all plane (elementary) bipartite graphs (see, e.g., [19, 20]).

The sextet polynomial was introduced by Hosoya and Yamaguchi in 1975 [13] as a counting polynomial in chemistry related to Kekulé structures. More precisely, it counts resonant sets of a given polycyclic aromatic hydrocarbon. Several interesting properties of this polynomial were obtained in [17], see also [12]. For example, it was shown that for a thin polyhex graph G (i.e. a benzenoid graph that has no coronene skeleton), the sextet polynomial evaluated at $x = 1$ coincides with the number of perfect matchings of G.

Daisy cubes were introduced in [14] as a subfamily of partial cubes which contains also Fibonacci and Lucas cubes. The connection between resonance graphs and daisy cubes was initially explored in [22], where it was shown that the resonance graph of a kinky benzenoid graph (i.e. a benzenoid graph without linear hexagons) is a daisy cube. Moreover, in [1] and [2], CERS and 2-connected outerplane bipartite graphs whose resonance graphs are daisy cubes were characterized, respectively. Additionally, the characterization was generalized to all plane bipartite graphs [3]. In particular, it turns out that if G is a plane elementary bipartite graph other than K_2, then its resonance graph $R(G)$ is a daisy cube if and only if the Fries number of G equals the number of finite faces of G, which in turn is equivalent to G being peripherally 2-colorable. Note that CERS that do not contain any linearly connected adjacent triple of finite faces are peripherally 2-colorable and that fibonaccenes also belong to this family of graphs [15].

Let G be a peripherally 2-colorable graph. Recently, a bijection was established between the set of maximal hypercubes of the resonance graph $R(G)$ and the set of maximal independent sets of the inner dual G^* of G, where G^* is a tree isomorphic to the τ-graph of $R(G)$ [4]. Moreover, an algorithm for a binary code labelling for the vertex set of the resonance graph $R(G)$ as a daisy cube with respect to the set of maximal independent sets of the inner dual G^* was obtained. Consequently, the existence of a bijection between the set of all perfect matchings of G and the set of all independent sets of the inner dual G^* was observed. However, it is not clear which perfect matching of G corresponds to a given independent set of G^* with respect to the mentioned algorithm.

In this paper, we firstly focus on the family of CERS that do not contain any linearly connected adjacent triple of finite faces, since from a chemical perspective, they offer a more intuitive graphical representation than general peripherally 2-colorable graphs, while also encompassing several interesting families of chemical graphs.

The paper is organized as follows. In Section 3, we describe a bijection f between the set of all perfect matchings of G and the set of all independent sets of the inner dual G^* such that any independent set X of G^* of cardinality k is mapped to the perfect matching $f(X) = M$ of G in which only the finite faces from X have M-links to all adjacent finite faces, where G is a CERS without any linearly connected adjacent triple of finite faces. Then, in Section 4, we establish the equality between the sextet polynomial of such a graph G and the independence polynomial of the inner dual of G. Moreover, we also introduce the link polynomial of G and show that it coincides with the above mentioned polynomials. We continue with the investigation of the derivative of all three discussed polynomials in Section 5. Finally, in Section 6 we generalize the established results to all peripherally 2-colorable graphs.

2 Preliminaries

Let G be a plane graph. We say that two faces of G are *adjacent* if they have an edge in common. We denote the edges lying on some face F of G by $E(F)$. The subgraph induced by the edges in $E(F)$ is the *periphery of* F and the periphery of the outer face is also called the *periphery of* G. The vertices of G that belong to the outer face are called *peripheral vertices* and the remaining vertices are *interior vertices*. Furthermore, an *outerplane graph* is a plane graph in which all vertices are peripheral vertices.

An *even ring system* is a 2-connected plane bipartite graph with all interior vertices of degree 3 and all peripheral vertices of degree 2 or 3. An outerplane even ring system is called *catacondensed even ring system* or shortly CERS [16]. Moreover, an even ring system whose inner faces are only hexagons is called a *benzenoid graph*.

The *distance* $d_G(u,v)$ between vertices u and v of a connected graph G is defined as the usual shortest path distance. The distance between two edges e and f of G, denoted by $d_G(e,f)$, is defined as the distance between corresponding vertices in the line graph of G.

Let F, F', F'' be three finite faces of a CERS G such that F, F' have the common edge e and F', F'' have the common edge f. In this case, the triple (F, F', F'') is called an *adjacent triple of finite faces*. Moreover, the adjacent triple of finite faces (F, F', F'') is *angularly connected* if the distance $d_G(e,f)$ is an even number and *linearly connected* otherwise.

The *inner dual* of a plane graph G is a graph whose vertices are the inner faces of G; two vertices are adjacent if and only if the corresponding faces are adjacent. Obviously, the inner dual of a CERS is always a tree, see Figure 1.

A path P of a graph G is called a *handle* if all internal vertices (if exist) of P are degree-2 vertices of G, and each end vertex of P has degree at least three in G [5]. A *nontrivial handle* is a handle with more than one edge.

A *perfect matching* M of a graph G is a subset of $E(G)$ such that every vertex of G is incident with exactly one edge from M. In chemical literature, perfect matchings are known as Kekulé structures (see [10] for

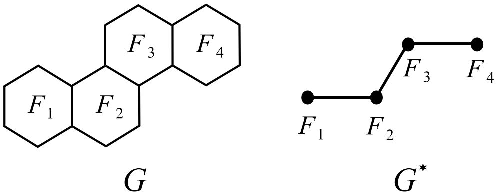

Figure 1. A benzenoid graph (CERS) G, which is a molecular graph of chrysene, and its inner dual G^*.

more details). The set of all perfect matchings of a graph G will be denoted by $\mathcal{M}(G)$ and the cardinality of this set by $\mathcal{K}(G)$. A bipartite graph G is *elementary* if and only if it is connected and each edge is contained in some perfect matching of G.

Let G be a graph and M a perfect matching of G. If H is a path or a cycle of G, then H is *M-alternating* if edges of H are alternately in M and out of M. It is clear that any nontrivial handle of G is M-alternating. In addition, for a nontrivial handle P with an odd number of edges, either both end edges of P or none of them belong to M. Furthermore, if G is a plane graph and F is a face of G, then F is *M-alternating* if the periphery of F is an M-alternating cycle.

If F, F' are adjacent inner faces of a CERS G, then the two edges on the periphery of F that have exactly one vertex on the periphery of F' are called the *link* from F to F'. It was proved in [16] that for a given perfect matching M and every link either both edges or none belong to M. Moreover, if M is a perfect matching of G such that the link from F to F' is contained in M, then we say that G has the *M-link* from F to F'. For example, for a graph G and perfect matching M shown on the left side of Figure 2, there is the M-link from F_7 to F_6 and also from F_7 to F_8.

Let G be a plane bipartite graph. The *resonance graph* $R(G)$ of G is the graph whose vertices are the perfect matchings of G, and two perfect matchings M_1, M_2 are adjacent if and only if their symmetric difference forms exactly one cycle that is the periphery of some finite face F of G, i.e. $E(F) = M_1 \oplus M_2$ [20].

A subset S of finite faces of a plane bipartite graph G is a *resonant set* of G [21] if the faces from S are pairwise vertex disjoint and $G - S$ is either empty or has a perfect matching (here $G - S$ denotes the graph obtained from G by deleting all the vertices of faces from S). Note that in literature resonant sets are sometimes referred to as *covers* [21], *sextet patterns* [12, 17], or *generalized Clar structures* [10].

For a string u of length n over $B = \{0, 1\}$, $u = (u_1, \ldots, u_n) \in B^n$, where $n \geq 1$, we will briefly write u as $u_1 \ldots u_n$. The *hypercube* Q_n of dimension n is defined in the following way: the vertices of Q_n are all binary strings from B^n, and two vertices of Q_n are adjacent if the corresponding binary strings differ in precisely one position. If G is a graph and $X \subseteq V(G)$, then $\langle X \rangle$ denotes the subgraph of G induced by X. Let $\leq$ be a partial order on B^n defined with $u_1 \ldots u_n \leq v_1 \ldots v_n$ if $u_i \leq v_i$ holds for all $i \in \{1, \ldots, n\}$. For $X \subseteq B^n$ we define the graph $Q_n(X)$ as the subgraph of Q_n with $Q_n(X) = \langle \{u \in B^n \mid u \leq x \text{ for some } x \in X\} \rangle$ and say that $Q_n(X)$ is a *daisy cube* (generated by X) [14].

Let G be a graph. A set of pairwise nonadjacent vertices of G is called an *independent set* of G. We denote by $\mathcal{I}(G)$ the set of all independent sets of G and by $i(G)$ the cardinality of the set $\mathcal{I}(G)$.

3 Constructing perfect matchings from independent sets of the inner dual

Let G be a CERS without any linearly connected adjacent triple of finite faces. In this section, we describe a bijection $f : \mathcal{I}(G^*) \to \mathcal{M}(G)$ between the set of all independent sets of the inner dual G^* of G and the set of all perfect matchings of G. We start with the following lemma, which follows by Lemma 3.1 in [3] and describes the structure of such graphs.

Lemma 1. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then each handle of G is a path on an odd number of edges.*

We proceed with the main result of this section.

Theorem 2. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then there exists a bijection $f : \mathcal{I}(G^*) \to \mathcal{M}(G)$ such that any independent set X of G^* of cardinality k is mapped to the perfect matching $f(X) = M$ of G in which only the finite faces from X have M-links to all adjacent finite faces.*

Proof. Let $F_1, F_2, \ldots, F_n$ be the finite faces of G. Recall that the inner dual G^* of G is a tree with vertices $F_1, F_2, \ldots, F_n$. Moreover, let $X \subseteq V(G^*) = \{F_1, F_2, \ldots, F_n\}$ be an independent set of G^*. Since X is an independent set of G^*, the finite faces of G in the set X are pairwise edge disjoint. Since G is a CERS, it follows that any two finite faces in X are also vertex disjoint because any vertex degree of G is at most 3. By Lemma 1, each handle of G is a path on an odd number of edges, so the induced subgraph $G - X$ is either empty or has a perfect matching. Therefore, X is a resonant set of G.

Define the perfect matching $f(X)$ of G in the following way: for any $i \in \{1, \ldots, n\}$, if $F_i \in X$, then $f(X)$ contains the links from F_i to all its adjacent finite faces (recall that this is possible by Lemma 1). Note that in this way, face F_i is $f(X)$-alternating.

Moreover, for any $i \in \{1, \ldots, n\}$, if $F_i \notin X$, then $f(X)$ does not contain any link from F_i to adjacent finite faces. Observe that since each handle of G is a path on an odd number of edges, the above stated conditions uniquely determine the perfect matching $f(X)$. So f is well-defined.

If X, Y are two distinct independent sets of G^*, then there exists a finite face F_i of G which is included in exactly one of the sets X, Y. Consequently, the perfect matchings $f(X)$ and $f(Y)$ differ in the edges of face F_i. Therefore, $f(X) \neq f(Y)$ and so f is injective.

Finally, we show that f is surjective. Let $M \in \mathcal{M}(G)$ be a perfect matching of G and X the set of all finite faces F of G such that F have M-links to all adjacent finite faces. Obviously, the faces in X are pairwise disjoint and therefore, X is an independent set of G^*. By the definition of function f, we also have $f(X) = M$. This completes the proof. ■

To show an example, let G be a CERS shown in Figure 2 that represents the molecular graph of a phenylene. The vertices in squares on the right side of the figure represent the independent set $X = \{F_2, F_5, F_7\}$ of the inner dual G^*. If f is a bijection from Theorem 2, then $f(X) = M$ is the perfect matching of G shown on the left side of the same figure.

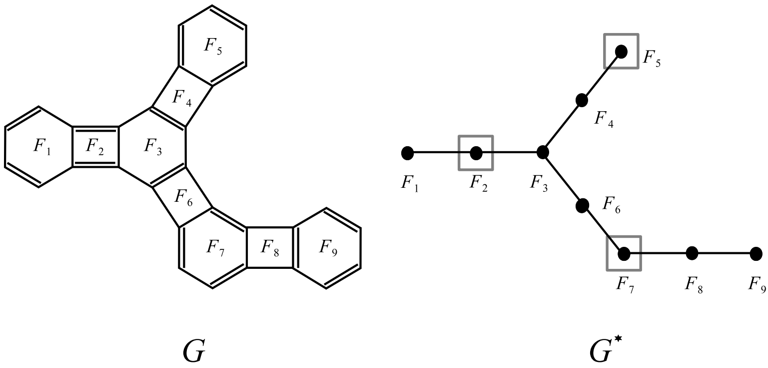

Figure 2. Phenylene (CERS) G with a perfect matching M and its inner dual G^* with the independent set X.

Remark. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Note that the existence of a bijection between sets $\mathcal{I}(G^*)$ and $\mathcal{M}(G)$ also follows from binary coding of perfect matchings described in [4]. More precisely, let $X \subseteq V(G^*) = \{F_1, F_2, \ldots, F_n\}$ be an independent set of G^* and $b(X) = b_1 b_2 \ldots b_n$ the binary code of length n defined in the following way:*

$$b_i = \begin{cases} 1\ ; & F_i \in X \\ 0\ ; & F_i \notin X \end{cases}$$

for any $i \in \{1, \ldots, n\}$. By Algorithm 2 from [4] it follows that the set

$$B = \{b(X) \mid X \text{ is an independent set of } G^*\}$$

is the vertex set of the daisy cube isomorphic to the resonance graph $R(G)$, see Figure 3. Obviously, the set $\mathcal{I}(G^*)$ has the same cardinality as the set B, which further has the same cardinality as the set $V(R(G)) = \mathcal{M}(G)$. Therefore, $|\mathcal{I}(G^*)| = |\mathcal{M}(G)|$ and there exists a bijection between $\mathcal{I}(G^*)$ and $\mathcal{M}(G)$.

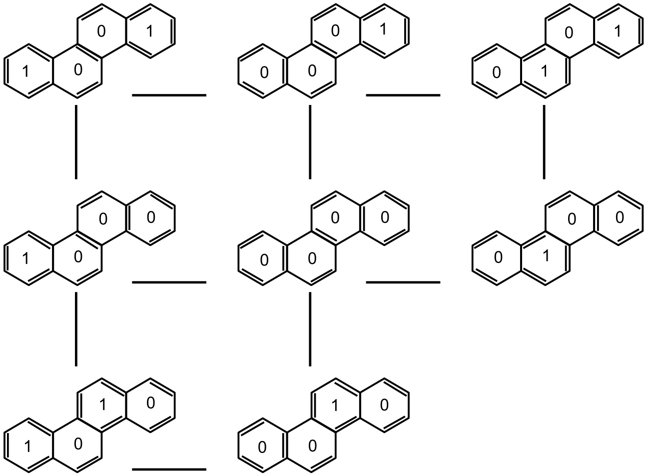

Figure 3. Binary codes as vertices of the resonance graph of graph G from Figure 1.

4 Equality between the independence polynomial and the sextet polynomial

In this section, we prove that if G is a CERS without any linearly connected adjacent triple of finite faces, then the independence polynomial of the inner dual G^* coincides with the sextet polynomial of graph G. In addition, we introduce a new polynomial, named the link polynomial, and prove that for CERS without any linearly connected adjacent triple of finite faces this polynomial equals both above mentioned polynomials.

Firstly, we define the first two polynomials. If G is a graph and $k \geq 0$, denote by $\mathcal{I}(G,k)$ the set of all independent sets of G with cardinality k. The cardinality of the set $\mathcal{I}(G,k)$ will be denoted as $i(G,k)$. Note that $i(G,0) = 1$ for any graph since the empty set is an independent set. The *independence polynomial* [11] of G is defined as

$$I(G;x) = \sum_{k\geq 0} i(G,k)x^k.$$

Recall that $i(G)$ is the number of all independent sets of G. Obviously, $i(G) = I(G; 1)$.

For example, the independence polynomial of the inner dual G^* of benzenoid graph G from Figure 1 is

$$I(G^*; x) = 1 + 4x + 3x^2.$$

Next, let G be a plane bipartite graph with a perfect matching. For $k \geq 0$, denote by $\mathcal{R}(G, k)$ the set of all resonant sets of G with cardinality k. The cardinality of the set $\mathcal{R}(G, k)$ will be denoted as $r(G, k)$. Note that $r(G, 0) = 1$ since the empty set is also a resonant set. The *sextet polynomial* [13] of G is defined as

$$B(G; x) = \sum_{k \geq 0} r(G, k) x^k.$$

In addition, by $r(G)$ we denote the number of all resonant sets of G. Obviously, $r(G) = B(G; 1)$. For example, the sextet polynomial of benzenoid graph G from Figure 3 is

$$B(G; x) = 1 + 4x + 3x^2,$$

which is equal to the independence polynomial of G^*.

Theorem 3. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then the independence polynomial of G^* equals the sextet polynomial of G:*

$$I(G^*; x) = B(G; x).$$

Proof. Let $k \geq 0$. We will show that $\mathcal{I}(G^*, k) = \mathcal{R}(G, k)$. For any $X \in \mathcal{I}(G^*, k)$, it follows by the proof of Theorem 2 that X is also a resonant set of G with cardinality k, so $\mathcal{I}(G^*, k) \subseteq \mathcal{R}(G, k)$.

On the other hand, for any $X \in \mathcal{R}(G, k)$, the finite faces from X are pairwise vertex disjoint since X is a resonant set. Therefore, X is an independent set of G^* with cardinality k, so $\mathcal{R}(G, k) \subseteq \mathcal{I}(G^*, k)$.

Consequently, for any $k \geq 0$ we have

$$i(G^*, k) = |\mathcal{I}(G^*, k)| = |\mathcal{R}(G, k)| = r(G, k),$$

which implies the equality of the two polynomials. ■

Next, we introduce so-called link polynomial, which will be used to prove some additional equalities.

Let G be a CERS. For $k \geq 0$, denote by $\mathcal{M}(G, k)$ the set of all perfect matchings M of G such that there are exactly k finite faces of G which have M-links to all adjacent finite faces. The cardinality of the set $\mathcal{M}(G, k)$ will be denoted as $\ell(G, k)$. We define the *link polynomial* of G in the following way:

$$L(G; x) = \sum_{k \geq 0} \ell(G, k) x^k. \tag{1}$$

Recall that $\mathcal{K}(G)$ is the number of all perfect matchings of G. It is clear that $\mathcal{K}(G) = L(G; 1)$.

Let G be a benzenoid graph from Figure 1. From Figure 3 we can see that $\ell(G, 0) = 1$, $\ell(G, 1) = 4$, $\ell(G, 2) = 3$, and $\ell(G, k) = 0$ for any $k \geq 3$. Hence,

$$L(G; x) = 1 + 4x + 3x^2.$$

Therefore, we prove the following result.

Theorem 4. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then the independence polynomial of G^* equals the link polynomial of G:*

$$I(G^*; x) = L(G; x).$$

Proof. Obviously, the set $\mathcal{I}(G^*)$ can be written as

$$\mathcal{I}(G^*) = \bigcup_{k \geq 0} \mathcal{I}(G^*, k),$$

where for any $k_1 \neq k_2$, the sets $\mathcal{I}(G^*, k_1)$ and $\mathcal{I}(G^*, k_2)$ are pairwise disjoint. Similarly, the set $\mathcal{M}(G)$ can be written as

$$\mathcal{M}(G) = \bigcup_{k \geq 0} \mathcal{M}(G,k),$$

where for any $k_1 \neq k_2$, the sets $\mathcal{M}(G,k_1)$ and $\mathcal{M}(G,k_2)$ are pairwise disjoint.

Let $k \geq 0$. Define f'_k as the restriction of the function $f : \mathcal{I}(G^*) \to \mathcal{M}(G)$ from Theorem 2 to the set $\mathcal{I}(G^*,k)$. By Theorem 2, the image of f'_k is contained in the set $\mathcal{M}(G,k)$. Let $f_k : \mathcal{I}(G^*,k) \to \mathcal{M}(G,k)$ be a function such that for any $X \in \mathcal{I}(G^*,k)$, $f_k(X) = f'_k(X)$. Obviously, since f is injective, it follows that f_k is also an injective function.

To show that f_k is surjective, let M be a perfect matching from $\mathcal{M}(G,k)$. Therefore, $M \in \mathcal{M}(G)$ and since f is surjective, there exists $X \in \mathcal{I}(G^*)$ such that $f(X) = M$. If $X \in \mathcal{I}(G^*,k_1)$, where $k_1 \neq k$, then $f(X) \in \mathcal{M}(G,k_1)$, which is a contradiction. Therefore, $X \in \mathcal{I}(G^*,k)$, so $f_k(X) = f(X) = M$. We have proved that f_k is surjective and consequently, f_k is a bijection.

This implies that for any $k \geq 0$, $|\mathcal{I}(G^*,k)| = |\mathcal{M}(G,k)|$ and also $i(G^*,k) = \ell(G,k)$, so the independence polynomial of G^* equals the link polynomial of G. ■

By Theorems 3 and 4 we immediately obtain that the link polynomial coincides with the sextet polynomial.

Corollary 5. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then the link polynomial of G equals the sextet polynomial of G:*

$$L(G;x) = B(G;x).$$

By Theorems 3, 4 and Corollary 5 we obtain also the following result.

Corollary 6. *Let G be a CERS without any linearly connected adjacent triple of finite faces. The number of perfect matchings of G equals the number of resonant sets of G and the number of independent sets of the inner dual G^*:*

$$\mathcal{K}(G) = r(G) = i(G^*).$$

Proof. Since $\mathcal{K}(G) = L(G;1)$, $r(G) = B(G;1)$, and $i(G^*) = I(G^*;1)$, the statement follows directly. ■

Note that the equality $\mathcal{K}(G) = r(G)$ was proved in [17] for so-called thin polyhex graphs. It would be interesting to generalize this equality to all CERS. However, the equality of the three polynomials does not hold for all CERS. For example, if G is the benzenoid graph of anthracene (formed of three linearly connected hexagons), then $B(G;x) = 1 + 3x$, $L(G;x) = 2 + 2x$, and $I(G^*;x) = 1 + 3x + x^2$.

5 Derivatives of the considered polynomials

We notice that the derivative of the sextet polynomial of graph G from Figure 1 evaluated at $x = 1$ is

$$B'(G;1) = 4 + 6 \cdot 1 = 10,$$

which is exactly the number of edges of the resonance graph $R(G)$ shown in Figure 3. Therefore, in this section we prove this equality for all CERS without any linearly connected adjacent triple of finite faces. Firstly, we connect the derivative of the link polynomial to the number of perfect matchings of some subgraphs of G. Note that for a CERS G and a face F of G, we denote by $G - F$ the graph obtained from G by deleting all the vertices of F.

Theorem 7. *Let G be a CERS without any linearly connected adjacent triple of finite faces. If $F_1, \ldots, F_n$ are the finite faces of G, then it holds*

$$L'(G;1) = \sum_{i=1}^{n} \mathcal{K}(G - F_i).$$

Proof. Obviously,

$$L'(G;1) = \sum_{k \geq 1} k \cdot \ell(G,k),$$

where $\ell(G,k) = |\mathcal{M}(G,k)|$ is the number of perfect matchings M of G such that exactly k finite faces of G has M-links to all adjacent finite faces. Note that in

$$\sum_{k\geq 1} k \cdot \ell(G,k),$$

any perfect matching $M \in \mathcal{M}(G,k)$ is counted k times. Therefore, we describe a function

$$g : \bigcup_{k\geq 1} \big(\mathcal{M}(G,k) \times \{1,\ldots,k\}\big) \to \bigcup_{i=1}^{n} \mathcal{M}(G - F_i).$$

Choose any

$$(M,j) \in \bigcup_{k\geq 1} \big(\mathcal{M}(G,k) \times \{1,\ldots,k\}\big).$$

Then there exists $k \geq 1$, such that $M \in \mathcal{M}(G,k)$ and $j \in \{1,\ldots,k\}$. Suppose that exactly the finite faces from the set $\{F_{s_1}, F_{s_2}, \ldots, F_{s_k}\}$ have M-links to all adjacent finite faces, where $s_1 < s_2 < \cdots < s_k$. Define

$$g(M,j) = M \setminus E(F_{s_j}),$$

which is a perfect matching of $G - F_{s_j}$, so $g(M,j) \in \mathcal{M}(G - F_{s_j})$ and also

$$g(M,j) \in \bigcup_{i=1}^{n} \mathcal{M}(G - F_i).$$

To prove that g is injective, let (M,j) and (M',j') be two elements of

$$\bigcup_{k\geq 1} \big(\mathcal{M}(G,k) \times \{1,\ldots,k\}\big)$$

such that $g(M,j) = g(M',j')$. Obviously, graphs $G - F_i$, $i \in \{1,\ldots,n\}$, have pairwise distinct sets of vertices. Therefore, the sets $\mathcal{M}(G - F_i)$, $i \in \{1,\ldots,n\}$, are pairwise disjoint. Consequently, there exists exactly one $i \in \{1,\ldots,n\}$ such that $g(M,j) = g(M',j') \in \mathcal{M}(G - F_i)$. Hence,

$$M \setminus E(F_i) = g(M,j) = g(M',j') = M' \setminus E(F_i)$$

and by the definition of function g, F_i has M-links and M'-links to all adjacent finite faces, which proves that $M = M'$. Moreover, there exists exactly one $k \geq 1$ such that $M = M' \in \mathcal{M}(G, k)$. Recall that the finite faces from the set $\{F_{s_1}, F_{s_2}, \ldots, F_{s_k}\}$ have M-links to all adjacent finite faces, where $s_1 < s_2 < \cdots < s_k$. Obviously, $F_{s_j} = F_i$ and also $F_{s_{j'}} = F_i$, so we obtain $j = j'$. This proves g is injective.

To show that g is surjective, let

$$M^* \in \bigcup_{i=1}^{n} \mathcal{M}(G - F_i).$$

Then there exists $i \in \{1, \ldots, n\}$ such that $M^* \in \mathcal{M}(G - F_i)$. Let M be the perfect matching of G such that $M^* \subseteq M$ and F_i has M-links to all adjacent finite faces. Since G is a CERS without any linearly connected adjacent triple of finite faces, such perfect matching M exists by Lemma 1. Obviously, G has at least one finite face which has M-links to all adjacent finite faces. So there exists $k \geq 1$ such that $M \in \mathcal{M}(G, k)$. Since F_i has M-links to all adjacent finite faces, by definition of function g there exists $j \in \{1, \ldots, k\}$ such that $g(M, j) = M \setminus E(F_i) = M^*$.

We have proved that g is bijective and therefore,

$$\left| \bigcup_{k \geq 1} \big(\mathcal{M}(G, k) \times \{1, \ldots, k\}\big) \right| = \left| \bigcup_{i=1}^{n} \mathcal{M}(G - F_i) \right|. \tag{2}$$

Obviously, the sets $\mathcal{M}(G, k)$, where $k \geq 1$, are pairwise disjoint and therefore, the sets $\mathcal{M}(G, k) \times \{1, \ldots, k\}$, where $k \geq 1$, are pairwise disjoint. Similarly, recall that the sets $\mathcal{M}(G - F_i)$, where $i \in \{1, \ldots, n\}$, are pairwise disjoint. Therefore, we get

$$\begin{aligned} \left| \bigcup_{k \geq 1} \big(\mathcal{M}(G, k) \times \{1, \ldots, k\}\big) \right| &= \sum_{k \geq 1} \big|\mathcal{M}(G, k) \times \{1, \ldots, k\}\big| \\ &= \sum_{k \geq 1} k \cdot \ell(G, k) = L'(G; 1) \end{aligned}$$

and

$$\left| \bigcup_{i=1}^{n} \mathcal{M}(G - F_i) \right| = \sum_{i=1}^{n} |\mathcal{M}(G - F_i)| = \sum_{i=1}^{n} \mathcal{K}(G - F_i).$$

The result now follows by Equation (2). ■

Since the link polynomial of G coincides with the sextet polynomial of G and also with the independence polynomial of G^*, where G is a CERS without any linearly connected adjacent triple of finite faces, we get the following result.

Corollary 8. *Let G be a CERS without any linearly connected adjacent triple of finite faces. If $F_1, \ldots, F_n$ are the finite faces of G, then it holds*

$$B'(G;1) = I'(G^*;1) = \sum_{i=1}^{n} \mathcal{K}(G - F_i).$$

Note that the equality $B'(G;1) = \sum_{i=1}^{n} \mathcal{K}(G - F_i)$ was proved in [17] for so-called thin polyhex graphs. Again, it would be interesting to generalize this result to all CERS. On the other hand, it is easy to see that equalities

$$L'(G;1) = I'(G^*;1) = \sum_{i=1}^{n} \mathcal{K}(G - F_i)$$

do not hold for all CERS. For example, consider the benzenoid graph of anthracene (formed of three linearly connected hexagons).

Next, we give the connection to the number of edges of the resonance graph.

Theorem 9. *Let G be a CERS with finite faces $F_1, \ldots, F_n$. Then the number of edges of the resonance graph $R(G)$ of G equals*

$$|E(R(G))| = \sum_{i=1}^{n} \mathcal{K}(G - F_i).$$

Proof. Let us define a function

$$h : E(R(G)) \to \bigcup_{i=1}^{n} \mathcal{M}(G - F_i).$$

Choose any edge M_1M_2 of the resonance graph $R(G)$. By definition of the resonance graph there exists exactly one finite face F_i of G such that

$E(F_i) = M_1 \oplus M_2$. Let

$$h(M_1M_2) = M_1 \setminus E(F_i) = M_2 \setminus E(F_i).$$

Obviously, $h(M_1M_2) \in \mathcal{M}(G - F_i)$, so h is well defined.

Firstly, we prove that h is injective. Let M_1M_2 and $M_1'M_2'$ be two edges of the resonance graph such that $h(M_1M_2) = h(M_1'M_2')$. Then there exist finite faces F_i and F_j, where $i, j \in \{1, \dots, n\}$, of G such that $E(F_i) = M_1 \oplus M_2$ and $E(F_j) = M_1' \oplus M_2'$. Obviously, $h(M_1M_2)$ is a perfect matching of the graph $G - F_i$ and $h(M_1'M_2')$ is a perfect matching of the graph $G - F_j$. If $i \neq j$, then the graphs $G - F_i$ and $G - F_j$ have distinct sets of vertices, so $h(M_1M_2) \neq h(M_1'M_2')$ and we obtain a contradiction. Therefore, we have proved that $F_i = F_j$. Moreover, since

$$\begin{aligned} M_1 \setminus E(F_i) &= M_2 \setminus E(F_i) = h(M_1M_2) \\ &= h(M_1'M_2') = M_1' \setminus E(F_i) = M_2' \setminus E(F_i), \end{aligned}$$

perfect matchings M_1, M_2, M_1', M_2' differ only in the edges of the face F_i. Since $M_1 \neq M_2$, $M_1' \neq M_2'$, and the periphery of F_i has only two perfect matchings, we obtain that $\{M_1, M_2\} = \{M_1', M_2'\}$. Consequently, $M_1M_2 = M_1'M_2'$ and so h is injective.

To show that h is surjective, choose any

$$M^* \in \bigcup_{i=1}^{n} \mathcal{M}(G - F_i).$$

We already know that there exists exactly one $i \in \{1, \dots, n\}$ such that $M^* \in \mathcal{M}(G - F_i)$. Obviously, the periphery of F_i has exactly two perfect matchings M_1^* and M_2^*. Let

$$M_1 = M^* \cup M_1^* \quad \text{and} \quad M_2 = M^* \cup M_2^*.$$

It is clear that $E(F_i) = M_1 \oplus M_2$ and hence, $M_1M_2 \in E(R(G))$. Moreover,

$$h(M_1M_2) = M_1 \setminus E(F_i) = M_1 \setminus M_1^* = M^*,$$

so h is bijective.

Therefore, since the sets $\mathcal{M}(G-F_i)$, where $i \in \{1,\ldots,n\}$, are pairwise disjoint, we get

$$|E(R(G))| = \left|\bigcup_{i=1}^{n} \mathcal{M}(G-F_i)\right| = \sum_{i=1}^{n} \mathcal{K}(G-F_i),$$

which completes the proof. ■

The following corollary follows directly by Theorem 7, Corollary 8, and Theorem 9.

Corollary 10. *Let G be a CERS without any linearly connected adjacent triple of finite faces. Then the number of edges of the resonance graph $R(G)$ of G equals*

$$|E(R(G))| = B'(G;1) = L'(G;1) = I'(G^*;1).$$

6 Generalization to peripherally 2-colorable graphs

In this section, we expand the obtained results to a wider family of graphs.

Let G be a plane elementary bipartite graph other than K_2. Then G is called *peripherally 2-colorable* if every vertex of G has degree 2 or 3, vertices with degree 3 (if exist) are all peripheral vertices of G, and G can be properly 2-colored black and white so that two vertices with the same color are nonadjacent and vertices with degree 3 (if exist) are alternatively black and white along the clockwise orientation of the periphery of G [3]. An example of a peripherally 2-colorable graph is shown in Figure 4. Obviously, a CERS without any linearly connected adjacent triple of finite faces is peripherally 2-colorable.

Let F_1, F_2 be two adjacent finite faces of a peripherally 2-colorable graph. The edges from the set $E(F_1) \setminus E(F_2)$ that have an end vertex on the periphery of F_2 are called the *link* from F_1 to F_2. Note that the link can be composed of two edges or in some cases of one edge, see Figure 4.

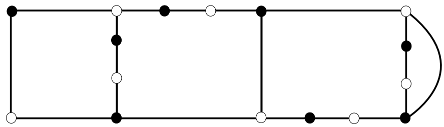

Figure 4. A peripherally 2-colorable graph.

Moreover, if M is a perfect matching of G such that the link from F_1 to F_2 is contained in M, then we say that G has the *M-link* from F_1 to F_2. Note that this definition extends the corresponding definition on CERS. We can now define the link polynomial of G in the same way as for CERS, see Equation 1.

However, it was shown in the proof of Theorem 3.5 from [3] that any peripherally 2-colorable graph G can be transformed to a CERS G' such that the resonance graphs $R(G)$ and $R(G')$ are isomorphic, see Figure 5. In addition, a bijection $\phi : \mathcal{M}(G) \to \mathcal{M}(G')$ between the sets of perfect matchings of G and G' was described such that the following holds true. Let F_1, F_2 be any two adjacent finite faces of G and let F_1', F_2' be the corresponding finite faces of G'. Moreover, let $e \in E(F_1) \setminus E(F_2)$ be an edge that has an end vertex on the periphery of F_2 and $e' \in E(F_1') \setminus E(F_2')$ an edge of G' that has an end vertex on the periphery of F_2'. Then for every perfect matching M of G, e is contained in M if and only if e' is contained in $\phi(M)$. It follows that that for a given perfect matching M of G and every link with two edges either both edges or none belong to M, since this is true for all CERS [16]. Furthermore, the link from F_1 to F_2 is contained in M if and only if the link from F_1' to F_2' is contained in $\phi(M)$. From the above discussion we immediately see that the link polynomial of G is equal to the link polynomial of G', i.e. $L(G; x) = L(G'; x)$.

Moreover, by the same arguments, a set $S = \{F_{s_1}, \ldots, F_{s_k}\}$ of finite faces of G is a resonant set of G if and only if the corresponding set $S' = \{F'_{s_1}, \ldots, F'_{s_k}\}$ is a resonant set of G'. This implies that the sextet polynomials of G and G' coincide: $B(G; x) = B(G'; x)$.

Finally, graphs G and G' have isomorphic inner duals, so their independence polynomials are equal: $I(G^*; x) = I((G')^*; x)$.

Consequently, all results from the previous sections can be generalized

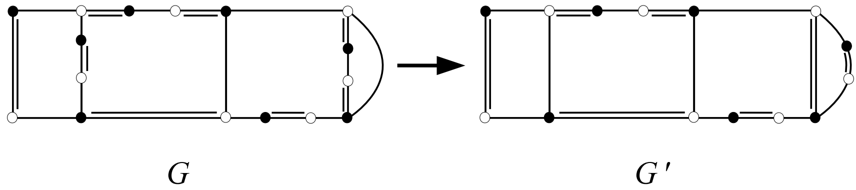

Figure 5. A peripherally 2-colorable graph G with a perfect matching M and the corresponding CERS G' with perfect matching $\phi(M)$.

to peripherally 2-colorable graphs.

Theorem 11. *If G is a peripherally 2-colorable graph, then there exists a bijection $f : \mathcal{I}(G^*) \to \mathcal{M}(G)$ such that any independent set X of G^* of cardinality k is mapped to the perfect matching $f(X) = M$ of G in which only the finite faces from X have M-links to all adjacent finite faces.*

Theorem 12. *If G is a peripherally 2-colorable graph, then*

$$B(G; x) = L(G; x) = I(G^*; x)$$

and

$$\mathcal{K}(G) = r(G) = i(G^*).$$

Theorem 13. *If G is a peripherally 2-colorable graph with finite faces $F_1, \ldots, F_n$, then*

$$B'(G; 1) = L'(G; 1) = I'(G^*; 1) = |E(R(G))| = \sum_{i=1}^{n} \mathcal{K}(G - F_i).$$

***Acknowledgment*:** Niko Tratnik acknowledges the financial support from the Slovenian Research Agency (research programme No. P1-0297 and project No. N1-0285). Petra Žigert Pleteršek acknowledges the financial support from the Slovenian Research Agency (research programme No. P1-0297 and project No. L7-4494).

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