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# Equivalence of Zhang–Zhang Polynomial and Cube Polynomial for Spherical Benzenoid Systems

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**Abstract**

Benzenoid systems or hexagonal systems are subgraphs of a hexagonal lattice. Open-ended carbon nanotubes alias tubulenes can be seen as an embedding of a benzenoid system to a surface of a cylinder with some perimeter edges being joined. Carbon nanotubes are interesting materials with some unusual properties and have therefore been of great interest for researchers in the last 20 years. We use a new term spherical benzenoid system for either a benzenoid system or a tubulene, since both of them can be embedded on a sphere.

Zhang–Zhang polynomial (also called Clar covering polynomial) of a spherical benzenoid system is a counting polynomial of resonant structures called Clar covers. Cube polynomial is a counting polynomial of induced hypercubes in a graph. In [39] authors established the one-to-one correspondence between Clar covers of a benzenoid system $G$ and hypercubes of its resonance graph $R(G)$. In this paper the equality of two polynomials is extended to spherical benzenoid systems using a different method of proving in one part.

## 1 Introduction

*Benzenoid graphs* are 2-connected planar graphs such that every inner face is a hexagon. Benzenoid graphs are generalization of *benzenoid systems*, also called *hexagonal systems*, which can be defined as benzenoid graphs that are also subgraphs of a hexagonal lattice. We refer to [18, 20] for more information about these graphs, especially for their chemical meaning as representation of benzenoid hydrocarbons. If we embed benzenoid systems on a surface of a cylinder and join some edges we obtain structures called open-ended carbon nanotubes (note that there are also closed-ended carbon nanotubes i.e. carbon nanotubes with caps). They were discovered in 1991 [25] and have been since then recognized as fascinating materials with nanometer dimensions, unusual electrical and mechanical properties. In 1996 Smalley group at Rice university successfully synthesized the aligned closed-ends carbon nanotubes [34], which have the almost unusual property of electrical conductivity and super-steel strength. Carbon nanotubes have attracted great attention in different research fields such as nanotechnology, artificial materials, and so on. For the details, see [12, 13, 40].

There are many papers regarding some topological indices of carbon nanotubes such as Wiener, Schultz, Szeged and Harary index; for example see [1, 2, 11, 15, 16]. On the other hand resonance graphs of carbon nanotubes are not so well investigated. A *resonance graph* $R(G)$ of a bipartite graph $G$ reflects the structure of perfect matchings of $G$. The concept is quite natural and has a chemical meaning, therefore it is not surprising that it has been independently introduced in the chemical literature [14, 17] as well as in the mathematical literature [37] under the name *Z-transformation graph*. A survey of some basic properties of resonance graph of benzenoid systems can be found in [36] and the structure of resonance graphs of some families of carbon nanotubes was considered in [43–45].

Main motivation for our research was a result of Zhang et al. [39] where they proved the equivalence of Zhang–Zhang polynomial of a benzenoid system $G$ and cube polynomial of its resonance graph $R(G)$.

Zhang–Zhang polynomial (also called Clar covering polynomial) of a benzenoid system $G$ was introduced by Zhang and Zhang [41] in 1996 and it counts Clar covers of $G$ with different number of hexagons. This polynomial unifies some topological indices such as the Clar number, the Kekulé count and the first Herndon number. Although these authors reported some chemical application of this polynomial [35, 42], intensive research along these lines started nearly 10 years later [21–24]. Basic properties of Zhang–Zhang polynomial and methods to compute it were developed in [4–6, 19, 21, 38]. In particular, Chou and Witek developed an automatic computation program for Zhang–Zhang polynomial of benzenoid systems [7, 8] and obtained many fruitful results, among them closed formulas for the determination of Zhang–Zhang polynomial of some benzenoid systems [9, 10].

Cube polynomial of a graph $H$ was introduced by Brešar et al. in [3] as a counting polynomial for the number of induced hypercubes in $H$ of different dimensions; $n$- dimensional hypercube is a graph whose vertices are all binary strings of length $n$ and two vertices are adjacent if their strings differ exactly in one position. The role of hypercubes as induced subgraphs of the resonance graph of benzenoid systems was established in different papers (see [26, 27, 31–33, 41]).

Our goal is to extend the equivalence of Zhang–Zhang polynomial and cube polynomial to open-ended carbon nanotubes. This paper is organized in the following way; definitions we use are given in the preliminaries, which are then continued by a section on some known results on hypercubes and resonant sets that are important for the next section about new results. We conclude this paper with an example.

## 2 Preliminaries

First we will formally define open-ended carbon nanotubes, also called *tubulenes* ( [28]). Choose any lattice point in the hexagonal lattice as the origin $O$. Let $\vec{a_1}$ and $\vec{a_2}$ be the two basic lattice vectors. Choose a vector $\vec{OA} = n\vec{a_1} + m\vec{a_2}$ such that $n$ and $m$ are two integers and at least one of them is not zero. Draw two straight lines $L_1$ and $L_2$ passing through $O$ and $A$ perpendicular to $OA$, respectively. By rolling up the hexagonal strip between $L_1$ and $L_2$ and gluing $L_1$ and $L_2$ such that $A$ and $O$ superimpose, we can obtain a hexagonal tessellation $\mathcal{HT}$ of the cylinder. $L_1$ and $L_2$ indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a *tubulene* $G$ is defined to be the finite graph induced by all the hexagons of $\mathcal{HT}$ that lie between $c_1$ and $c_2$, where $c_1$ and $c_2$ are two vertex-disjoint cycles of $\mathcal{HT}$ encircling the axis of the cylinder. The vector $\vec{OA}$ is called the *chiral vector* of $G$ and the cycles $c_1$ and $c_2$ are the two open-ends of $G$.

For any tubulene $G$, if its chiral vector is $n\vec{a_1} + m\vec{a_2}$, $G$ will be called an $(n, m)$-type tubulene, see Figure 1.

Now we can define a new family of graphs: graph $G$ is a *spherical benzenoid system* if $G$ is either a benzenoid system or a tubulene. Spherical benzenoid systems can be embedded on a sphere and are bipartite graphs.

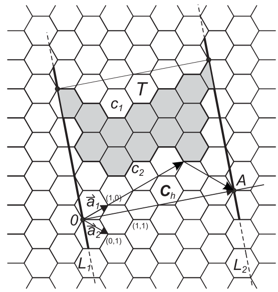


Figure 1: Illustration of a $(4, 2)$-type tubulene.

An *1-factor* of a spherical benzenoid system $G$ is a spanning subgraphs of $G$ such that every vertex has degree one. Edges of 1-factor form an independent set of edges i.e. a *perfect matching* of $G$ (in the chemical literature these are known as Kekulé structures; for more details see [20]). Let $M$ be a perfect matching of $G$. A hexagon $h$ of $G$ is $M$-*alternating* if edges of $h$ appear alternately in and off the perfect matching $M$. A perfect matching of a hexagon of $G$ is called a *sextet*.

Let $G$ be a spherical benzenoid system. A *Clar cover* is a spanning subgraph of $G$ such that every component of it is either a hexagon or an edge. Set of hexagons in a Clar cover is a *resonant set* of $G$. Resonant set with the maximum number of hexagons is a *Clar formula* of $G$. Number of hexagons in the Clar formula is a *Clar number* $Cl(G)$ of $G$. It is not difficult to see that if $P$ is a resonant set of a spherical benzenoid system $G$, then $G - P$ is empty or has a perfect matching (this fact was proved in [29, 30] for benzenoid systems and can be extended to spherical benzenoid systems). A resonant set $P$ such that $G - P$ is empty or has a unique perfect matching is called a *canonical* resonant set.

The *resonance graph* $R(G)$ of a spherical benzenoid system $G$ is the graph whose vertices are the perfect matchings of $G$, and two perfect matchings are adjacent whenever their symmetric difference forms an edge set of a hexagon of $G$.

Let $G$ be a spherical benzenoid system. *Zhang–Zhang polynomial* of $G$ is defined in the following way:

$$ZZ(G, x) = \sum_{k=0}^{Cl(G)} z(G, k)x^k,$$

where $z(G, k)$ is the number of Clar covers of $G$ with $k$ hexagons. Note that for a spherical benzenoid system $G$ $z(G,0)$ equals the number of vertices of $R(G)$ and $z(G,1)$ equals the number of edges of $R(G)$.

Let $H$ be a graph. *Cube polynomial* of $H$ is defined as follows:

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

where $\alpha_i(H)$ denotes the number of induced subgraphs of $H$ that are isomorphic to the $i$-dimensional hypercube.

Now we can write the main result of Zhang et al. which was our motivation:

**Theorem 2.1** *[39] For a benzenoid system $G$ with a perfect matching, we have*

$$ZZ(G,x) = C(R(G),x) .$$

# 3 Hypercubes and resonant sets

In [31] (and later in [32], [33]) authors considered the relation between resonant sets of a benzenoid system $G$ and subgraphs of its resonance graph $R(G)$ that are isomorphic to hypercubes. To a resonant set of cardinality $k$ for some positive integer $k$ we can associate a unique subgraph of $R(G)$ isomorphic to a $k$-dimensional hypercube if $P$ is a canonical resonant set, otherwise we can associate as many (vertex-disjoint) subgraphs of $R(G)$ isomorphic to the $k$-dimensional hypercube as the number of perfect matchings in $G-P$.

For a benzenoid system $G$ let $\mathcal{H}(R(G))$ be the set of all hypercubes of its resonance graph $R(G)$ and let $\mathcal{RS}(G)$ be the set of all resonant sets of $G$. The main result of [31] is:

**Theorem 3.1** *[31] Let $G$ be a benzenoid system possessing at least one perfect matching. Then there exists a surjective map $f : \mathcal{H}(R(G)) \longrightarrow \mathcal{RS}(G)$, where $|f(Q)| = k$ for a $k$-dimensional hypercube $Q$ of $R(G)$.*

Proof of this result and relation between resonant sets of $G$ and hypercubes of $R(G)$ can also be applied to spherical benzenoid systems since the embedding of the hexagonal lattice to a surface of a cylinder does not affect proofs. We could have used the same proof as in [31], but in the next section we will prove stronger result (using some ideas from [31]) such that Theorem 3.1, extended to spherical benzenoid systems, will be just a corollary.

# 4 Main result

**Lemma 4.1** *Let $G$ be a spherical benzenoid system with a perfect matching. Then there exists a surjective mapping from the set of Clar covers of $G$ (with at least one hexagon) to the set of resonant sets of $G$.*

**Proof.** Let $G$ be a spherical benzenoid system with a perfect matching and let $g$ be a mapping from the set od Clar covers of $G$ to the set of resonant sets of $G$ defined in the following way: for a Clar cover $C$ with $k$-hexagons $h_1, h_2, \ldots, h_k$ let $g(C)$ be the set of hexagons $\{h_1, h_2, \ldots, h_k\}$. From the definitions of Clar cover and resonant set it follows that $g$ is a well-defined mapping.

Now, let $P = \{h_1, h_2, \ldots, h_k\}$, $1 \leq k \leq Cl(G)$, be a resonant set of $G$. Therefore hexagons $h_1, h_2, \ldots, h_k$ are pairwise disjoint and $G - P$ is either empty or has a perfect matching. Let $M$ be a perfect matching of $G$ such that hexagons $h_1, h_2, \ldots, h_k$ are $M$-alternating. Then the subgraph of $G$ induced with edges $M \cup \left(\cup_{i=1}^{k} E(h_i)\right)$ is the Clar cover of $G$ with $k$ hexagons. ■

Our main result is a generalization of Theorem 2.1 from [39] to spherical benzenoid systems. First two lemmas of the proof are proved almoust analogously as in Theorem 2.1 and the proof of the third lemma is new and shorter.

**Theorem 4.2** *Let $G$ be a spherical benzenoid system. Then Zhang–Zhang polynomial of $G$ equals cube polynomial of its resonance graph $R(G)$ i.e.*

$$ZZ(G, x) = C(R(G), x)\,.$$

**Proof.** Let $k$ be a nonnegative integer. For a spherical benzenoid system $G$ we denote by $\mathbb{Z}(G, k)$ the set of all Clar covers of $G$ with exactly $k$ hexagons. On the other hand, consider a graph $H$; the set of subgraphs of $H$ that are isomorphic to a $k$-dimensional hypercube is denoted by $\mathbb{Q}_k(H)$. Let us define a mapping $f_k$ from the set of Clar covers of a spherical benzenoid system $G$ with $k$ hexagons to the set of subgraphs of the resonance graph $R(G)$ isomorphic to the $k$-dimensional hypercube

$$f_k : \mathbb{Z}(G,k) \longrightarrow \mathbb{Q}_k(R(G))$$

in the following way: for a Clar cover $C \in \mathbb{Z}(G,k)$ consider those perfect matchings $M_1$, $M_2$, ..., $M_i$ of $G$ that each hexagon in $C$ is $M_j$-alternating and each isolated edge of $C$ is in $M_j$, for all $j = 1, 2, \ldots, i$. Assign $f_k(C)$ as an induced subgraph of $R(G)$ with vertices $M_1, M_2, \ldots, M_i$.

Note first that in case when $k = 0$ Clar covers are without hexagons, i.e. Clar covers are perfect matchings of a spherical benzenoid system and if $C$ is such Clar cover then $f_k(C)$ is a vertex of the resonance graph and the mapping is obviously bijective. So from now on $k$ will be a positive integer.
The following lemma shows that $f_k$ is a well-defined mapping.

**Lemma 4.3** *For each Clar cover $C \in \mathbb{Z}(G,k)$ we have $f_k(C) \in \mathbb{Q}_k(R(G))$.*

**Proof.** We can apply similar proof as in [39]:
It is sufficient to show that $f_k(C)$ is isomorphic to the $k$-dimensional hypercube $Q_k$. Let $h_1, h_2, \ldots, h_k$ be hexagons of $C$. Obviously, every hexagon of $C$ has two possible perfect matchings. Let us call these "possibility 0" and "possibility 1". For any vertex $M$ of $f_k(C)$ let $b(M) = (b_1, b_2, \ldots, b_k)$, where $b_i = 1$ if on $h_i$ possibility 1 is selected, and $b_i = 0$ otherwise, $i = 1, 2, \ldots, k$. It is obvious that $b : V(f_k(C)) \to V(Q_k)$ is a bijection. For $M' \in V(f_k(C))$, let $b(M') = (b'_1, b'_2, \ldots, b'_k)$. If $M$ and $M'$ are adjacent in $f_k(C)$ then $M \oplus M' = E(h_i)$ for some $i, 1 \le i \le k$. Therefore, $b_j = b'_j$ for each $j \neq i$ and $b_i \neq b'_i$, which implies $(b_1, b_2, \ldots, b_k)$ and $(b'_1, b'_2, \ldots, b'_k)$ are adjacent in $Q_k$. Conversely, if $(b_1, b_2, \ldots, b_k)$ and $(b'_1, b'_2, \ldots, b'_k)$ are adjacent in $Q_k$, it follows that $M$ and $M'$ are adjacent in $f_k(C)$. Hence $b$ is an isomorphism between $f_k(C)$ and $Q_k$. ■
The following lemma shows that $f_k$ is an injective mapping.

**Lemma 4.4** *The mapping $f_k : \mathbb{Z}(G,k) \longrightarrow \mathbb{Q}_k(R(G))$ is injective for each positive integer $k$.*

**Proof.** We can apply the same proof as in [39].
Let $C$ and $C'$ be distinct Clar covers from $\mathbb{Z}(G,k)$. If $C$ and $C'$ contain the same set

of hexagons, then the isolated edges of $C$ and $C'$ are distinct. Therefore, $f_k(C)$ and $f_k(C')$ are disjoint induced subgraphs of $R(G)$ and thus $f_k(C) \neq f_k(C')$. Suppose $C$ and $C'$ contain different sets of hexagons and let $h$ be a hexagon in $C - C'$. Hence at least one edge $e$ of $h$ does not belong to $C'$. From the definition of the function $f_k$, $e$ is thus unsaturated by those perfect matchings that correspond to the vertices in $f_k(C')$. However, there exist vertices $M_1$ and $M_2$ of $f_k(C)$ ($M_1$ and $M_2$ are perfect matchings of $G$) such that $M_1 \oplus M_2 = E(h)$ because $h$ is a hexagon in $C$. Hence $e$ is saturated by one of $M_1$ or $M_2$, say $M_1$. As a result, $M_1 \notin V(f_k(C'))$ and $f_k(C) \neq f_k(C')$. ■

The following lemma shows that $f_k$ is a surjective mapping.

**Lemma 4.5** *The mapping $f_k : \mathbb{Z}(G,k) \longrightarrow \mathbb{Q}_k(R(G))$ is surjective for each positive integer $k$.*

**Proof.** Let $k$ be a positive integer and $Q \in \mathbb{Q}_k(R(G))$. Since $Q$ is a subgraph of $R(G)$ isomorphic to a $k$-dimensional hypercube, vertices of $Q$ can be identified with binary strings $(u_1, u_2, \ldots, u_k)$, so that two vertices of $Q$ are adjacent in $Q$ if and only if their binary strings differ in precisely one position. Consider the following vertices of $Q$: $M = (0,0,0,\ldots,0)$, $N^1 = (1,0,0,\ldots,0)$, $N^2 = (0,1,0,\ldots,0)$, $\ldots$, $N^k = (0,0,0,\ldots,1)$. It is obvious that $MN^i$ is an edge of $R(G)$ for every $i, 1 \leq i \leq k$. By definition of $R(G)$, the symmetric difference of perfect matchings $M$ and $N^i$ is the edge set of a hexagon of $G$. We denote this hexagon by $h_i$ and we obtain the set of hexagons $\{h_1, \ldots, h_k\}$ of the spherical benzenoid system $G$. Similar as in the proof of Theorem 2 in [31] we can show that the following two claims hold true:

1. The hexagons $h_i$, $1 \leq i \leq k$, are pairwise disjoint.

2. Let $XY$ be an edge of $Q$. If the binary representations of $X$ and $Y$ differ at the $j$-th place, then the symmetric difference $X \oplus Y$ is the edge set of the hexagon $h_j$.

We notice that $M^0 = M = (0,0,0,\ldots,0)$, $M^1 = N^1 = (1,0,0,\ldots,0)$, $M^2 = (1,1,0,\ldots,0)$, $\ldots$, $M^k = (1,1,1,\ldots,1)$ is the path in $Q$ and by second claim, the edge $M^iM^{i+1}$ corresponds to the hexagon $h_{i+1}$ for every $i, 0 \leq i \leq k-1$. So going from $M^0$ to $M^k$ the perfect matchings only change in pair-wise disjoint hexagons $h_1, \ldots, h_k$, hence the perfect matching $M^k$ contains a sextet of each hexagon in $\{h_1, \ldots, h_k\}$. Since $Q$ is connected graph it follows that every vertex of $Q$ contains a sextet of each hexagon from $\{h_1, \ldots, h_k\}$ and also vertices of $Q$ differ only on edges of exactly these same hexagons.

Let $C$ be a subgraph of $G$, induced with edges in the set $M^k \cup E(h_1) \cup \ldots \cup E(h_k)$. It is easy to see that $C$ is a Clar cover with $k$ hexagons and $V(f_k(C)) = V(Q)$. Since both $Q$ and $f_k(C)$ are induced subgraphs of the resonance graph, it follows $f_k(C) = Q$. ■

From Lemmas 4.3, 4.4, 4.5 follows the equality of two polynomials:

$$ZZ(G, x) = C(R(G), x)\,,$$

what concludes the proof of Theorem 4.2. ■

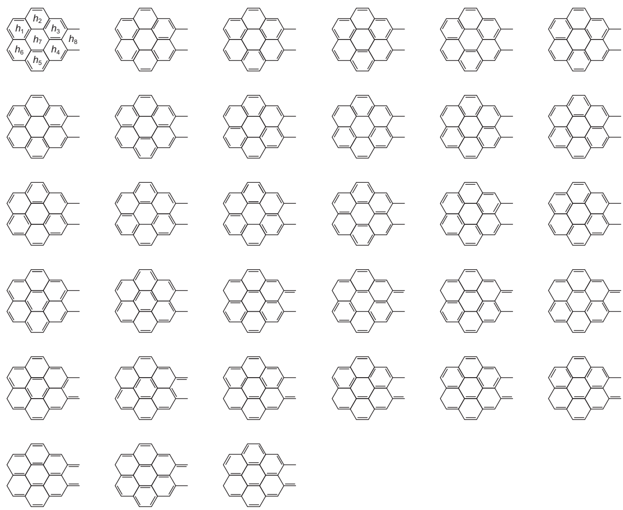


Figure 2: Perfect matchings of a $(2, 2)$-type tubulene $G$.

Using Lemma 4.1 and Theorem 4.2 we obtain the following result from [31], extended to spherical benzenoid systems.

**Corollary 4.6** *Let $G$ be a spherical benzenoid system possessing at least one perfect matching. Then there exists a surjective map $f : \mathcal{H}(R(G)) \longrightarrow \mathcal{RS}(G)$, where $|f(Q)| = k$ for a $k$-dimensional hypercube $Q$ of $R(G)$.*

## 5 Example

We will conclude with an example of a spherical benzenoid system $G$ that is similar to a very well known benzenoid system named coronene. Graph $G$ is a $(2,2)$-type tubulene consisted of 8 hexagons denoted by $h_1, \ldots, h_8$, see Figure 2. On that figure we can see all 33 perfect matchings of $G$ what is then the number of vertices in the resonance graph $R(G)$.

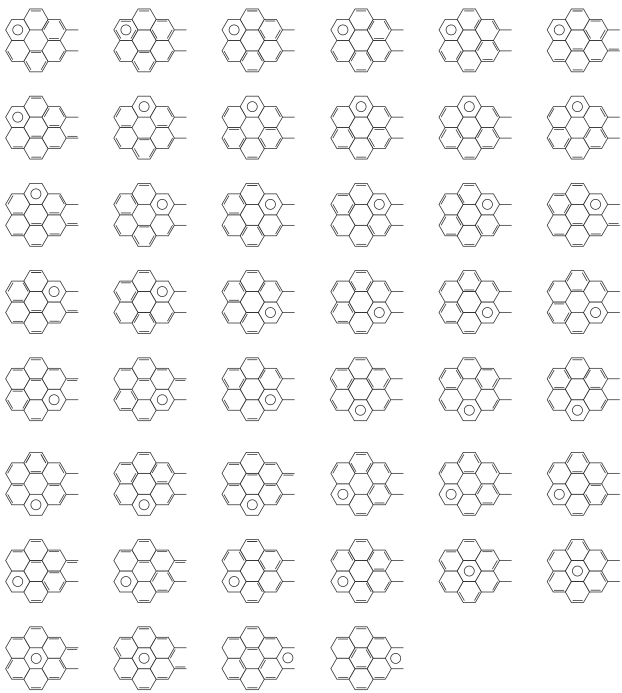

Figure 3: Clar covers of $G$ with one hexagon.

As we can see on Figure 3 there are 46 Clar covers of $G$ with one hexagon and this is the number of edges of the resonance graph $R(G)$.

There are 18 Clar covers of $G$ with exactly two hexagons (see Figure 4) and this is the number of subgraphs of $R(G)$ that are isomorphic to a 2-dimensional hypercube.

On Figure 5 we can see both maximum cardinality Clar covers of $G$, what means that $Cl(G) = 3$, and the number of induced 3-dimensional hypercubes in $R(G)$ is two.

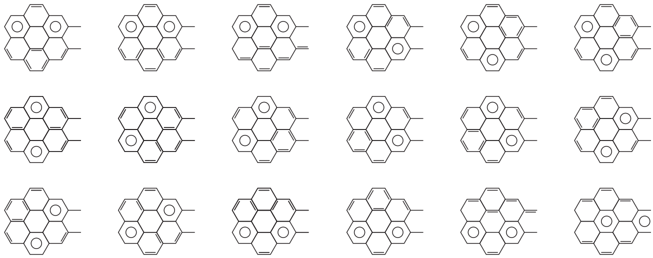

Figure 4: Clar covers of $G$ with two hexagons.

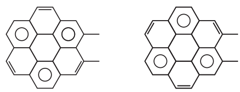

Figure 5: Clar covers of $G$ with three hexagons.

The resonance graph $R(G)$ of the $(2,2)$-type tubulene $G$ can be seen on Figure 6 and Zhang–Zhang polynomial of $G$ is equal to the cube polynomial of $R(G)$:

$$ZZ(G,x) = C(R(G),x) = 2x^3 + 18x^2 + 46x + 33\,.$$

Let us remark that labels $h_i$ for $i = 1,2,\ldots,8$ of edges on Figure 6 shows that the symmetric
difference of corresponding perfect matchings (end-vertices of an edge) are edges of the hexagon $h_i$. Also note that the resonance graph $R(G)$ has three connected components, one consisting of a single vertex (i.e. the perfect matching of $G$ without alternating hexagons).

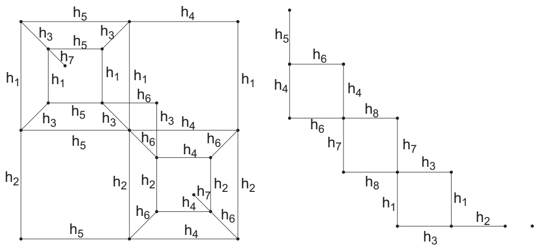

Figure 6: Resonance graph $R(G)$ of $G$.

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