On k-resonant fullerene graphs^{*}

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Abstract

A fullerene graph F is a 3-connected plane cubic graph with exactly 12 pentagons and the remaining hexagons. Let M be a perfect matching of F. A cycle C of Fis M-alternating if the edges of C appear alternately in and off M. A set \mathcal{H} of disjoint hexagons of F is called a resonant pattern (or sextet pattern) if F has a perfect matching M such that all hexagons in \mathcal{H} are M-alternating. A fullerene graph F is k-resonant if any i ($0 \le i \le k$) disjoint hexagons of F form a resonant pattern. In this paper, we prove that every hexagon of a fullerene graph is resonant and all leapfrog fullerene graphs are 2-resonant. Further, we show that a 3-resonant fullerene graph has at most 60 vertices and construct all nine 3-resonant fullerene graphs, which are also k-resonant for every integer k > 3. Finally, sextet polynomials of the 3-resonant fullerene graphs are computed.

Keywords: Fullerene graph; Perfect matching; Resonant pattern; k-resonance; Sextet polynomial AMS 2000 subject classification: 05C70, 05C90

1 Introduction

A *fullerene graph* is a 3-connected plane cubic graph with exactly 12 pentagonal faces and the other faces being hexagonal. Fullerene graphs have been studied in mathematics as trivalent polyhedra for a long time [9, 12], for example, the dodecahedron is the fullerene graph with 20 vertices. Fullerene graphs have been studied in chemistry as fullerene molecules which have extensive applications in physics, chemistry and material science [6].

Let G be a plane 2-connected graph. A *perfect matching* or 1-factor M of G is a set of independent edges such that every vertex of G is incident with exactly one edge in M.

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A cycle C of G is M-alternating if the edges of C appear alternately in and off M. For a fullerene graph F, every edge of F belongs to a perfect matching of F [16, 4]. A hexagon h of a fullerene graph F is resonant if F has a perfect matching M such that h is M-alternating. It was proved that every hexagon of a normal benzenoid system is resonant [28]. This result was generalized to normal coronoid systems [30] and plane elementary bipartite graphs [33]. However a fullerene graph is a non-bipartite graph. It is natural to ask if every hexagon of a fullerene graph is resonant. The present paper first uses Tutte's 1-factor theorem to give a positive answer to this question.

A set \mathcal{H} of disjoint hexagons of a fullerene graph F is a resonant pattern (or sextet pattern), in other words, such hexagons are mutually resonant, if F has a perfect matching M such that every hexagon in \mathcal{H} is M-alternating; equivalently, if $F - \mathcal{H}$ has a perfect matching, where $F - \mathcal{H}$ denotes the subgraph obtained from F by deleting all vertices of \mathcal{H} together with their incident edges. The maximum cardinality of resonant patterns of F is called the *Clar number* of F [3], and the maximum number of M-alternating hexagons over all perfect matchings M of F is called the *Fries number* of F [8]. Graver [10] explored some connections among the Clar number, the face independence number and the Fries number of a fullerene graph, and obtained a lower bound for the Clar number of leapfrog fullerene graphs with icosahedral symmetry. Zhang and Ye [31] showed that the Clar number of a fullerene graph F_n with n vertices satisfies $c(F_n) \leq \lfloor \frac{n-12}{6} \rfloor$, which is sharp for infinitely many fullerene graphs, including C₆₀ whose Clar number is 8 [1]. Shiu, Lam and Zhang [24] computed the Clar polynomial and the sextet polynomial of C₆₀ by showing that every hexagonal face independent set of C₆₀ is also a resonant pattern.

A fullerene graph is k-resonant if any i $(0 \le i \le k)$ disjoint hexagons are mutually resonant. So k-resonant fullerene graphs are also (k - 1)-resonant for integer $k \ge 1$. Hence a fullerene graph with each hexagon being resonant is 1-resonant. Zheng [34, 35] characterized general k-resonant benzenoid systems. In particular, he showed that every 3-resonant benzenoid system is also k-resonant $(k \ge 3)$. This result also holds for coronoid systems [2, 18], open-ended nanotubes [29], toroidal polyhexes [25, 32] and Klein-bottle polyhexes [26]. For a recent survey on k-resonant benzenoid systems, refer to [13].

Here we consider k-resonant fullerene graphs. We show that all leapfrog fullerene graphs are 2-resonant and a 3-resonant fullerene graph has at most 60 vertices. We construct all 3-resonant fullerene graphs, and show that they are all k-resonant for every integer $k \geq 3$. This result is consistent with the aforementioned results. Finally, sextet polynomials of the 3-resonant fullerene graphs are computed.

2 1-resonance of fullerene graphs

Let G be a plane graph admitting a perfect matching with vertex-set V(G) and edge-set E(G). Use ∂G denote the boundary of G, i.e. the boundary of the infinite face of G. For a face f of G, let V(f) and E(f) be the sets of vertices and edges of f, respectively. If G is a 2-connected plane graph, then each face of G is bounded by a cycle. For convenience, a face is often represented by its boundary if unconfused. In particular, for a fullerene graph F, any pentagon, a cycle with length five, and any hexagon, a cycle with length six, of F must bound a face since F is cyclically 5-edge connected [5, 31]. For a plane graph G, a face f of G adjoins a subgraph G' of G if f is not a face of G' and f has an edge in common with G'. The faces adjoining G' are always called adjacent faces of G'. A subgraph H of G is called nice in [20] or central in [23] if G - V(H) has a perfect matching. So a resonant pattern of G can be viewed as a central subgraph of G. A graph G is cyclically k-edge connected if deleting fewer than k edges of G can not separate G into two components each of which contains a cycle. By Tutte's Theorem on perfect matchings of graphs ([20], Theorem 3.1.1), we have the following result.

Lemma 2.1. A subgraph H of a graph G is central if and only if for any $S \subseteq V(G - H)$,

$$C_o(G - H - S) \le |S|,$$

where $C_o(G - H - S)$ is the number of odd components of G - H - S.

Theorem 2.2. Let G be a cyclically 4-edge connected cubic graph with a 6-length cycle. Then for every 6-length cycle H of G, either H is central or G - H is bipartite.

Proof: Let H be a 6-length cycle in G. If G - H has a perfect matching, then the theorem holds. If not, then by Lemma 2.1 there exists an $S \subset V(G - H)$ such that $C_o(G - H - S) \ge$ |S| + 2 by parity, i.e. $|S| \le C_o(G - H - S) - 2$. Since G is cubic, S sends out at most $3|S| \le 3C_o(G - H - S) - 6$ edges.

Let $G_1, G_2, ..., G_k$ be all odd components of G-H-S, where $k = C_o(G-H-S)$. Because G is cyclically 4-edge connected and cubic, it has no cut edges. Every G_i (i = 1, 2, ..., k) sends odd number edges, hence at least three edges, to $H \cup S$. So $\bigcup_{i=1}^k G_i$ sends out at least $3C_o(G-H-S)$ edges to either S or H. Since H is a 6-length cycle, there are at most 6 edges between H and $\bigcup_{i=1}^k G_i$. So $\bigcup_{i=1}^k G_i$ sends at least $3C_o(G-H-S) - 6$ edges to S. Hence there are precisely $3C_o(G-H-S) - 6$ edges between S and $\bigcup_{i=1}^k G_i$. So S is an independent set, and every G_i sends out exactly 3 edges, and G-H-S has no even component. In addition, since G is cyclically 4-edge connected, every G_i is a tree. We claim that each G_i is a singular vertex. If not, then an odd component G_i has at least 2 vertices. So G_i has at least two leaves. Every leaf of G_i is adjacent to at least two vertices in $S \cup H$. So G_i sends at least four edges out, contradicting the fact that every G_i sends precisely three edges out.

Therefore G - H is a bipartite graph with bipartition (S, V(G - H - S)). This completes the proof of the theorem.

Lemma 2.3. [5, 21] Every fullerene graph is cyclically 5-edge connected.

By Lemma 2.3 and Theorem 2.2, we immediately have the following result.

Theorem 2.4. Every hexagon of a fullerene graph is resonant.

Proof: Let F be a fullerene graph and H be a hexagon of F. It is obvious that F - H is not bipartite. By Theorem 2.2 and Lemma 2.3, H is central. That means H is resonant.

3 2-resonant fullerene graphs

Let F be a fullerene graph. The *leapfrog operation* on F is defined [7] as follows: for any face f of F, add a new vertex v_f in f and join v_f to all vertices in V(f) to obtain a new triangular graph F'; then take the geometry dual of the graph F' and denote it by F^* (see Figure 1). Clearly, F^* is a fullerene graph since every vertex of F' is 6-degree excluding exactly 12 5-degree vertices and every face of F' is a triangle. The edges of F^* cross the edges of $F \subset F'$ in the geometry dual operation form a perfect matching M^0 of F^* . A fullerene graph is called *leapfrog fullerene* if it arises from a fullerene graph by the leapfrog operation. Several characterizations of leapfrog fullerenes have been given; see Liu, Klein and Schmalz [19], Fowler and Pisanski [7], and Graver [10, 11]. For example, a fullerene graph is a leapfrog fullerene if and only if it has a perfect Clar structure (i.e. a set of disjoint faces including all vertices); and if and only if it has a Fries structure (i.e. a perfect matching which avoids edges in pentagons and is alternating on the maximal number n/3 of hexagons).

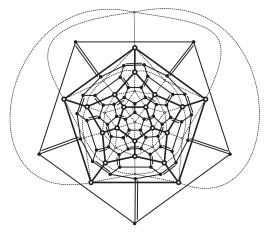


Figure 1: The leapfrog operation on the dodecahedron F_{20} and the perfect matching M^0 of C_{60} (double edges).

Let F^* be a leapfrog fullerene graph arising from F. A face f of F^* is called a *heritable* face if it lies completely in some face of F, and a fresh face, otherwise. For example, C₆₀ is the leapfrog fullerene graph of the dodecahedron and every pentagon is a heritable face and all hexagons are fresh faces. The perfect matching M^0 corresponds to the Fries structure of C₆₀ (see Figure 1). For a leapfrog fullerene graph, we have the following result.

Lemma 3.1. Let F be a leapfrog fullerene graph. Then every fresh face is M^0 -alternating and all heritable faces are independent.

Let F be a leapfrog fullerene and f a heritable face of F. A subgraph of F consisting of f together with all adjacent (fresh) faces is called the *territory* of f, and denoted by T[f]. For two heritable faces f_1 and f_2 , it is easily seen that there are at most 2 common fresh faces in their territories, which are adjacent.

Theorem 3.2. Every leapfrog fullerene graph is 2-resonant.

Proof: Let F be a leapfrog fullerene graph and f_1, f_2 any two disjoint hexagons. If both f_1 and f_2 are fresh faces, then clearly M^0 is alternating on both of them by Lemma 3.1. So suppose that at least one of them is a heritable face, say f_1 . Let us denote the six fresh hexagons in $T[f_1]$ by h_0, h_1, \ldots, h_5 in clockwise order. If f_2 is fresh, then $f_2 \nsubseteq T[f_1]$ and it adjoins at most one of h_0, h_1, \ldots, h_5 since F is a leapfrog fullerene graph. If f_2 adjoins none of h_1, h_3 and h_5 , let $M_1 := M^0 \oplus h_1 \oplus h_3 \oplus h_5$; otherwise, let $M_1 := M^0 \oplus h_0 \oplus h_2 \oplus h_4$. Then M_1 is a perfect matching and alternating on both f_1 and f_2 . So, in the following, we suppose both f_1 and f_2 are heritable. Let h'_0, h'_1, \ldots, h'_5 be the six fresh hexagons of $T[f_2]$ in clockwise order. If $T[f_1]$ and $T[f_2]$ have a common hexagon, then they have exactly two common adjacent hexagons. Assume $h_{i_0} = h'_{j_0}$ for some $i_0, j_0 \in \mathbb{Z}_6$. Let $M_2 := M^0 \oplus h_{i_0} \oplus h_{i_0}$ $h_{i_0+2} \oplus h_{i_0+4} \oplus h'_{j_0+2} \oplus h'_{j_0+4}$. It is clear that M_2 is a perfect matching alternating on both f_1 and f_2 . Now suppose $T[f_1]$ and $T[f_2]$ have no common hexagons. If no face in $T[f_2]$ adjoins one of h_1, h_3 and h_5 , let $M_3 := M^0 \oplus h_1 \oplus h_3 \oplus h_5 \oplus h'_1 \oplus h'_3 \oplus h'_5$; otherwise, let $M_3 := M^0 \oplus h_0 \oplus h_2 \oplus h_4 \oplus h'_1 \oplus h'_3 \oplus h'_5$. Then M_3 is also a perfect matching alternating on both f_1 and f_2 . So the theorem holds.



Figure 2: The dodecahedron F_{20} (left) and the fullerene graph F_{24} with a perfect matching M (right).

There exist 2-resonant fullerene graphs which are non-leapfrog. The dodecahedron F_{20} is a trivial example. The fullerene graph F_{24} , as shown in Figure 2 (right), is 2-resonant since the two hexagons are simultaneously *M*-alternating. Another non-trivial example is C₇₀.

Lemma 3.3. C_{70} is 2-resonant.

Proof: C_{70} has two perfect matchings M_1 and M_2 as shown in Figure 3. It has a total 25 of hexagons. The hexagons other than h_1, h_3, h_5, h_7 and h_9 are all M_1 -alternating. Let $M_3 := M_1 \oplus h_2 \oplus h_4 \oplus h_6 \oplus h_8 \oplus h_{10}$. Then the hexagons other than $h_{11}, h_{12}, h_{13}, h_{14}$ and h_{15} are all M_3 -alternating. We choose any pair of disjoint hexagons h and h' in C_{70} . If $h, h' \notin \{h_1, h_3, h_5, h_7, h_9\}$, then h and h' are simultaneously M_1 -alternating. If $h, h' \notin \{h_{11}, h_{12}, h_{13}, h_{14}, h_{15}\}$, then h and h' are simultaneously M_3 -alternating. So suppose $h \in \{h_1, h_3, h_5, h_7, h_9\}$ and $h' \in \{h_{11}, h_{12}, h_{13}, h_{14}, h_{15}\}$. By symmetry, we may assume $h = h_1$. If $h' \in \{h_{12}, h_{15}\}$, we may let $h' = h_{12}$ by the symmetry of h_{12} and h_{15} . Then both h and h' are M_4 -alternating. Finally, if $h' \in \{h_{13}, h_{14}\}$, then h and h' are simultaneously M_4 -alternating.

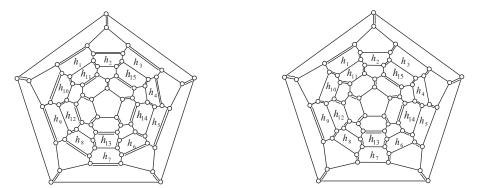


Figure 3: C_{70} with two perfect matchings M_1 (left) and M_2 (right).

On the other hand, we can construct infinitely many fullerene graphs which are not 2resonant. Let R_5 and R_6 be the graphs obtained by deleting the outer pentagon from F_{20} and by deleting the outer hexagon from F_{24} , respectively (see Figure 4).

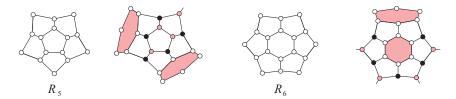


Figure 4: R_5 and R_6 and the illustration for the proof of Theorem 3.4.

Theorem 3.4. Let F be a fullerene graph different from F_{20} and F_{24} . If F contains R_5 or R_6 as subgraphs, then F is not 2-resonant.

Proof: First suppose $R_5 \subset F$. Since F is different from F_{20} , there are at least two disjoint hexagons of F adjoining R_5 . Let \mathcal{H} be the set of these two hexagons (shadowed hexagons in Figure 4). Then there is a set S of four vertices of Figure 4 such that $F - \mathcal{H} - S$ contains five isolated vertices (black vertices of R_5 in Figure 4). So \mathcal{H} is not a resonant pattern.

Now suppose $R_6 \subset F$. Since F is different from F_{24} , at least one hexagon of F adjoins R_6 . Let \mathcal{H} be the set consisting of this hexagon together with the center hexagon of R_6 . Similarly, it is easy to see that \mathcal{H} is not a resonant pattern (see Figure 4).

Using R_5 and R_6 as caps, we can construct infinitely many non-2-resonant nanotubes, which are, of course, 1-resonant fullerene graphs. It is interesting to characterize 2-resonant fullerene graphs. Since each leapfrog fullerene graph is 2-resonant and has no adjacent pentagons, we now propose an open problem as follows.

Open problem 3.5. Is every fullerene graph without adjacent pentagons 2-resonant?

4 Substructures of 3-resonant fullerene graphs

We first present a forbidden subgraph G^* as shown in Figure 5 of 3-resonant fullerene graphs: The three hexagons of G^* are not mutually resonant since deleting the three hexagons isolates the vertex v. Let f be a face of a fullerene graph F. A vertex v outside f is *adjacent* to f if v has a neighbor (a vertex adjacent to v) in the boundary of f. Hence the forbidden subgraph can be described a vertex being adjacent to each of three disjoint hexagons.



Figure 5: A forbidden subgraph G^* of 3-resonant fullerene graphs.

Theorem 4.1. Let F be a 3-resonant fullerene graph. Then $|V(F)| \leq 60$.

Proof: Since F is 3-resonant, then F contains no G^* . So any $v \in V(F)$ is adjacent to at least one pentagon of F. On the other hand, for any pentagon f of F, there are at most 5 vertices in V(F - V(f)) adjacent to it. Hence $|V(F)| \le 12 \times 5 = 60$ since F has exactly 12 pentagons. So the theorem holds.

We now discuss maximal pentagonal fragments and pentagonal rings as substructures of fullerene graphs in next two subsections, which will play important roles in construction of 3-resonant fullerene graphs.

4.1 Pentagonal fragments

A fragment B of a fullerene graph F is a subgraph of F consisting of a cycle together with its interior. A fragment B is said to be *pentagonal* if its every inner face is a pentagon. A pentagonal fragment B of a fullerene graph F is maximal if all faces adjoining B are hexagons. For a pentagonal fragment B, use $\gamma(B)$ denote the minimum number of pentagons adjoining a pentagon in B. For example, $\gamma(R_5) = 3$.

The following two lemmas due to Ye and Zhang are useful.

Lemma 4.2. [27] Let B be a fragment of a fullerene graph F and W the set of 2-degree vertices on the boundary ∂B . If $0 < |W| \le 4$, then $T = F - (V(B) \setminus W)$ is a forest and (1) T is K_2 if |W| = 2;

(2) T is $K_{1,3}$ if |W| = 3;

(3) T is the union of two K_2 's, or a 3-length path, or T_0 as shown in Figure 6 if |W| = 4.



Figure 6: Trees K_2 , $K_{1,3}$ and T_0 .

Lemma 4.3. [27] Let B be a pentagonal fragment of a fullerene graph F. Then (1) $R_5 \subseteq B$ if $\gamma(B) \ge 3$; (2) B has a pentagon adjoining exactly two adjacent pentagons of B if $\gamma(B) = 2$.

A turtle is a pentagonal fragment consisting of six pentagons as illustrated in Figure 7. $\gamma(B) = 1$ if B is a turtle. The following theorem characterizes the maximal pentagonal fragments of 3-resonant fullerene graphs.

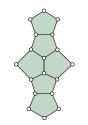


Figure 7: The turtle.

Theorem 4.4. Let F be a 3-resonant fullerene graph different from F_{20} and B a maximal pentagonal fragment of F. Then B is either a pentagon or a turtle.

Proof: For a set \mathcal{H} of at most three disjoint hexagons of F, we have that \mathcal{H} is a sextet pattern, that is, $F - \mathcal{H}$ has a perfect matching, since F is 3-resonant. This fact will be used repeatedly. Let B be a maximal pentagonal fragment of F. By Theorem 3.4, B contains no R_5 . Lemma 4.3 implies $\gamma(B) \leq 2$. If $\gamma(B) = 0$, then B is a pentagon. So suppose that $\gamma(B) > 0$.

Case 1. $\gamma(B) = 1$. Then B has a pentagon f_0 with a unique adjacent pentagon f_1 . The other four faces adjacent to f_0 are all hexagons since B is maximal, and denoted by h_1, h_2, h_3 and h_4 such that h_i is adjacent to $h_{i+1}(1 \le i \le 3)$ and both h_1 and h_4 are also adjacent to f_1 . Further, let f_2 and f_3 be the other faces adjacent to f_1 as illustrated in Figure 8(a).

If one of f_2 and f_3 is a hexagon, say f_2 , then $F - \{h_2, h_4, f_2\}$ has an isolated vertex; that is impossible. Hence both f_2 and f_3 must be pentagons and thus belong to B since Bis maximal. Let $f_4 \neq f_1$ be the face adjacent to both f_2 and f_3 . Then f_4 is a pentagon; otherwise, $F - \{h_1, h_4, f_4\}$ would have an isolated vertex. Let f_5 be the face adjacent to f_4 but not adjacent to f_2 and f_3 . Then f_5 is also a pentagon; otherwise, one component of $F - \{h_1, h_4, f_5\}$ would be $K_{1,3}$, which has no perfect matchings. Thus $G := \bigcup_{i=0}^5 f_i \subseteq B$ is a turtle. It suffices to show that B = G; that is, all faces adjoining G are hexagons. Besides

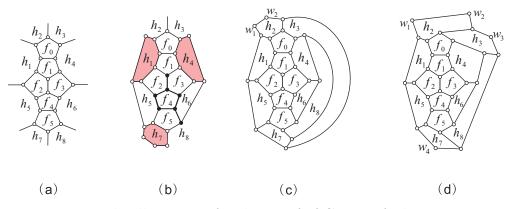


Figure 8: The illustration for the proof of Case 1 of Theorem 4.4.

the four faces h_1, \ldots, h_4 , let h_5, h_6, h_7 and h_8 be the remaining four faces adjoining G as illustrated in Figure 8(a). It can be seen that h_1, \ldots, h_8 are different from each other. Since h_1, h_2, h_3 and h_4 are hexagons, it remains to show that h_5, h_6, h_7 and h_8 are hexagons. Let $G' := G \cup (\bigcup_{i=1}^8 h_i).$

We claim that both h_5 and h_6 are hexagons. Since $R_5 \nsubseteq B$, one of h_5 and h_6 must be a hexagon, say h_5 , by the symmetry of G. Suppose to the contrary that h_6 is a pentagon. Then h_7 is a pentagon; otherwise, h_1, h_4 and h_7 are disjoint hexagons, and $F - \{h_1, h_4, h_7\}$ would have an odd component with seven vertices (see Figure 8(b)). If h_8 is a pentagon, then G' is a fragment with only two 2-degree vertices w_1 and w_2 on h_2 (see Figure 8(c)). This contradicts that F is 3-edge connected since the two edges coming out G_1 from w_1 and w_2 form an edge-cut of F. So h_8 must be a hexagon and the fragment G' contains four 2-degree vertices w_1, w_2, w_3 and w_4 (see Figure 8(d)). By Lemma 4.2(3), there are at most four faces of F outside G'. These faces must be all pentagons since the fragment G' contains exactly eight pentagons. So w_1 and w_4 must be adjacent in F, and w_2 and w_3 are also adjacent in F, resulting in a face of F with size three. This contradiction establishes the claim.

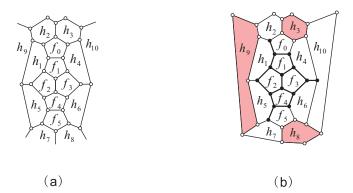


Figure 9: The illustration for the proof of Case 1 of Theorem 4.4.

Further, we claim that both h_7 and h_8 are hexagons. Without loss of generality, suppose to the contrary that h_7 is a pentagon. The faces h_9 and h_{10} faces of F adjoining G' as shown in Figure 9(a) are distinct and disjoint. Then $G'' := G' \cup h_9 \cup h_{10}$ is a fragment. If both h_8 and h_9 are hexagons, then h_3 , h_8 and h_9 are disjoint by Lemma 2.3, and $F - \{h_3, h_8, h_9\}$ would have an odd component with 15 vertices (see Figure 9(b)). Hence at least one of h_8 and h_9 is a pentagon, and G'' is a fragment with at most four and at least two 2-degree vertices. By Lemma 4.2, it can be analyzed analogously that that G'' can not be a subgraph of F. Hence both h_7 and h_8 are hexagons. So all faces of F adjoining G are hexagons and B = G.

Case 2. $\gamma(B) = 2$. Lemma 4.3 implies that B contains a pentagon f_0 which has exactly two adjacent pentagons f_1 and f_2 in B. Let h_1, h_2 and h_3 be the other faces (hexagons) adjacent to f_0 as shown in Figure 10(a).

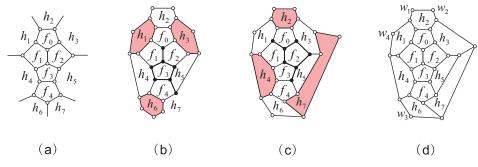


Figure 10: The illustration for the proof of Case 2 of Theorem 4.4.

Let $f_3 \neq f_0$ be the face of F adjacent to both f_1 and f_2 . Similarly, f_3 is a pentagon; otherwise, disjoint hexagons h_1, h_3 and f_3 are not mutually resonant. Let h_4, f_4, h_5 be the

other adjacent faces of f_3 as shown in Figure 10(a). If f_4 is a hexagon, then one component of $F - \{h_1, h_3, f_4\}$ is $K_{1,3}$. So f_4 is also a pentagon in B. Since $R_5 \nsubseteq B$, at least one of h_4 and h_5 is a hexagon, say h_4 . If h_5 is also a hexagon, then one component of $F - \{h_2, h_4, h_5\}$ is $K_{1,3}$. So h_5 is a pentagon.

Let h_6 and h_7 be the other two adjacent faces of f_4 as shown in Figrue 10. If h_6 is a hexagon, then $\{h_1, h_3, h_6\}$ is not a resonant pattern since $F - \{h_1, h_3, h_6\}$ has an odd component with seven vertices (see Figure 10(b)). Hence h_6 is a pentagon. Similarly, h_7 must be a pentagon; if not, $\{h_2, h_4, h_7\}$ is not a resonant pattern (see Figure 10(c)). Now, we have a fragment $G := (\bigcup_{i=0}^4 f_i) \cup (\bigcup_{j=1}^7 h_j)$ with four 2-degree vertices w_1, w_2, w_3 and w_4 (see Figure 10(d)). By Lemma 4.2(3), it can be similarly checked that $G \nsubseteq F$; that is, $\gamma(B) = 2$ is impossible.

4.2 Pentagonal rings

For an integer $l \geq 3$, let $\{f_i | i \in \mathbb{Z}_l\}$ be a cyclic sequence of l faces (polygons) of a fullerene graph F such that two consecutive faces f_i and f_{i+1} ($i \in \mathbb{Z}_l$) intersect only at an edge, denoted by e_i , and two non-consecutive faces f_i and f_j are disjoint. The subgraph $R := \bigcup_{i \in \mathbb{Z}_l} f_i$ is called a *polygonal ring* of F if $\{e_i | i \in \mathbb{Z}_l\}$ is a matching of F, and l is called the *length* of the polygonal ring R, denoted by l(R). A polygonal ring R is called a *pentagonal ring* if every f_i of R is a pentagon ($i \in \mathbb{Z}_{l(R)}$) (see Figure 11). The R_5 and R_6 in Figure 4 are two pentagonal rings with length five and six, respectively.

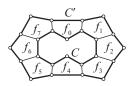


Figure 11: A pentagonal ring R of length eight with s(R) = 2 and s'(R) = 6.

Let R be a pentagonal ring of F consisting of pentagons $f_1, \ldots, f_{l(R)}$. As a subgraph of F, R has two faces different from the f_i $(i = 1, \ldots, l(R))$. Without loss of generality, we suppose that C and C' are the boundaries of the central interior face and exterior face, respectively, and C and C' have s(R) and s'(R) 2-degree vertices, respectively, with $s(R) \leq s'(R)$. We call C and C' the *inner cycle* and the *outer cycle* of R, respectively. Then s'(R) + s(R) = l(R), $s(R) \leq \lfloor \frac{l(R)}{2} \rfloor$, and $s(R) \neq 1$ and $s'(R) \neq 1$.

Let G be the subgraph of F induced by the vertices on C and its interior, and r(R), $n_6(R)$ and $n_5(R)$ the numbers of vertices, hexagons and pentagons within C, respectively.

We claim that r(R) and s(R) have the same parity. We have

$$|V(G)| = r(R) + l(R) + s(R),$$

and

$$|E(G)| = \frac{2l(R) + 3s(R) + 3r(R)}{2}$$

By Euler's formula |V(G)| - |E(G)| + |F(G)| = 1, where $|F(G)| (= n_5(R) + n_6(R))$ is the number of the interior faces of G, we have

$$n_5(R) + n_6(R) = \frac{1}{2}(s(R) + r(R) + 2).$$
(1)

Further, by $|E(G)| = \frac{1}{2}(5n_5(R) + 6n_6(R) + s(R) + l(R))$, we have

$$5n_5(R) + 6n_6(R) = 2s(R) + 3r(R) + l(R)).$$
(2)

Combining Eqs. (1) and (2), we have that

$$n_5(R) = 6 + s(R) - l(R), \tag{3}$$

and

$$n_6(R) = l(R) + \frac{1}{2}(r(R) - s(R)) - 5.$$
(4)

Equation (4) implies that $r(R) \equiv s(R) \pmod{2}$.

For a fullerene graph F, let

$$\psi_l(F) := \min\{s(R) \mid R \text{ is a pentagonal ring of } F \text{ with length } l\}.$$
(5)

For example, $\psi_5(F_{20}) = 0$ and $\psi_6(F_{24}) = 0$. Further, let

$$\tau(F) := \min\{l(R) | R \text{ is a pentagonal ring of } F\}.$$
(6)

For example, $\tau(F_{20}) = 5$ and $\tau(F_{24}) = 6$.

Lemma 4.5. For any fullerene graph F with a pentagonal ring, $5 \le \tau(F) \le 12$.

Proof: Because F has exactly 12 pentagons, $\tau(F) \leq 12$. Further, if F contains a pentagonal ring R with $l(R) \leq 4$, then s(R) = s'(R) = 2 since F has no squares as faces. Hence l(R) = 4, and by Lemma 4.2 (1) F has two edges connecting the two 2-degree vertices of R lying on the inner cycle and lying on the outer cycle respectively, which would result in one face of size at most four in F, a contradiction. Hence $\tau(F) \geq 5$.

The following lemma is due to Kutnar and Marušič.

Lemma 4.6. [17] Let F be a fullerene graph containing a polygonal ring R of length five, and let C and C' be the inner cycle and the outer cycle of R, respectively. Then either (1) C or C' is the boundary of a face, or

(2) both C and C' are of length 10, and the five faces of R are all hexagonal.

By Lemma 4.6 we immediately have

Corollary 4.7. If a fullerene graph F contains a pentagonal ring R of length five, then R is just R_5 .

Lemma 4.8. There is no fullerene graph F with $\tau(F) = 7$.

Proof: Suppose to the contrary that F is a fullerene graph with $\tau(F) = 7$. Let R be a pentagonal ring of F with length l(R) = 7. Then $s(R) \leq \lfloor \frac{l(R)}{2} \rfloor = 3$. So s(R) = 2 or 3. By Lemma 4.2, whenever s(R) = 2 or 3, F would contain a R_6 (see Figure 12), contradicting that $\tau(F) = 7$.



Figure 12: The illustration for the proof of Lemma 4.8.

Lemma 4.9. A fullerene graph F with $\tau(F) = 11$ is not 3-resonant.

Proof: Let R be a pentagonal ring of F with length $l(R) = \tau(F) = 11$ and $s(R) = \psi_{11}(F)$. Let C be the inner cycle of R. By Eq. (3), $n_5(R) = s(R) - 5$, and $\psi_{11}(F) = s(R) \ge 5$. On the other hand, $\psi_{11}(F) = s(R) \le \lfloor \frac{l(R)}{2} \rfloor = 5$. So $\psi_{11}(F) = s(R) = 5$ and $n_5(R) = 0$; that is, there are no pentagons within C.

Let v_1, v_2, v_3, v_4 and v_5 be the five 2-degree vertices clockwise on C. If two of these five vertices are adjacent in F, then by Lemma 4.2 it follows that the two vertices are consecutive, say v_1, v_2 , and the other three vertices v_3, v_4 and v_5 have a common neighbor within C, denoted by w. Let h be the face of F containing v_1, v_2, v_3, w and v_5 . Note that any two of v_1, v_2, \ldots, v_5 are not adjacent on C. So $|h| \ge 7$, a contradiction. If any two of v_1, v_2, \ldots, v_5 have no common neighbor within C, then the five faces adjoining R along Cform a polygonal ring R' with C as the outer cycle. Since |C| = 16, the inner cycle of R'bounds a face f' of F by Lemma 4.6. Note $s(R) \equiv r(R) \pmod{2}$. So f' is a pentagon, contradicting $n_5(R) = 0$.

So there exist two vertices of v_1, \ldots, v_5 with a common neighbor within C. They must be consecutive by Lemma 4.2, so say v_1 and v_2 . By Lemma 4.2 and $n_5(R) = 0$, the subgraph of F induced by R together with all vertices within C is isomorphic to the graph in Figure 13(a). Let f be the face adjacent to R along a 4-length path on the boundary of R (see Figure 13(b)). If f is a pentagon, then F contains a pentagonal ring R' with length l(R') = 10 (see Figure 13(b)). Then $11 = \tau(F) \leq l(R') = 10$, that is a contradiction. So suppose f is a hexagon. Then F contains the forbidden subgraph of 3-resonant fullerene graph in Figure 5; see also Figure 13(c). Hence F is not 3-resonant.

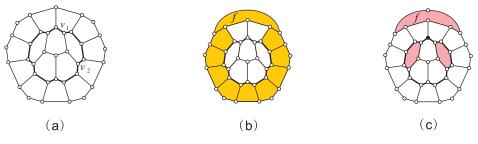


Figure 13: The illustration of Lemma 4.9.

5 Construction of k-resonant $(k \ge 3)$ fullerene graphs

For a pentagon f of a fullerene graph F, if it dose not lie in any pentagonal ring of F, then it must lie in some maximal pentagonal fragment of F. In particular, if F is a 3-resonant fullerene graph containing no pentagonal rings, then by Theorem 4.4 the maximal pentagonal fragment of F containing any given pentagon is either a pentagon or a turtle.

Lemma 5.1. Let F be a fullerene graph without pentagonal rings. Then F is 3-resonant if and only if F is either C_{60} or F_{36}^1 shown in Figure 14. Further, both C_{60} and F_{36}^1 are k-resonant for any integer $k \geq 3$.

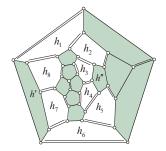


Figure 14: The fullerene graph F_{36}^1 with a perfect matching M.

Proof: Let F be a 3-resonant fullerene graph without pentagonal rings as subgraphs. Then F is different from F_{20} since F_{20} contains a pentagonal ring R_5 . So by Theorem 4.4, every maximal pentagonal fragment of F is either a pentagon or a turtle. If F contains no turtles as maximal pentagonal fragments, then every pentagon of F is adjacent only to hexagons. Hence F satisfies IPR (isolated pentagon rule). By Theorem 4.1, F is C_{60} since it is the unique fullerene graph with no more than 60 vertices and without adjacent pentagons.

Now suppose that F contains a turtle B as a maximal pentagonal fragment. Denote clockwise the hexagons adjoining B by $h_1, h_2, ..., h_8$ as shown in Figure 15(a). Let $G_0 :=$ $B \cup h_3 \cup h_4 \cup h_7 \cup h_8$. Then h_1, h_2, h_5 and h_6 are four hexagons adjoining G_0 . The other two faces adjoining G_0 are denoted by h' and h'' such that h' is adjacent to both h_7 and h_8 . By Lemma 2.3, h' is disjoint from h_2 and h_5 . If h' is a hexagon, then $\mathcal{H} = \{h', h_2, h_5\}$ is not a resonant pattern since $F - \mathcal{H}$ has a component with 15 vertices (see Figure 15(b)), contradicting that F is 3-resonant. So h' must be a pentagon. By the symmetry of G_0 , h'' is also pentagonal. Hence the fragment G_1 , consisting of G_0 together with its all adjacent faces, has exactly four 2-degree vertices on its boundary (see Figure 15(c)). By Lemma 4.2(3), Fis isomorphic to the graph (d) in Figure 15, that is F_{36}^1 in Figure 14.

Conversely, each of fullerene graphs C_{60} and F_{36}^1 has a perfect matching, illustrated by double edges in Figures 1 and 14 respectively, so that all hexagons are alternating. Hence C_{60} and F_{36}^1 are k-resonant for any integer $k \ge 1$ since any disjoint hexagons are mutually resonant.

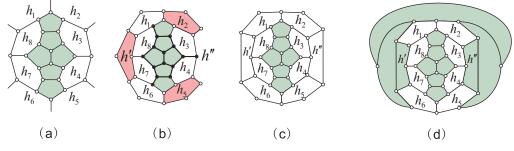


Figure 15: The illustration for the proof of Lemma 5.1.

From now on we discuss 3-resonant fullerene graphs with a pentagonal ring. By Lemmas 4.5, 4.8 and 4.9, we have that $\tau(F) = 5, 6, 8, 9, 10$ or 12. Such cases will be discussed in next five lemmas.

Lemma 5.2. Let F be a fullerene graph with $\tau(F) = 5$ or 6. Then F is 3-resonant if and only if it is either F_{20} or F_{24} (Figure 2). Further, F_{20} and F_{24} are k-resonant for any integer $k \geq 3$.

Proof: Since both F_{20} and F_{24} are 2-resonant and contain no more than two hexagons, they are also k-resonant for any integer $k \geq 3$.

Now let F be a 3-resonant fullerene graph. If $\tau(F) = 5$, then F contains pentagonal ring R_5 by Corollary 4.7. So F is F_{20} by Theorem 3.4.

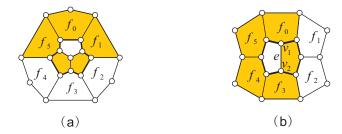


Figure 16: The illustration for the proof of Lemma 5.2.

Now suppose $\tau(F) = 6$. Let R be a pentagonal ring with length $l(R) = \tau(F) = 6$ and let C and C' be the inner cycle and the outer cycle of R, respectively. Let f_0, f_1, \ldots, f_5 be the six pentagons of R in clockwise order. Then $1 \neq s(R) \leq \lfloor \frac{6}{2} \rfloor = 3$. If s(R) = 0, then R is R_6 and F is just F_{24} by Theorem 3.4.

If s(R) = 3, there are three 2-degree vertices on C and also three 2-degree vertices on C'. By Lemma 4.2, the three 2-degree vertices on C have a common neighbor within C. Hence F contains a R_5 (see Figure 16(a)), contradicting $\tau(F) = 6$. If s(R) = 2, there are two 2-degree vertices v_1, v_2 on C. By Lemma 4.2, v_1 and v_2 are adjacent in F (see Figure 16(b)). Hence F contains a R_5 , also contradicting $\tau(F) = 6$.

Lemma 5.3. Let F be a fullerene graph with $\tau(F) = 8$. Then F is 3-resonant if and only if F is F_{28} shown in Figure 17. Further, F_{28} is also k-resonant for any integer $k \ge 3$.

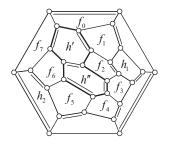


Figure 17: The fullerene graph F_{28} with a perfect matching.

Proof: Similar to the proof of Lemma 5.1 we can show readily that F_{28} is k-resonant for any integer $k \geq 3$.

Conversely, let F be a 3-resonant fullerene graph with $\tau(F) = 8$. Let R be a pentagonal ring of F with length $l(R) = \tau(F) = 8$ and $s(R) = \psi_8(F)$. Let C and C' be the inner cycle and the outer cycle of R, respectively, and f_0, f_1, \ldots, f_7 the eight pentagons of R in clockwise order. Obviously, $2 \le \psi_8(F) = s(R) \le \lfloor \frac{l(R)}{2} \rfloor = 4$.

Case 1. $\psi_8(F) = 4$. By Lemma 4.2(3), the subgraph G of F induced by R together with all vertices within C is isomorphic to one of the four graphs shown in Figure 18. If G is isomorphic to the graph (a) or (b), then F contains a pentagonal ring with length six, contradicting $\tau(F) = 8$. If G is isomorphic to the graph (c) or (d), then F contains a pentagonal ring R' with length eight and s(R') = 2, contradicting $\psi_8(F) = 4$ (refer to Eq. (5)).

Case 2. $\psi_8(F) = 3$. By Lemma 4.2 (2) and Eqs. (3) and (4), we have r(R) = 1, $n_5(R) = 1$ and $n_6(R) = 2$. Hence F contains a pentagonal ring R' with length eight and s(R') = 2; see Figure 19. So $3 = \psi_8(F) \le s(R') = 2$ by (5), a contradiction.

Case 3. $\psi_8(F) = 2$. Then R contains two 2-degree vertices u_1 and u_2 on C. By Lemma 4.2(1), u_1 and u_2 are adjacent in F, and lie on two pentagons f_i and f_{i+4} for some $i \in \mathbb{Z}_8$, respectively (say i = 2, and see Figure 20 (a)). So there are exactly two adjacent hexagons

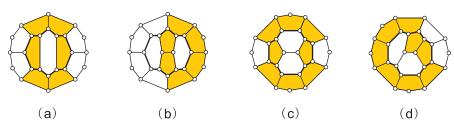


Figure 18: The illustration for Case 1 of the proof of Lemma 5.3.



Figure 19: The illustration for Case 2 of the proof of Lemma 5.3.

h' and h'' within C. Let h_1 and h_2 be the two faces outside C' such that h_1 is adjacent to faces f_1 , f_2 and f_3 , while h_2 is adjacent to faces f_5 , f_6 and f_7 (see Figure 20 (a)). Then h_1 and h_2 are distinct and disjoint. If both h_1 and h_2 are hexagons, let v, v_1 and v_2 be three vertices on C' as shown in Figure 20 (a) and let $S := \{v\}$ and $\mathcal{H} := \{h_1, h_2, h'\}$. Then $F - \mathcal{H} - S$ has two isolated vertices v_1 and v_2 . By Lemma 2.1, \mathcal{H} is not a resonant pattern, contradicting that F is 3-resonant. So at least one of h_1 and h_2 , say h_1 , is a pentagon. If h_2 is a hexagon, let h_3 and h_4 be the other two adjacent faces of h_1 as shown in Figure 20 (b). By Lemma 4.2(3), it follows that both h_3 and h_4 are hexagons. Hence F is the fullerene graph F_{30} shown in Figure 20 (b). Clearly, $\mathcal{H} := \{h_2, h_4, h''\}$ is not resonant. So both h_1 and h_2 are pentagons. By Lemma 4.2, F is the fullerene graph F_{28} shown in Figure 17. \Box

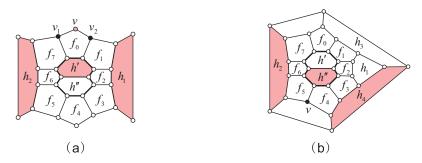


Figure 20: The illustration for Case 3 of the proof of Lemma 5.3.

Lemma 5.4. Let F be a fullerene graph with $\tau(F) = 9$. Then F is 3-resonant if and only if F is F_{32} as shown in Figure 21. Further, F_{32} is k-resonant for any integer $k \ge 3$.

Proof: Let F be a 3-resonant fullerene graph with $\tau(F) = 9$. Let R be a pentagonal ring of F with length l(R) = 9 and $s(R) = \psi_9(F)$. Let C and C' be the inner cycle and the outer

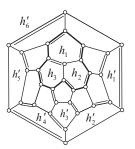


Figure 21: The fullerene graph F_{32} with a perfect matching.

cycle of R, respectively. If s(R) = 2, by by Lemma 4.2 (1) the two 2-degree vertices on C must be adjacent in F. Then the two faces f and f' within C satisfy |f| + |f'| = |C| + 2 = 13. Hence F has a face of size larger than 6, a contradiction. So $3 \le \psi_9(F) = s(R) \le \lfloor \frac{l(R)}{2} \rfloor = 4$. Let f_0, f_1, \ldots, f_8 be the nine pentagons of R in clockwise order.

Case 1. $\psi_9(F) = 4$. Let G be the subgraph of F induced by the vertices of R together with the vertices within C. By Eqs. (3) and (4), $n_5(R) = 1$ and $n_6(R) = 2 + \frac{1}{2}r(R)$. By Lemma 4.2(3), either r(R) = 0 and $n_6(R) = 2$, or r(R) = 2 and $n_6(R) = 3$. By Lemma 4.2, G is isomorphic to the graph (a) in Figure 22 if the former holds, and G is isomorphic to either the graph (b) or (c) in Figure 22 if the latter holds.

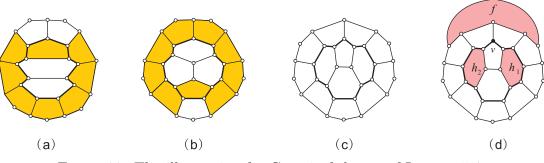


Figure 22: The illustration for Case 1 of the proof Lemma 5.4.

If G is isomorphic to the graph (a), then F contains a pentagon ring with length eight, contradicting $\tau(F) = 9$. If G is isomorphic to the graph (b), then F contains a pentagonal ring R' with length 9 and s(R') = 3, contradicting $\psi_9(F) = 4$. So suppose G is isomorphic to the graph (c). Let f be the face adjoining R along a 4-length path as shown in Figure 22 (d). If f is a pentagon, then F contains a pentagonal ring with length 8 which consists of seven pentagons of R and f, contradicting $\tau(F) = 9$. So f is a hexagon. Then disjoint hexagons f, h_1 and h_2 form a forbidden substructure of 3-resonant fullerene graphs (see Figures 22(d) and 5).

Case 2. $\psi_9(F) = 3$. By Lemma 4.2(2) and Eqs (3) and (4), we have r(R) = 1, $n_5(R) = 0$ and $n_6(R) = 3$. Denote the three hexagons within C by h_1, h_2 and h_3 . The three 2-degree vertices on C must lie on the pentagons f_i , f_{i+3} and f_{i+6} for some $i \in \mathbb{Z}_9$ (say i = 1, and see Figure 23 (a)). Let h'_1, h'_2, \ldots, h'_6 be the six faces adjoining R clockwise along C' such that h'_1 is adjacent to f_0, f_1 and f_2 (see Figure 23(a)). If at least two of h'_1, h'_3 and h'_5 are hexagons, say h'_1 and h'_5 , then h'_1, h'_5 and h_1 also form a forbidden substructure of 3-resonant fullerene graphs (see Figure 23(a)), contradicting that F is 3-resonant. If only one of h'_1, h'_3 and h'_5 is a hexagon, then by Lemma 4.2(3), F has a face with size seven, a contradiction. So all of h'_1, h'_3 and h'_5 are pentagons. By Lemma 4.2(2), F is isomorphic to the graph (b) in Figure 23; that is F_{32} in Figure 21.

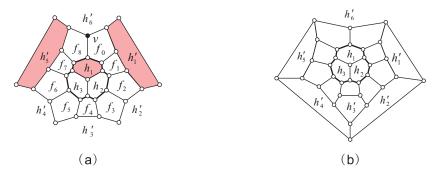


Figure 23: The illustration for Case 2 of the proof of Lemma 5.4.

Conversely, it needs to show that F_{32} is k-resonant for any integer $k \ge 3$. Since there are no more than two disjoint hexagons in F_{32} , it suffices to show that any two disjoint hexagons of F_{32} are mutually resonant. By symmetry, we only consider $\{h_1, h'_4\}$ and $\{h_1, h'_6\}$. Let M be the perfect matching of F_{32} consisting of the double edges illustrated in Figure 21. Clearly, h_1, h'_4 and h'_6 are all M-alternating. Hence both $\{h_1, h'_4\}$ and $\{h_1, h'_6\}$ are resonant patterns of F_{32} .

Lemma 5.5. Let F be a fullerene graph with $\tau(F) = 10$. Then F is 3-resonant if and only if F is either F_{36}^2 or F_{40} shown in Figure 24. Further, F_{36}^2 and F_{40} are k-resonant for any integer $k \geq 3$.

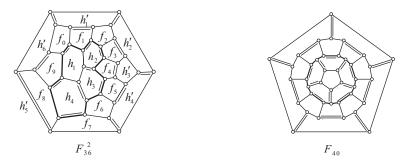


Figure 24: The fullerene graphs F_{36}^2 and F_{40} .

Proof: Let F be a 3-resonant fullerene graph with $\tau(F) = 10$. Let R be a pentagonal ring of F with length $l(R) = \tau(F) = 10$ and $s(R) = \psi_{10}(F)$. Let C be the inner cycle of R and f_0, \ldots, f_9 the pentagons of R in clockwise order. Clearly, $\psi_{10}(F) \ge 2$. If $\psi_{10}(F) = 2$, then the two 2-degree vertices of R on C are adjacent in F by Lemma 4.2. Then there are two faces h_0 and h_1 of F within C such that $|h_0| + |h_1| = l(R) + s(R) + 2 = 14$ since the edge within C is counted twice in $|h_0| + |h_1|$. So at least one of h_0 and h_1 has size more than six, a contradiction. If $\psi_{10}(F) = 3$, then the three 2-degree vertices of R on C together with vertices within C induce a $K_{1,3}$ by Lemma 4.2(2). Hence there are three faces h_0, h_1, h_2 of F within C and $\sum_{i \in \mathbb{Z}_3} |h_i| = l(R) + s(R) + 6 = 19$. So at least one of h_0, h_1 and h_2 has size no less than seven, a contradiction, too. So $4 \le \psi_{10}(F) = s(R) \le \lfloor \frac{l(R)}{2} \rfloor = 5$.

Case 1. $\psi_{10}(F) = 4$. By Eqs. (3) and (4), $n_5(R) = 0$ and $n_6(R) = 3 + \frac{1}{2}r(R)$. By Lemma 4.2(3), r(R) = 0 or 2.

If r(R) = 0 and $n_6(R) = 3$, the four 2-degree vertices on C belong to four pentagons f_i, f_{i+1}, f_{i+5} and f_{i+6} for some $i \in \mathbb{Z}_{10}$, say i = 3 (see Figure 25(a)). Let h_1, h_2 and h_3 be the three hexagons within C such that $h_1 \cap f_2 \neq \emptyset, h_2 \cap f_3 \neq \emptyset$ and $h_3 \cap f_4 \neq \emptyset$. Let f be the common adjacent face of f_2, f_3, f_4 and f_5 (see Figure 25(a)). If f is a pentagon, then F contains a pentagonal ring $(R - \{f_3, f_4\}) \cup f$ with length 9, contradicting $\tau(F) = 10$. So suppose f is a hexagon. Then $\mathcal{H} := \{f, h_1, h_3\}$ is not a resonant pattern since $F - \mathcal{H}$ has an isolated vertex (the black vertex in Figure 25 (a)), contradicting that F is 3-resonant.

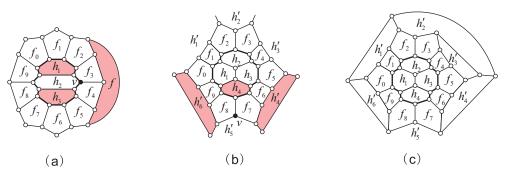


Figure 25: The illustration for Case 1 of the proof of Lemma 5.5.

So suppose r(R) = 2 and $n_6(R) = 4$. By Lemma 4.2(3), the four 2-degree vertices on C together with all vertices within C induce a T_0 . Hence, the four 2-degree vertices belong to the pentagons f_j , f_{j+3} , f_{j+5} and f_{j+8} for some $j \in \mathbb{Z}_{10}$, say j = 1 (see Figure 25(b)). Let h_1, h_2, h_3 and h_4 be the four hexagons within C in clockwise order and $h_1 \cap f_0 \neq \emptyset$. Let $h'_1, h'_2, \dots h'_6$ be the faces adjoining R in clockwise order along its boundary such that $h'_1 \cap f_1 \neq \emptyset$ (see Figure 25 (b)). By Lemmas 2.3 and 4.6, they are pairwise distinct. If both h'_4 and h'_6 are hexagons, then $\mathcal{H} := \{h_4, h'_4, h'_6\}$ is not a resonant pattern since $F - \mathcal{H}$ has an isolated vertex v, contradicting that F is 3-resonant. So one of h'_4 and h'_6 is a pentagon, say h'_6 . By the symmetry, one of h'_1 and h'_3 is a pentagon. If h'_1 is a pentagon, then F would have a pentagonal ring of length nine, contradicting $\tau(F) = 10$. So h'_3 is a pentagon, and both h'_1 and h'_4 are hexagons. By Lemma 4.2(3), it follows that F is the graph (c) in Figure

25; that is also F_{36}^2 in Figure 24.

Case 2. $\psi_{10}(F) = 5$. By Eqs. (3) and (4), $n_5(R) = 1$ and $n_6(R) = 5 - \frac{1}{2}(5 - r(R))$.

If there exist two vertices of R on C having a common neighbor within C, let G be the subgraph induced by R together with all vertices within C. By Lemma 4.2, it follows that G is isomorphic to the graph (a) or the graph (b) in Figure 26. If G is isomorphic to the graph (a), then F contains a pentagonal ring R' with length 10 and s(R') = 4. Hence $s(R') = 4 < \psi_{10}(F) \leq s(R')$, a contradiction. So suppose G is isomorphic to the graph (b). Let f be the face adjoining R along a 4-length path (see Figure 26, the common adjacent face f of $f_2, ..., f_5$). If f is a pentagon, then F contains a pentagonal ring with length 9 (the pentagonal ring $(R - \{f_3, f_4\}) \cup f$ in Figure 26), contradicting $\tau(F) = 10$. So suppose f is a hexagon. Then F has a set \mathcal{H} of three mutually disjoint hexagons such that $f \in \mathcal{H}$ and $F - \mathcal{H}$ has an isolated vertex v (the black vertex in Figure 26 (b)), contradicting that F is 3-resonant. So there is no k-resonant fullerene graph satisfying the condition.

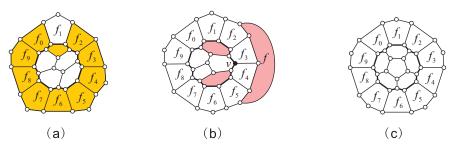


Figure 26: The illustration for Case 2 of the proof of Lemma 5.5.

Otherwise, any two 2-degree vertices on C have distinct neighbors within C: If two 2degree vertices on C are adjacent, by Lemma 4.2(2) the other three 2-degree vertices on Cwould have one common neighbor within C, a contradiction. Then the five faces adjacent to R within C form a ring R' of F with C as its outer cycle. Note that the edges of R'connecting its outer cycle and inner cycle form a cyclic 5-edge-cut of F. Since |C| = 15, the inner cycle of R' bounds a face f' of F by Lemma 4.6. So f' is a pentagon. Therefore the subgraph G induced by R together with all vertices within C is isomorphic to the graph (c) in Figure 26. An analogous argument yields that the five faces adjacent G along its boundary are hexagons and F - G is a pentagon. So F is F_{40} as shown in Figure 24.

Finally it suffices to prove that F_{36}^2 and F_{40} are k-resonant for every integer $k \ge 3$. For F_{40} , it has a perfect matching illustrated in Figure 24 that is alternating on all hexagons. Hence F_{40} is k-resonant for all $k \ge 1$. For F_{36}^2 , let $G_1 := h_1 \cup h_2 \cup h_3 \cup h_4$ and $G_2 := h'_1 \cup h'_2 \cup h'_4 \cup h'_5$. Then G_1 and G_2 are disjoint, and the restrictions of perfect matching M illustrated in Figure 24 on G_1 and G_2 are also their perfect matchings. That means that the union of perfect matchings of G_1 and G_2 can be extended to a perfect matching of F_{36}^2 . For each of G_1 and G_2 , it is easy to see that any disjoint hexagons are mutually resonant. Hence any disjoint hexagons of F_{36}^2 forms a sextet pattern. **Lemma 5.6.** Let F be a fullerene graph with $\tau(F) = 12$. Then F is 3-resonant if and only if F is F_{48} shown in Figure 27. Further, F_{48} is k-resonant for any integer $k \ge 3$.

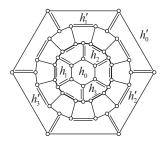


Figure 27: The fullerene graph F_{48} with a perfect matching M_0 .

Proof: Let F be a 3-resonant fullerene graph with $\tau(F) = 12$. Let R be the pentagonal ring of F with length l(R) = 12 and C the inner cycle of R. Since F has exactly 12 pentagons, there is no pentagons within C and hence $n_5(R) = 0$. By Eqs (3) and (4), s(R) = 6and $n_6(R) = 4 + \frac{1}{2}r(R)$. Let v_0, v_1, \ldots, v_5 be the six 2-degree vertices of R on C arranged clockwise.

If two 2-degree vertices on C are connected by an edge of F through the interior of C, then by Lemma 4.2 (1) and (3), the other four 2-degree vertices are connected by two edges of F since every face within C is a hexagon. Then r(R) = 0, the subgraph of F induced by the vertices of R is isomorphic to the graph G_1 as shown in Figure 28 (left) and F is the fullerene graph as shown in Figure 28 (right). Then the three shadowed disjoint hexagons in Figure 28 (right) are not mutually resonant, contradicting that F is 3-resonant.

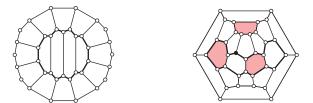


Figure 28: The subgraph G_1 (left) and the fullerene graph containing G_1 (right).

So we may suppose each 2-degree vertex on C has a neighbor within C. Then $r := r(R) \ge 2$. Let G be the subgraph induced by the vertices within C and m the number of edges of G. Since C has six 2-degree vertices, 3r - 2m = 6.

If G is not connected, then G is a forest since F is cyclically 5-edge connected. Then $m = r - \omega$, where $\omega \ge 2$ is the number of components of G. So $3r - 2(r - \omega) = 6$, and $r = 6 - 2\omega \le 2$. Therefore r = 2 and G consists of two isolated vertices, denoted by u, v. We may assume that $N(u) = \{v_0, v_1, v_2\}$ and $N(v) = \{v_3, v_4, v_5\}$. Let f be the face within C containing vertices v_0, u, v_2, v_3, v and v_5 . Note that the six 2-degree vertices are not adjacent on C. So $v_2v_3 \notin E(f)$ and $v_5v_0 \notin E(f)$. Therefore $|f| \ge 8$, a contradiction.

So suppose that G is connected. Let ∂G be the boundary of G which is a closed walk. Note that a cut-edge of G will contribute 2 to $|\partial G|$. Let x be the number of inner faces of G. By Euler's formula, m = r - 1 + x. So 3r - 2(r - 1 + x) = 6, and r = 4 + 2x. On the other hand, since every inner face of G is also a face of F, every inner face of G is a hexagon. So $|\partial G| + 6x = 2m = 2r - 2 + 2x = 2(4 + 2x) - 2 + 2x = 6 + 6x$. Hence $|\partial G| = 6$.

If x = 0, then G is a tree. Since $|\partial G| = 6$, G has three edges. So G is isomorphic to a $K_{1,3}$ or a 3-length path. Hence the subgraph of F induced by $V(R \cup G)$ is isomorphic to either G_2 or G_3 shown in Figure 29. Whenever $G_2 \subset F$ or $G_3 \subset F$, F has three disjoint hexagons which are not mutually resonant (see Figure 29).

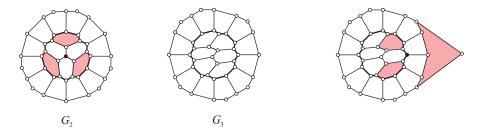


Figure 29: The subgraphs G_2 and G_3 .

Hence x > 0. Since the length of every cycle of G is at least 6 and $|\partial G| = 6$, ∂G is a 6-length cycle. Since F is cubic, there are six edges connecting the 2-degree vertices v_0, v_1, \ldots, v_5 to vertices of G. So G is a hexagon. By the symmetry of R, F is the fullerene graph F_{48} shown in Figure 27.

Conversely, it suffices to show that F_{48} is k-resonant for $k \geq 3$. Let M_0 be the perfect matching of F_{48} illustrated in Figure 27. Let f_0, f_1, f_2, f_3 and f'_0, f'_1, f'_2, f'_3 be the hexagons marked in F_{48} (see Figure 27), and let $M_1 := M_0 \oplus f_1 \oplus f_2 \oplus f_3$, $M_2 := M_0 \oplus f'_1 \oplus f'_2 \oplus f'_3$ and $M_3 := M_0 \oplus f_1 \oplus f_2 \oplus f_3 \oplus f'_1 \oplus f'_2 \oplus f'_3$. Let \mathcal{H} be any set of mutually disjoint hexagons of F_{48} . If $h_0, h'_0 \notin \mathcal{H}$, then every hexagon of \mathcal{H} is M_0 -alternating. If $h'_0 \notin \mathcal{H}$ but $h_0 \in \mathcal{H}$, then every hexagon of \mathcal{H} is M_1 -alternating. If $h_0 \notin \mathcal{H}$ but $h'_0 \in \mathcal{H}$, then every hexagon of \mathcal{H} is M_2 -alternating. If $\{h_0, h'_0\} \subseteq \mathcal{H}$, then $\mathcal{H} = \{h_0, h'_0\}$ and both h_0 and h'_0 are M_3 -alternating. Thus F_{48} is k-resonant for $k \geq 3$.

Summarizing the above results (Lemmas 5.1-5.6), we have the following main theorem.

Theorem 5.7. A fullerene graph F is 3-resonant if and only if F is one of F_{20} , F_{24} , F_{28} , F_{32} , F_{36}^1 , F_{36}^2 , F_{40} , F_{48} and C_{60} . Further, these nine fullerene graphs are all k-resonant for every integer $k \ge 1$.

From Theorem 5.7, we arrive immediately at the following result.

Theorem 5.8. A fullerene graph F is 3-resonant if and only if it is k-resonant for any integer $k \geq 3$.

6 Sextet polynomials of 3-resonant fullerene graphs

The sextet polynomial of a benzenoid system G for counting sextet patterns was introduced by Hosoya and Yamaguchi [15] as follows:

$$B_G(x) = \sum_{i=0}^{C(G)} \sigma(G, i) x^i,$$
(7)

where $\sigma(G, i)$ denotes the number of sextet patterns of G with *i* hexagons, and C(G) the Clar number of G. The sextet polynomial of C₆₀ is computed [24] as

$$B_{C_{60}}(x) = 5x^8 + 320x^7 + 1240x^6 + 1912x^5 + 1510x^4 + 660x^3 + 160x^2 + 20x + 1.$$
 (8)

For a detailed discussion and review of sextet polynomials, see [14, 22].

Since any independent hexagons of a 3-resonant fullerene graph form a sextet pattern, we can compute easily the sextet polynomials of the other eight 3-resonant fullerene graphs as follows, by counting sets of disjoint hexagonal faces.

$$B_{F_{20}}(x) = 1,$$

$$B_{F_{24}}(x) = (x+1)^2 = x^2 + 2x + 1,$$

$$B_{F_{28}}(x) = (2x+1)^2 = 4x^2 + 4x + 1,$$

$$B_{F_{32}}(x) = (3x+1)^2 = 9x^2 + 6x + 1,$$

$$B_{F_{36}^1}(x) = 2x^4 + 16x^3 + 20x^2 + 8x + 1,$$

$$B_{F_{36}^2}(x) = (x^2 + 4x + 1)^2 = x^4 + 8x^3 + 18x^2 + 8x + 1,$$

$$B_{F_{40}}(x) = (5x^2 + 5x + 1)^2 = 25x^4 + 50x^3 + 35x^2 + 10x + 1, \text{ and}$$

$$B_{F_{48}}(x) = (2x^3 + 9x^2 + 7x + 1)^2 = 4x^6 + 36x^5 + 109x^4 + 130x^3 + 67x^2 + 14x + 1.$$
(9)

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References

- S. El-Basil, Clar sextet theory of buckminsterfullerene (C₆₀), J. Mol. Struct. (Theochem) 531 (2000) 9-21.
- [2] R. Chen and X. Guo, k-coverable coronoid systems, J. Math. Chem. 12 (1993) 147-162.
- [3] E. Clar, The Aromatic Sextet (Wiley, London, 1972).
- [4] T. Došlić, On lower bounds of number of perfect matchings in fullerene graphs, J. Math. Chem. 24 (1998) 359-364.

- [5] T. Došlić, Cyclical edge-connectivity of fullerene graphs and (k,6)-cages, J. Math. Chem. 33 (2003) 103-112.
- [6] P.W. Fowler and D.E. Manolopoulos, An Atlas of Fullerenes (Oxford Univ. Press, Oxford, 1995).
- [7] P. Fowler and T. Pisanski, Leapfrog transformation and polyhedra of Clar type, J. Chem. Soc. Faraday Trans. 90(19) (1994) 2865-2871.
- [8] K. Fries, Bicyclic compounds and their comparison with naphthalene III, Justus Liebigs Ann. Chem. 454 (1972) 121-324.
- [9] M. Goldberg, A class of multi-symmetric polyhedra, Tôhoku Math. J. 43 (1937) 104-108.
- [10] J.E. Graver, Kekulé structures and the face independence number of a fullerene, Europ. J. Combin. 28 (2007) 1115-1130.
- [11] J.E. Graver, Encoding fullerenes and geodesic domes, SIAM. J. Discrete Math. 17 (4) (2004) 596-614.
- [12] B. Grünbaum, *Convex Polytopes* (Wiley, New York, 1967).
- [13] X. Guo, k-resonant benzenoid systems and k-cycle resonant graphs, MATCH Commun. Math. Comput. Chem. 57 (2006) 153-168.
- [14] I. Gutman, Topological properties of benzenoid system. IX. On the sextet polynomial, Z. Nathrforsch, 37a (1982) 69-73.
- [15] H. Hosoya and T. Yamaguchi, Sextet polynomial. A new enumeration and proof technique for the resonance theory applied to the aromatic hydrocarbons, Tetrehedron Lett. 16 (52) (1975) 4659-4662.
- [16] D.J. Klein and X. Liu, Theorems for carbon cages, J. Math. Chem. 11 (1992) 199-205.
- [17] K. Kutnar and D. Marušič, On cyclic edge-connectivity of fullerenes, Discrete Appl. Math. 156 (10) (2008) 1661-1669.
- [18] K. Lin and R. Chen, k-coverable polyhex graphs, Ars Combin. 43 (1996) 33-48.
- [19] X. Liu, D.J. Klein and T.G. Schmalz, Preferable fullerenes and Clar-sextet cages, Full. Sci. Tech. 2 (1994) 405-422.
- [20] L. Lovász and M. D. Plummer, *Matching Theory*, Ann. Discrete Math., Vol. 29 (North-Holland, Amsterdam, 1986).
- [21] Z. Qi and H. Zhang, A note on the cyclical edge-connectivity of fullerene graphs, J. Math. Chem. 43 (2008) 134-140.
- [22] M. Randić, Aromaticity of polycyclic conjugated hydrocarbons, Chem. Rev. 103 (9) (2003) 3449-3605.
- [23] N. Robertson, P.D. Seymour and R. Thomas, Permanents, Pfaffian orientations, and even directed circuits, Ann. Math. 150 (1999) 929-975.

- [24] W.C. Shiu, P.C.B. Lam and H. Zhang, Clar and sextet polynomials of buckminsterfullerene, J. Mol. Struct. (Theochem) 662 (2003) 239-248.
- [25] W.C. Shiu, P.C.B. Lam and H. Zhang, k-resonance in toroidal polyhexes, J. Math. Chem. 38 (4) (2005) 451-466.
- [26] W.C. Shiu and H. Zhang, A complete characterization for k-resonant Klein-bottle polyhexes, J. Math. Chem. 43 (2008) 45-59.
- [27] D. Ye and H. Zhang, Extremal fullerene graphs with the maximum Clar number, Discrete Appl. Math. 157 (2009) 3152-3173.
- [28] F. Zhang and R. Chen, When each hexagon of a hexagonal system covers it, Discrete Appl. Math. 30 (1991) 63-75.
- [29] F. Zhang and L. Wang, k-resonance of open-ended carbon nanotubes, J. Math. Chem. 35(2) (2004) 87-103.
- [30] F. Zhang and M. Zheng, Generalized hexagonal systems with each hexagon being resonant, Discrete Appl. Math. 36 (1992) 67-73.
- [31] H. Zhang and D. Ye, An upper bound for the Clar number of fullerene graphs, J. Math. Chem. 41 (2007) 123-133.
- [32] H. Zhang and D. Ye, k-resonant toroidal polyhexes, J. Math. Chem. 44 (1) (2008) 270-285.
- [33] H. Zhang and F. Zhang, Plane elementary bipartite graphs, Discrete Appl. Math. 105 (2000) 291-311.
- [34] M. Zheng, k-resonant benzenoid systems, J. Mol. Struct. (Theochem) 231 (1991) 321-334.
- [35] M. Zheng, Construction of 3-resonant benzenoid systems, J. Mol. Struct. (Theochem) 277 (1992) 1-14.