On 2-Cores of Resonance Graphs of Fullerenes

Tomislav Došlić\textsuperscript{a}, Niko Tratnik\textsuperscript{b}, Dong Ye\textsuperscript{c}, Petra Žigert Pleteršek\textsuperscript{b,d}

\textsuperscript{a}Faculty of Civil Engineering, University of Zagreb, Croatia
\textsuperscript{b}Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia
\textsuperscript{c}Department of Mathematical Sciences, Middle Tennessee State University, USA
\textsuperscript{d}Faculty of Chemistry and Chemical Engineering, University of Maribor, Slovenia

e-mail: doslic@grad.hr, niko.tratnik1@um.si, dong.ye@mtsu.edu, petra.zigert@um.si

(Received September 1, 2016)

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 \cite{14} and later for open-ended carbon nanotubes \cite{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 Kekulé 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 \cite{3, 4} as well as in the mathematical literature \cite{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
M₂-alternating cycle. If h₁ and h₂ are edge disjoint, then there exists another perfect matching M₂' of G such that M₂' = M₁ ⊕ E(h₂) and M₃ = M₂' ⊕ E(h₁). Hence M₁M₂'M₃ and M₁M₂M₃ are two internally vertex-disjoint paths joining M₁ and M₃.

So in the following assume that h₁ and h₂ share edges. Since G is a fullerene and hence 3-connected, h₁ and h₂ share exactly one edge. By Lemma 3.1, G has two disjoint M₁-alternating hexagons since M₁ ∈ V(H) − V(H₁). Without loss of generality, assume that one of the two M₁-alternating hexagons is h₁ and the other is h₃. Consider the following cases:

Case 1. E(h₂) ∩ E(h₃) = ∅.

Let M₂' = M₁ ⊕ E(h₃), M₃' = M₂' ⊕ E(h₁), M₄' = M₃' ⊕ E(h₂) and M₃ = M₄' ⊕ E(h₃). Then M₁M₂'M₃'M₄M₃ is another path joining M₁ and M₃, which is internally disjoint from M₁M₂M₃. (See Figure 1.) So the theorem holds.

![Figure 1](https://example.com/figure1.png)

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

Case 2. E(h₂) ∩ E(h₃) ≠ ∅.

Then h₂ and h₃ have exactly one edge in common. Since M₃ ∈ V(H) − V(H₁), Lemma 3.1 implies that G has another M₃-alternating hexagon disjoint from h₂, say h₄.

Subcase 2.1. E(h₁) ∩ E(h₄) = ∅.

Since h₄ is disjoint from both h₁ and h₂, it follows that h₄ is also an M₁-alternating hexagon. Let M₂' = M₁ ⊕ E(h₄), M₃' = M₂' ⊕ E(h₁), M₄' = M₃' ⊕ E(h₂) and M₃ = M₄' ⊕ E(h₄). Then M₁M₂'M₃'M₄M₃ is another path joining M₁ and M₃, which is internally vertex-disjoint from M₁M₂M₃.

Subcase 2.2. E(h₁) ∩ E(h₄) ≠ ∅.
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](image)

**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 $M_1 M'_1 M'_2 M'_3 M'_4 M'_5 M_3$ joining $M_1$ and $M_3$, which is internally vertex-disjoint from $M_1 M_2 M_3$. (For example, see Figure 3.) This completes the proof of Case 2.

![Figure 3](image)

**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.

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).

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 $M_1$.](image)

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 $R(G)$.](image)

**Acknowledgment:** Supported in part by the Ministry of Science of Slovenia under grants P1–0297. Partial support of the Croatian Science Foundation (research project BioAmp-Mode (Grant no. 8481)) is gratefully acknowledged by the first author, as well as partial support of the Croatian Ministry of Science, Education and Sports through bilateral Croatian-Slovenian and Croatian-Chinese projects.
References


