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On 2-Cores of Resonance Graphs of Fullerenes

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Abstract

A fullerene G is a 3-regular 3-connected plane graph consisting of only pentagonal and hexagonal faces. The resonance graph $R(G)$ of G reflects the structure of the set of its perfect matchings. In this paper we show that if a connected component of the resonance graph of a fullerene is not a path, then this component without vertices of degree one (its 2-core) is 2-connected, extending thus analogous results already established for benzenoid systems [14] and later for open-ended carbon nanotubes [11].

1 Introduction

The concept of the resonance graph appears quite naturally in the study of perfect matchings of molecular graphs of hydrocarbons that represent Kekulé structures of corresponding hydrocarbon molecules. The resonance graph of a molecular graph carries many important information on Kekué structures. For example, the maximum degree of the resonance graph is the Fries number of the molecule. Therefore, it is not surprising that it has been independently introduced in the chemical [3, 4] as well as in the mathematical literature [14] (under the name Z-transformation graph) and then later rediscovered in

[9, 8]. Some basic properties of resonance graphs were shown for benzenoid systems in [14] and for open-ended carbon nanotubes (tubulenes) in [11]. For a survey on resonance graphs see also [13].

Resonance graphs of fullerenes were introduced in [10] and their basic properties were investigated in [12]. The established properties were found to be similar to the properties of resonance graphs of benzenoid systems and tubulenes, except that the problem of 2-connectedness of their components remained unsolved. The aim of this paper is to settle this problem by showing that if a connected component of the resonance graph of a fullerene is not a path, then this component without vertices of degree one is 2-connected.

In the next section some basic definitions are given. In Section 3 the main result is proved, followed by two examples showing the necessity of conditions in the main theorem.

2 Preliminaries

A *benzenoid system* consists of a cycle C of the infinite hexagonal lattice together with all hexagons inside C. A *benzenoid graph* is the underlying graph of a benzenoid system.

A *fullerene* G is a 3-connected 3-regular plane graph such that every face is bounded by either a pentagon or a hexagon. By Euler's formula, it follows that the number of pentagonal faces of a fullerene is exactly 12. For more information on fullerenes see [1].

A *1-factor* of a graph G is a spanning subgraph of G such that every vertex has degree one. The edge set of a 1-factor is called a *perfect matching* of G, which is a set of independent edges covering all vertices of G. In chemical literature, perfect matchings are known as Kekulé structures (see [5] for more details). Petersen's theorem states that every bridgeless 3-regular graph always has a perfect matching [6]. 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*.

Let G be a fullerene or a benzenoid graph. The *resonance graph* $R(G)$ is the graph whose vertices are the perfect matchings of G, and two perfect matchings are adjacent whenever their symmetric difference forms a hexagon of G.

Let G be a connected graph and $v \in V(G)$. Vertex v is a *cut-vertex* if its removal disconnects G. A connected graph with at least three vertices is *2–connected* if it does not contain a cut-vertex.

For a graph G let $V_1(G)$ be the set of all vertices in G that have degree one. The graph induced by $V(G) - V_1(G)$ is called the *2-core* of G.

A graph G is *cyclically k-edge-connected* if G can not be separated into two components, each containing a cycle, by deleting at most $k-1$ edges. Došlić [2] has proved the following theorem about cyclic edge-connectivity of fullerenes (see also [7]).

Theorem 2.1 ([2] and [7]) *Every fullerene G is cyclically 5-edge-connected.*

3 Main result

In this section we prove that if a connected component of the resonance graph of a fullerene is not a path, then the 2-core of this component is 2-connected. The following technical lemma (Lemma 3.2 in [12]) will be used in the proof of our main result.

Lemma 3.1 ([12]) *Let G be a fullerene and H a connected component of its resonance graph $R(G)$ such that H is not a path. If $M \in V(H) - V_1(H)$, then we can find in the fullerene G at least two disjoint hexagons which are M-alternating cycles.*

Now we can prove the main result of this paper.

Theorem 3.2 *Let G be a fullerene, and H be a connected component of the resonance graph $R(G)$ such that H is not a path. Then the 2-core of H is 2-connected.*

Proof. Let $U = H - V_1(H)$. Since H is connected and all vertices in $V_1(H)$ have degree one, it follows that U is connected. Note that, if U has a cut-vertex M, then any path joining two vertices from different components of $U - M$ must contain M. Therefore, in order to prove the 2-connectedness of U, it is enough to prove the following:

For any path $M_1M_2M_3$ of length 2 in U, there is another path $M_1M_2' \ldots M_3$ which is internally vertex-disjoint from $M_1M_2M_3$.

Let $M_1M_2M_3$ be a path. Suppose that h_1 and h_2 are such hexagons of G that $M_2 = M_1 \oplus E(h_1)$ and $M_3 = M_2 \oplus E(h_2)$. So h_1 is an M_1–alternating cycle and h_2 is an

M_2–alternating cycle. If h_1 and h_2 are edge disjoint, then there exists another perfect matching M_2' of G such that $M_2' = M_1 \oplus E(h_2)$ and $M_3 = M_2' \oplus E(h_1)$. Hence $M_1M_2'M_3$ and $M_1M_2M_3$ are two internally vertex-disjoint paths joining M_1 and M_3.

So in the following assume that h_1 and h_2 share edges. Since G is a fullerene and hence 3-connected, h_1 and h_2 share exactly one edge. By Lemma 3.1, G has two disjoint M_1-alternating hexagons since $M_1 \in V(H) - V(H_1)$. Without loss of generality, assume that one of the two M_1-alternating hexagons is h_1 and the other is h_3. Consider the following cases:

Case 1. $E(h_2) \cap E(h_3) = \emptyset$.

Let $M_2' = M_1 \oplus E(h_3)$, $M_3' = M_2' \oplus E(h_1)$, $M_4' = M_3' \oplus E(h_2)$ and $M_3 = M_4' \oplus E(h_3)$. Then $M_1M_2'M_3'M_4'M_3$ is another path joining M_1 and M_3, which is internally disjoint from $M_1M_2M_3$. (See Figure 1.) So the theorem holds.

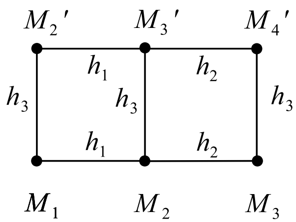

Figure 1. A part of the resonance graph of a fullerene in Case 1.

Case 2. $E(h_2) \cap E(h_3) \neq \emptyset$.

Then h_2 and h_3 have exactly one edge in common. Since $M_3 \in V(H) - V(H_1)$, Lemma 3.1 implies that G has another M_3-alternating hexagon disjoint from h_2, say h_4.

Subcase 2.1. $E(h_1) \cap E(h_4) = \emptyset$.

Since h_4 is disjoint from both h_1 and h_2, it follows that h_4 is also an M_1-alternating hexagon. Let $M_2' = M_1 \oplus E(h_4)$, $M_3' = M_2' \oplus E(h_1)$, $M_4' = M_3' \oplus E(h_2)$ and $M_3 = M_4' \oplus E(h_4)$. Then $M_1M_2'M_3'M_4'M_3$ is another path joining M_1 and M_3, which is internally vertex-disjoint from $M_1M_2M_3$.

Subcase 2.2. $E(h_1) \cap E(h_4) \neq \emptyset$.

Then h_1 and h_4 have exactly one edge in common. If $E(h_3) \cap E(h_4) \neq \emptyset$, then the four edges in $E(h_1)\cap E(h_2)$, $E(h_1)\cap E(h_4)$, $E(h_2)\cap E(h_3)$ and $E(h_3)\cap E(h_4)$ form a cyclic edge-cut of G, a contradiction to Theorem 2.1. So in the following assume that $E(h_3) \cap E(h_4) = \emptyset$.

Recall that h_1 and h_3 are disjoint, and h_2 and h_4 are disjoint. Note that both h_1 and h_3 are M_1-alternating, and both h_2 and h_4 are M_3-alternating, where $M_3 = M_1 \oplus E(h_1) \oplus E(h_2)$. Hence, the subgraph Q induced by h_1, h_2, h_3 and h_4 has to be one of the two configurations in Figure 2.

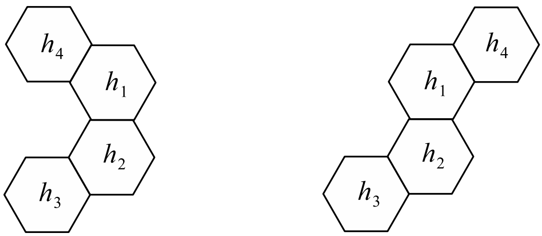

Figure 2. Possible configurations of hexagons h_1, h_2, h_3 and h_4 in Subcase 2.2.

Let $M_1' = M_1 \oplus E(h_3)$, $M_2' = M_1' \oplus E(h_1)$, $M_3' = M_2' \oplus E(h_4)$, $M_4' = M_3' \oplus E(h_3)$ and $M_5' = M_4' \oplus E(h_2)$. Then $M_3 = M_1 \oplus E(h_1) \oplus E(h_2) = M_5' \oplus E(h_4)$. Therefore, $H - V(H_1)$ has another path $M_1M_1'M_2'M_3'M_4'M_5'M_3$ joining M_1 and M_3, which is internally vertex-disjoint from $M_1M_2M_3$. (For example, see Figure 3.) This completes the proof of Case 2.

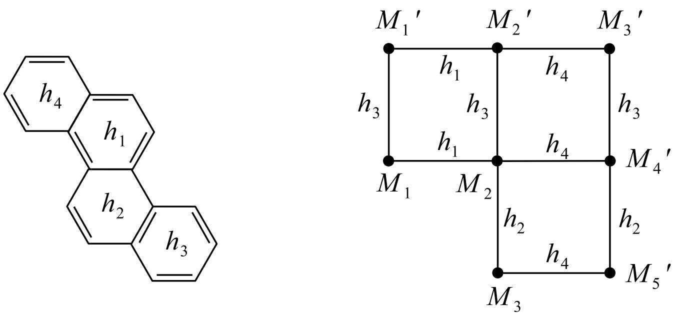

Figure 3. A perfect matching M_1 and a part of the resonance graph in Subcase 2.2.

Combining Case 1 and Case 2, we can conclude that the graph $U = H - V_1(H)$ does not contain a cut-vertex. Therefore, $H - V_1(H)$ is 2–connected. ■

To see that the conditions in Theorem 3.2 are really necessary, we first show an example of a fullerene G and a connected component H_1 of its resonance graph $R(G)$ such that H_1 is a path with more than two vertices. Let G be a fullerene in Figure 4 and let N_1 be its perfect matching.

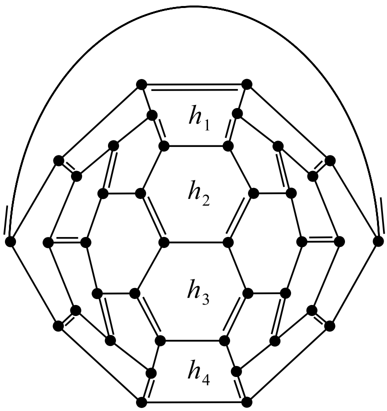

Figure 4. A fullerene G with a perfect matching N_1.

Moreover, let H_1 be the connected component of $R(G)$ containing N_1. Obviously, going through H_1 we can rotate only hexagons h_1, h_2, h_3, and h_4, since the edges of the other hexagons that are in the perfect matchings of H_1 must be fixed. Hence, graph H_1 is isomorphic to the resonance graph of a benzenoid graph, formed by these four hexagons. Therefore, H_1 is isomorphic to P_5 (see Figure 5).

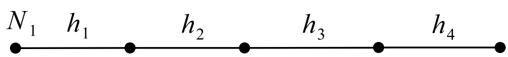

Figure 5. Connected component H_1 of the resonance graph $R(G)$.

It is also natural to ask whether there exists a fullerene G such that one component of its resonance graph $R(G)$ is not a path and contains a vertex of degree one. Otherwise the restriction on vertices of degree more than one in non-path component of $R(G)$ in Theorem 3.2 would not be necessary. The next example shows that the answer to the question is positive.

Let G be a fullerene as in Figure 4 and let M_1 be its perfect matching, see Figure 6. Obviously, in M_1 only hexagon h_3 is a sextet, therefore, the degree of M_1 in $R(G)$ is one.

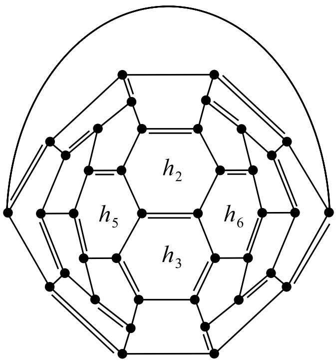

Figure 6. A fullerene G with a perfect matching M_1.

Furthermore, let H_2 be a connected component of $R(G)$ containing M_1. Obviously, going through H_2 we can rotate only hexagons h_2, h_3, h_5, and h_6, since the edges of the other hexagons that are in the perfect matchings of H_2 must be fixed. Hence, graph H_2 is isomorphic to the resonance graph of a benzenoid graph, formed by these hexagons. Therefore, graph H_2 can be easily obtained (see Figure 7). Clearly, H_2 is not a path and contains vertices of degree one.

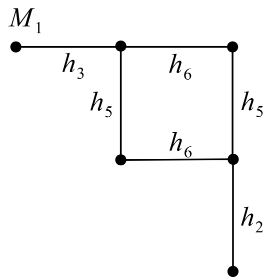

Figure 7. Connected component H_2 of the resonance graph $R(G)$.

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