

# Resonance graphs of fullerenes\*

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## Abstract

A fullerene  $G$  is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. The resonance graph  $R(G)$  of  $G$  reflects the structure of its perfect matchings. The Zhang-Zhang polynomial of a fullerene is a counting polynomial of resonant structures called Clar covers. The cube polynomial is a counting polynomial of induced hypercubes in a graph.

In the present paper we show that the resonance graph of every fullerene is bipartite and each connected component has girth 4 or is a path. Also, the equivalence of the Zhang-Zhang polynomial of a fullerene and the cube polynomial of its resonance graph is established. Furthermore, it is shown that every subgraph of the resonance graph isomorphic to a hypercube is an induced subgraph in the resonance graph. For benzenoid systems and tubulenes each connected component of the resonance graph is the covering graph of a distributive lattice; for fullerenes this is not true, as we show with an example.

*Keywords:* Fullerene, resonance graph, Zhang-Zhang polynomial, cube polynomial, Kekulé structure, perfect matching, distributive lattice, median graph.

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## 1 Introduction

A fullerene is a molecule of carbon in the form of a hollow sphere, ellipsoid, tube, or many other shapes. The first fullerene molecule was discovered 30 years ago. In graph theory, a fullerene is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. Kekulé structures of an unsaturated hydrocarbon represent the possible positions of double bonds in the molecule, which corresponds to a perfect matching of a molecular graph. In recent years, a lot of research has been done on the symmetries of fullerenes and their Kekulé structure counts. The concept of the resonance graph of a fullerene was introduced in [9]. The resonance graph of a hydrocarbon reflects the structure of its perfect matchings. There are many results on resonance graphs of benzenoid systems [14] and open-ended carbon nanotubes (tubulenes) [11, 19], but nothing has been done on resonance graphs of fullerenes.

In the present paper we investigate basic properties of resonance graphs of fullerenes. It is shown that the resonance graph of every fullerene is bipartite and each connected component has girth 4 or is a path. Further, the equivalence of Zhang-Zhang polynomial of a fullerene and the cube polynomial of its resonance graph is established. The corresponding results are already known for benzenoid systems and tubulenes (see [14, 12, 11, 17, 3]). Moreover, we prove that every subgraph of the resonance graph of a fullerene that is isomorphic to a hypercube is actually an induced subgraph. We also give an example of a fullerene such that one of the connected components of its resonance graph is not the covering graph of a distributive lattice. This is surprising since all such components are covering graphs of distributive lattices in the case of benzenoid systems and tubulenes (see [15, 13]).

## 2 Preliminaries

A fullerene  $G$  is a 3-regular plane graph consisting only of pentagonal and hexagonal faces. By Euler's formula it follows that the number of pentagonal faces is exactly 12 in every fullerene.

A 1-factor of a fullerene  $G$  is a spanning subgraph of  $G$  such that every vertex has degree one. Edges of the 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 [5]). Petersen's theorem states that in a bridgeless 3-regular graph, there is always a perfect matching [8]. Therefore, a fullerene always has at least one perfect matching.

Let  $M$  be a perfect matching of  $G$ . A hexagon  $h$  of  $G$  is  $M$ -alternating if the edges of  $h$  appear alternately in and out the perfect matching  $M$ . Such a hexagon  $h$  is also called a sextet.

The resonance graph  $R(G)$  of a fullerene  $G$  is the graph whose vertices are the perfect matchings of  $G$ , and two perfect matchings  $M_1$  and  $M_2$  are adjacent whenever their symmetric difference  $M_1 \oplus M_2$  forms a set of edges of exactly one hexagon of  $G$ .

Let  $G$  be a fullerene. A Clar cover is a spanning subgraph of  $G$  such that every component of it is either a hexagon or an edge. The set of hexagons in a Clar cover is a resonant set of  $G$ . A resonant set with the maximum number of hexagons is a Clar formula of  $G$ . The number of hexagons in the Clar formula is a Clar number  $Cl(G)$  of  $G$ . The Zhang-Zhang polynomial of  $G$  (also called the Clar covering polynomial, see [18]) is defined in

the following way:

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

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

The  $n$ -dimensional hypercube  $Q_n$  is the graph whose vertices are all binary strings of length  $n$  and two vertices are adjacent if and only if their strings differ exactly in one position. A Lucas cube  $\Lambda_n$  is the graph whose vertex set is the set of all binary strings of length  $n$  without consecutive 1's and also without 1 in the first and the last bit. The edges are defined analogously as for the hypercube.

Let  $H$  be a graph. The *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.

The *Cartesian product*  $G \square H$  of graphs  $G$  and  $H$  is the graph with the vertex set  $V(G) \times V(H)$  and  $(a, x)(b, y) \in E(G \square H)$  whenever  $ab \in E(G)$  and  $x = y$ , or, if  $a = b$  and  $xy \in E(H)$ .

Let  $\mathbf{P} = (P, \leq)$  be a poset, i.e.  $\leq$  is a binary relation on  $P$ , which is reflexive, antisymmetric and transitive. For  $x, y \in P$ , a *lower bound* of  $x$  and  $y$  is an element  $z \in P$  such that  $z \leq x$  and  $z \leq y$ . A lower bound  $z$  of  $x$  and  $y$  is said to be the *greatest lower bound* (if it exists) if  $z' \leq x$  and  $z' \leq y$ ,  $z' \in P$ , imply that  $z' \leq z$ . If  $x$  and  $y$  have a greatest lower bound, then it is unique and denoted by  $x \wedge y$ . Similarly we can define the least upper bound  $x \vee y$  whenever it exists. A *lattice* is a poset in which every pair of elements have the least upper bound and the greatest lower bound. Further, when operations  $\wedge$  and  $\vee$  of a lattice admit distributive laws we call it a *distributive lattice*. By  $x < y$  we mean that  $x \leq y$  and  $x \neq y$ . We say that  $y$  *covers*  $x$  if  $x < y$  and  $x < a \leq y$  imply  $a = y$ . The *covering graph*  $\mathcal{C}(\mathbf{P})$  of a poset  $\mathbf{P}$  is a graph whose vertices are elements of  $P$  and  $x, y \in P$  are adjacent in  $\mathcal{C}(\mathbf{P})$  if and only if  $x$  covers  $y$  or  $y$  covers  $x$ .

Let  $G$  be a graph. A *median* of a triple of vertices  $u, v, w$  of  $G$  is a vertex  $z$  that lies on a shortest  $u, v$ -path, on a shortest  $u, w$ -path and on a shortest  $v, w$ -path. Note that  $z$  can be one of the vertices  $u, v, w$ . A graph is a *median graph* if every triple of its vertices has a unique median. These graphs were first introduced in [1] by Avann. Median graphs arise naturally in the study of ordered sets and distributive lattices. It is known that trees and grid graphs are examples of median graphs.

A graph  $H$  is a *retract* of  $G$  if there are homomorphisms (edge-preserving functions)  $f : V(H) \rightarrow V(G)$  and  $g : V(G) \rightarrow V(H)$  such that  $g(f(a)) = a$  for every  $a \in V(H)$ . Note that if  $H$  is a retract of  $G$  it is convenient to take  $H$  as a subgraph of  $G$  and  $f$  to be an inclusion map. It is known that median graphs can be characterized as retracts of hypercubes [2].

### 3 Some results about resonance graphs of fullerenes

In this section we will prove some basic properties of resonance graphs of fullerenes. The first theorem claims that the resonance graph of every fullerene is a bipartite graph. In the proof we use the concept of the dual graph  $G^*$ , which has a vertex for each face of  $G$ . The dual graph has an edge whenever two faces of  $G$  are separated from each other by an edge.

**Theorem 3.1.** *Let  $G$  be a fullerene. Then its resonance graph  $R(G)$  is bipartite.*

*Proof.* It is known that  $R(G)$  is bipartite if and only if  $R(G)$  does not contain an odd cycle. Let  $C = M_0M_1 \dots M_t$  be a cycle in  $R(G)$ , where  $M_0 = M_t$ . Hence there exists a sequence of hexagons  $h_1, h_2, \dots, h_t$  such that  $E(h_i) = M_{i-1} \oplus M_i$  for every  $i \in \{1, 2, \dots, t\}$ . For every hexagon  $h$  of a fullerene  $G$  we define  $\delta(h)$  to be the number of times  $h$  appears in the sequence  $h_1, h_2, \dots, h_t$ . We will show that  $\delta(h)$  is an even number for every hexagon  $h$  of  $G$ . We consider two options:

- (i) Let  $h$  be a hexagon with an edge  $e$  lying on some pentagon of  $G$ . We know that  $M_0 = M_0 \oplus E(h_1) \oplus E(h_2) \oplus \dots \oplus E(h_t)$ , hence there must be an even number of terms in the sequence  $h_1, h_2, \dots, h_t$  containing the edge  $e$ . Since  $h$  is the only hexagon of  $G$  that contains  $e$ ,  $\delta(h)$  must be even.
- (ii) Now suppose that no edge of  $h$  lies on a pentagon. Let  $G^*$  be the dual graph of some planar drawing of  $G$  and let  $p_0$  be a pentagon of  $G$  such that  $d_{G^*}(h, p_0) = \min\{d(h, p) \mid p \text{ pentagon of } G\}$ . Furthermore, let  $h, h_1, \dots, h_n, p_0$  be a shortest path from  $h$  to  $p_0$  in  $G^*$ . Let  $e$  be the common edge of  $h$  and  $h_1$ . Similar as in (i) we can see that  $\delta(h) + \delta(h_1)$  is even. Assume that  $\delta(h)$  is odd. Then  $\delta(h_1)$  must be odd. Let  $e'$  be the common edge of  $h_1$  and  $h_2$  – see Figure 1. But  $\delta(h_2)$  is odd too since  $\delta(h_1) + \delta(h_2)$  is even. If we repeat this discussion we obtain that  $\delta(h_n)$  is odd. But the hexagon  $h_n$  contains an edge lying on pentagon  $p_0$  and therefore, by (i),  $\delta(h_n)$  must be even. This contradiction shows that  $\delta(h)$  is even.

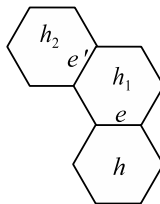


Figure 1: Hexagons  $h, h_1$  and  $h_2$ .

We have proved that  $\delta(h)$  is an even number for every hexagon  $h$  of  $G$ . Hence  $t = \sum_{h \in T} \delta(h)$  is even, i.e.  $C$  is an even cycle. □

Next we show that every connected component (different from a path) of the resonance graph of a fullerene has girth 4. We begin with the following lemma.

**Lemma 3.2.** *Let  $G$  be a fullerene and  $H$  a connected component of the resonance graph  $R(G)$  such that  $H$  is not a path. If  $V_1(H)$  is the set of all vertices in  $H$  that have degree one and  $M \in V(H) - V_1(H)$ , then we can find in a fullerene  $G$  at least two disjoint hexagons which are  $M$ -alternating cycles.*

*Proof.* The proof is the same as the proof of Lemma 3.1 in [11]. □

With Lemma 3.2 the following theorem is almost obvious.

**Theorem 3.3.** *Let  $G$  be a fullerene and  $H$  a connected component of the resonance graph  $R(G)$ . Then  $H$  is either a path or a graph of girth 4.*

*Proof.* Suppose that  $H$  is not a path. The set of all vertices in  $V(H)$  which have degree one will be denoted by  $V_1(H)$ . If the set  $V(H) - V_1(H)$  is empty it follows that  $H$  is the path  $P_2$ , which is a contradiction since  $H$  is not a path. Hence, let  $M \in V(H) - V_1(H)$ .

By Lemma 3.2, in a fullerene  $G$  there are two disjoint hexagons  $h_1$  and  $h_2$  which are  $M$ -alternating cycles. Thus,  $M$  lies in a 4-cycle  $MM_1M_2M_3$  where  $M_1 = M \oplus E(h_1)$ ,  $M_2 = M_1 \oplus E(h_2)$  and  $M_3 = M_2 \oplus E(h_1)$ . By Theorem 3.1 the resonance graph  $R(G)$  is bipartite, therefore,  $H$  is bipartite too. Hence, there is no 3-cycle in  $H$ . Since every vertex lies in some 4-cycle, the girth of  $H$  is 4 and the proof is completed. □

### 4 Equivalence of Zhang-Zhang polynomial and cube polynomial for fullerenes

In this section we prove that the Zhang-Zhang polynomial of every fullerene equals the cube polynomial of its resonance graph. The same result was proved in [17] for benzenoid systems and in [3] for tubulenes. However, the proof in [17] cannot be applied in our case, since it is based on directed resonance graph (which is not defined for fullerenes, since fullerenes are not bipartite). Therefore, we combine ideas from [10], [17] and [3] to prove the following theorem:

**Theorem 4.1.** *Let  $G$  be a fullerene. Then the Zhang-Zhang polynomial of  $G$  equals the 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 fullerene  $G$  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 induced 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 fullerene  $G$  with  $k$  hexagons to the set of induced 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  $M_1, M_2, \dots, M_i$  of  $G$  that each hexagon in  $C$  is  $M_j$ -alternating and each isolated edge of  $C$  is in  $M_j$ , for all  $j = 1, 2, \dots, i$ . Assign  $f_k(C)$  as an induced subgraph of  $R(G)$  with vertices  $M_1, M_2, \dots, M_i$ .

Note first that in case when  $k = 0$  Clar covers are without hexagons, i.e. Clar covers are perfect matchings of a fullerene and if  $C$  is such a 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.

First show that  $f_k$  is a well-defined mapping.

**Lemma 4.2.** *For each Clar cover  $C \in \mathbb{Z}(G, k)$  we have  $f_k(C) \in \mathbb{Q}_k(R(G))$ .*

*Proof.* The proof in [17] is based on proper and improper alternating cycles, which are not well defined in our case. But we can apply the same proof as in [3]:

It is sufficient to show that  $f_k(C)$  is isomorphic to the  $k$ -dimensional hypercube  $Q_k$ . Let  $h_1, h_2, \dots, h_k$  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  $b(M) = (b_1, b_2, \dots, b_k)$ , where  $b_i = 1$  if on  $h_i$  possibility 1 is selected, and  $b_i = 0$  otherwise,  $i = 1, 2, \dots, k$ . It is obvious that  $b : V(f_k(C)) \rightarrow V(Q_k)$  is a bijection. For  $M' \in V(f_k(C))$ , let  $b(M') = (b'_1, b'_2, \dots, b'_k)$ . If  $M$  and  $M'$  are adjacent in  $f_k(C)$  then  $M \oplus M' = E(h_i)$  for some  $i, 1 \leq i \leq k$ . Therefore,  $b_j = b'_j$  for each  $j \neq i$  and  $b_i \neq b'_i$ , which implies  $(b_1, b_2, \dots, b_k)$  and  $(b'_1, b'_2, \dots, b'_k)$  are adjacent in  $Q_k$ . Conversely, if  $(b_1, b_2, \dots, b_k)$  and  $(b'_1, b'_2, \dots, b'_k)$  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. For the proof see [17, 3].

**Lemma 4.3.** *The mapping  $f_k : \mathbb{Z}(G, k) \rightarrow \mathbb{Q}_k(R(G))$  is injective for each positive integer  $k$ .*

The next lemma was proved in [17] for benzenoid systems. Here we extend it to fullerenes.

**Lemma 4.4.** *Let  $G$  be a fullerene. If the resonance graph  $R(G)$  contains a 4-cycle  $M_1M_2M_3M_4$ , 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.* We can apply the proof of Lemma 2.4 in [17]. □

To prove that the mapping  $f_k$  is surjective, we apply a similar proof as in [3], but to prove Claim 1 and Claim 2 in the proof, we use Lemma 4.4 (which is shorter). We give the whole proof since notation from it is then used in the proof of Proposition 4.8.

**Lemma 4.5.** *The mapping  $f_k : \mathbb{Z}(G, k) \rightarrow \mathbb{Q}_k(R(G))$  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  $(u_1, u_2, \dots, u_k)$ , 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  $Q$ :  $M = (0, 0, 0, \dots, 0)$ ,  $N^1 = (1, 0, 0, \dots, 0)$ ,  $N^2 = (0, 1, 0, \dots, 0)$ ,  $\dots$ ,  $N^k = (0, 0, 0, \dots, 1)$ . 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  $\{h_1, \dots, h_k\}$  of fullerene  $G$ . If two of these hexagons were the same, for example if  $h_i = h_j$  for  $i, j \in \{1, \dots, k\}$  and  $i \neq j$ , then  $N^1 = N^2$  - a contradiction. Hence, we have the set of  $k$  distinct hexagons. In the next claim we show that these hexagons are pairwise disjoint.

**Claim 4.6.** *The hexagons  $h_i, 1 \leq i \leq k$ , are pairwise disjoint.*

*Proof.* Let  $i, j \in \{1, \dots, k\}$  and  $i \neq j$ . Let  $W$  be a vertex of  $Q$  having exactly two 1's and these are in the  $i$ th and  $j$ th position. Obviously,  $MN^1WN^2$  is a 4-cycle and therefore, by Lemma 4.4,  $h_i$  and  $h_j$  are disjoint hexagons.  $\square$

**Claim 4.7.** *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  $h_j$ .*

*Proof.* We can apply the same proof as in [10]:

Without loss of generality assume that  $j = 1$ . Let  $X = (0, \dots)$  and  $Y = (1, \dots)$ . Let  $s$  be the number of 1's in  $X$ . Consider the path  $X^0, X^1, \dots, X^s$  in  $Q$ , where  $X^i$  has exactly  $i$  1's and these are in the same position as the first  $i$  1's in  $X$ . Furthermore, consider the path  $Y^0, Y^1, \dots, Y^s$  in  $Q$ , where  $Y^i$  differ from  $X^i$  in precisely the first position. Obviously,  $X^i$  and  $Y^i$  are adjacent in  $Q$  and we also notice that  $X^0 = M, Y^0 = N^1, X^s = X, Y^s = Y$ . We use induction to prove that the symmetric difference of  $X^i$  and  $Y^i$  is the hexagon  $h_1$ . If  $i = 0$ , this follows from the definition of the hexagon  $h_1$ . Now suppose that the statement holds for  $i = r$ , i.e. the symmetric difference of  $X^r$  and  $Y^r$  is the hexagon  $h_1$ . Consider the cycle  $X^r X^{r+1} Y^{r+1} Y^r$ . By the inductive assumption and Lemma 4.4 it follows that the symmetric difference of  $X^{r+1}$  and  $Y^{r+1}$  is the hexagon  $h_1$ . Therefore, the symmetric difference of  $X^s = X$  and  $Y^s = Y$  is the hexagon  $h_1$ .  $\square$

We notice that  $M^0 = M = (0, 0, 0, \dots, 0)$ ,  $M^1 = N^1 = (1, 0, 0, \dots, 0)$ ,  $M^2 = (1, 1, 0, \dots, 0)$ ,  $\dots$ ,  $M^k = (1, 1, 1, \dots, 1)$  is the path in  $Q$  and by Claim 2, the edge  $M^i M^{i+1}$  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  $h_1, \dots, h_k$ , hence the perfect matching  $M^k$  contains a sextet of each hexagon in  $\{h_1, \dots, h_k\}$ . Since  $Q$  is connected graph it follows that every vertex of  $Q$  contains a sextet of each hexagon from  $\{h_1, \dots, h_k\}$  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  $M^k \cup E(h_1) \cup \dots \cup E(h_k)$ . 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  $f_k(C) = Q$ .  $\square$

Lemma 4.2, Lemma 4.3 and Lemma 4.5 together imply Theorem 4.1.  $\square$

In the proof of Theorem 4.1 we considered just induced subgraphs of the resonance graph that are isomorphic to a hypercube. It is natural to ask what happens if we consider all subgraphs that are isomorphic to a hypercube. In the next proposition we show that every subgraph of the resonance graph of a fullerene that is isomorphic to a hypercube is actually an induced subgraph. The same can be shown for benzenoid systems and tubulenes.

**Proposition 4.8.** *Let  $G$  be a fullerene. Then every subgraph of  $R(G)$ , isomorphic to a hypercube, is induced subgraph in  $R(G)$ .*

*Proof.* Let  $Q$  be a subgraph of the resonance graph, isomorphic to the  $k$ -dimensional hypercube. If  $k = 0$ , the proposition is obvious. So let  $k \geq 1$ . Let  $F$  and  $F'$  be two distinct vertices in  $Q$  such that they are not adjacent in  $Q$ . It suffices to prove that  $F$  and  $F'$  are not adjacent in  $R(G)$ . Let all notation be the same as in the proof of Lemma 4.5. Since  $F$  and  $F'$  are not adjacent in  $Q$ , their binary representations differ in more than one coordinate. Since every coordinate represents position of double bonds of one of the hexagons  $h_1, \dots, h_k$ ,  $F$  and  $F'$  differ in double bonds of more than one hexagon. Hence, they are not adjacent in the resonance graph  $R(G)$ .  $\square$

## 5 Example

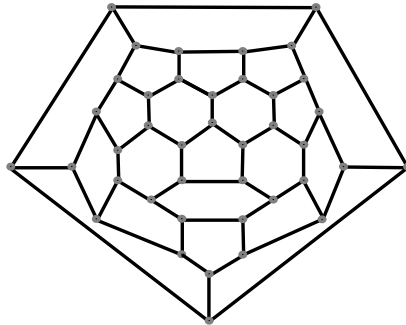


Figure 2: A fullerene  $G$  with two rings consisting of  $5 + 5$  hexagons.

In Figure 2 we can see an example of a fullerene  $G$  with 10 hexagon faces, forming two disjoint rings, each having 5 hexagons. A subgraph of fullerene  $G$  induced on one of those two rings is a graph called cyclic fibonacene which resonance graph is isomorphic to a Lucas cube  $\Lambda_5$  (see [20]). Since the two rings of hexagons are disjoint and the union of their vertex sets is the vertex set of  $G$ , one of the components of the resonance graph of  $G$  is isomorphic to the Cartesian product of two 5-dimensional Lucas cubes,  $\Lambda_5 \square \Lambda_5 = H$ , see Figure 3. The Clar number of fullerene  $G$  is obviously 4, since there is no resonant set of size 5 in  $G$ . Since a Clar cover with  $k$  hexagons induces a  $k$ -dimensional hypercube in the corresponding resonance graph, the largest induced hypercubes in  $H$  are of size 4. It is easy to see that every perfect matching with 4 sextets is a vertex of  $H$ . It is also not difficult to check that there is no maximal resonant set with 3 hexagons in  $G$ . Therefore all components of the resonance graph of  $G$  different from  $H$  contain at most 2-dimensional hypercubes (due to their large number only the component  $H$  of the resonance graph  $R(G)$  is drawn in Figure 3).

To conclude the example, we calculate the first two coefficients of Zhang-Zhang polynomial using cube polynomial of a fullerene from Figure 2. Since we already know that graph  $H$  from Figure 3 includes all 3-dimensional and 4-dimensional hypercubes of resonance graph  $R(G)$ , it suffices to count them in  $H$ . The number of 4-dimensional hypercubes in  $H$  is 25 and the number of 3-dimensional hypercubes in  $H$  is 75 (see Figure 3) therefore, the number of Clar covers with 4 and 3 hexagons is 25 and 75, respectively.

## 6 Distributive lattice structure and median graphs

We have already mentioned that the resonance graph (or each connected component of the resonance graph) of every benzenoid graph or tubulene is the covering graph of some distributive lattice. For the details see [6, 15, 13]. Therefore it is interesting that this result is no longer true (in general) for resonance graphs of fullerenes. Here we give an example of a fullerene such that a connected component of its resonance graph is not the covering graph of a distributive lattice.

In Figure 3 we can see the largest connected component  $H$  of the resonance graph of fullerene  $G$  from Figure 2. It is obvious that the diameter of  $H$ ,  $\text{diam}(H)$  is 8, since the



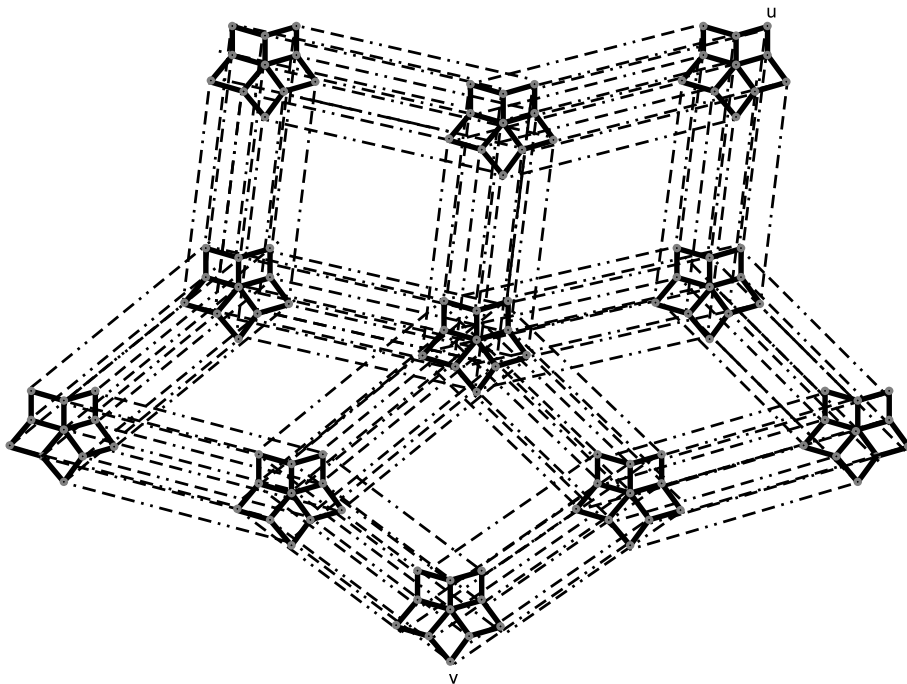


Figure 3: The largest connected component  $H$  of the resonance graph of fullerene  $G$ .

distance between vertices  $u$  and  $v$  from Figure 3 is 8. To show that graph  $H$  is not the covering graph of any distributive lattice, we use Theorem 6.1. Before stating the theorem, we introduce some notation.

Let  $2^n$  denote the distributive lattice of all subsets of an  $n$ -element set. Then the covering graph  $\mathcal{C}(2^n)$  is an  $n$ -dimensional hypercube. Also, if  $(L, \leq)$  is a lattice, then a linearly ordered set  $C \subseteq L$  is called a *chain*. For a chain  $C$  of  $L$  we define its *length* by  $l(C) = |C| - 1$ . Then the *length*  $l(L)$  of  $L$  is the maximum of the lengths of the chains in  $L$ . Now the following result can be stated.

**Theorem 6.1.** [4] *A finite graph  $G$  is the covering graph of a distributive lattice of length  $n$  if and only if  $G$  is a retract of  $\mathcal{C}(2^n)$  and  $\text{diam}(G) = n$ .*

It follows from Theorem 6.1 that if  $H$  is the covering graph of some distributive lattice, then  $H$  is a retract of a 8-dimensional hypercube  $Q_8$ . But it is obvious from Figure 3 that the degree of the vertex in the center of  $H$  is 10 and, therefore,  $H$  cannot be a subgraph of  $Q_8$ , since all the vertices in  $Q_8$  have degree 8. Hence,  $H$  is not the covering graph of any distributive lattice.

Next we consider the relationship between resonance graphs of fullerenes and median graphs. It was shown that the resonance graph (or its connected component) of a benzenoid graph or a tubulene is always a median graph (see [16, 13]). Both proofs rely on a distributive lattice structure for resonance graphs, which cannot be established for fullerenes. Since covering graphs of distributive lattices and median graphs are closely connected [4], it is

natural to ask if resonance graphs of fullerenes are not (in general) median graphs. However, we can easily show that graph  $H$  in Figure 3 is a median graph. To this end, let us introduce the following procedure.

Let  $G$  be a graph. Suppose  $V(G) = V_1 \cup V_2$ , where  $V_1 \cap V_2 \neq \emptyset$ , each  $\langle V_i \rangle$  (an induced subgraph of  $G$  with vertices  $V_i$ ) is an isometric subgraph of  $G$ , and no edge of  $G$  joins  $V_1 \setminus V_2$  to  $V_2 \setminus V_1$ . An *expansion* of  $G$  with respect to  $V_1$  and  $V_2$  is a graph  $H$  obtained from  $G$  by the following steps.

- i) Replace each  $v \in V_1 \cap V_2$  by vertices  $v_1$  and  $v_2$ , and insert the edge  $v_1v_2$ .
- ii) Insert edges between  $v_1$  and all neighbours of  $v$  in  $V_1 \setminus V_2$ ; insert edges between  $v_2$  and all neighbours of  $v$  in  $V_2 \setminus V_1$ .
- iii) Insert the edges  $v_1u_1$  and  $v_2u_2$  if  $v, u \in V_1 \cap V_2$  are adjacent in  $G$ .

An expansion is *convex* if  $\langle V_1 \cap V_2 \rangle$  is a convex subgraph of  $G$ . Now we can state the following well-known theorem, which is called Mulder’s Convex Expansion Theorem.

**Theorem 6.2.** [7] *A graph is a median graph if and only if it can be obtained from the one-vertex graph by a convex expansion procedure.*

It is easy to check that the Lucas cube  $\Lambda_5$  can be obtained from a one-vertex graph by a convex expansion procedure (see Figure 4), therefore,  $\Lambda_5$  is a median graph.

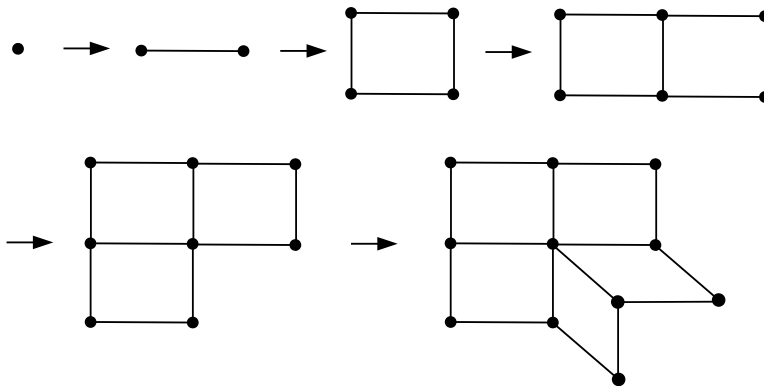


Figure 4: A convex expansion procedure for  $\Lambda_5$ .

Since the Cartesian product of median graphs is another median graph, graph  $H$  from Figure 3 is median. Since we do not know any example of a fullerene such that some connected component of its resonance graph is not a median graph, we propose the following conjecture.

**Conjecture 6.3.** *Let  $G$  be a fullerene. Then every connected component of the resonance graph  $R(G)$  is a median graph.*

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