# 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 $F$ is $M$-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 $i(0 \leq i \leq k)$ 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
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## 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 $M$.

[^0]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 $c\left(F_{n}\right) \leq\left\lfloor\frac{n-12}{6}\right\rfloor$, which is sharp for infinitely many fullerene graphs, including $\mathrm{C}_{60}$ whose Clar number is 8 [1]. Shiu, Lam and Zhang [24] computed the Clar polynomial and the sextet polynomial of $\mathrm{C}_{60}$ by showing that every hexagonal face independent set of $\mathrm{C}_{60}$ is also a resonant pattern.

A fullerene graph is $k$-resonant if any $i(0 \leq i \leq k)$ disjoint hexagons are mutually resonant. So $k$-resonant fullerene graphs are also $(k-1)$-resonant for integer $k \geq 1$. 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 $(k \geq 3)$. 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 $\partial G$ 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 $G^{\prime}$ of $G$ if $f$ is not a face of $G^{\prime}$ and $f$ has an edge in common with $G^{\prime}$. The faces adjoining $G^{\prime}$ are always called adjacent faces of $G^{\prime}$. 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 $S \subseteq V(G-H)$,

$$
C_{o}(G-H-S) \leq|S|
$$

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 $C_{o}(G-H-S) \geq$ $|S|+2$ by parity, i.e. $|S| \leq C_{o}(G-H-S)-2$. Since $G$ is cubic, $S$ sends out at most $3|S| \leq 3 C_{o}(G-H-S)-6$ edges.

Let $G_{1}, G_{2}, \ldots, G_{k}$ 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 $G_{i}(i=1,2, \ldots, k)$ sends odd number edges, hence at least three edges, to $H \cup S$. So $\cup_{i=1}^{k} G_{i}$ sends out at least $3 C_{o}(G-H-S)$ edges to either $S$ or $H$. Since $H$ is a 6 -length cycle, there are at most 6 edges between $H$ and $\cup_{i=1}^{k} G_{i}$. So $\cup_{i=1}^{k} G_{i}$ sends at least $3 C_{o}(G-H-S)-6$ edges to $S$. Hence there are precisely $3 C_{o}(G-H-S)-6$ edges between $S$ and $\cup_{i=1}^{k} G_{i}$. 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 $F^{\prime}$; then take the geometry dual of the graph $F^{\prime}$ and denote it by $F^{*}$ (see Figure (1). Clearly, $F^{*}$ is a fullerene graph since every vertex of $F^{\prime}$ is 6-degree excluding exactly 125 degree vertices and every face of $F^{\prime}$ is a triangle. The edges of $F^{*}$ cross the edges of $F \subset F^{\prime}$ 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 $\mathrm{C}_{60}$ (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, $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ (see Figure 11). 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 $T\left[f_{1}\right]$ by $h_{0}, h_{1}, \ldots, h_{5}$ in clockwise order. If $f_{2}$ is fresh, then $f_{2} \nsubseteq T\left[f_{1}\right]$ 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 $h_{0}^{\prime}, h_{1}^{\prime}, \ldots, h_{5}^{\prime}$ be the six fresh hexagons of $T\left[f_{2}\right]$ in clockwise order. If $T\left[f_{1}\right]$ and $T\left[f_{2}\right]$ have a common hexagon, then they have exactly two common adjacent hexagons. Assume $h_{i_{0}}=h_{j_{0}}^{\prime}$ for some $i_{0}, j_{0} \in \mathbb{Z}_{6}$. Let $M_{2}:=M^{0} \oplus h_{i_{0}} \oplus$ $h_{i_{0}+2} \oplus h_{i_{0}+4} \oplus h_{j_{0}+2}^{\prime} \oplus h_{j_{0}+4}^{\prime}$. It is clear that $M_{2}$ is a perfect matching alternating on both $f_{1}$ and $f_{2}$. Now suppose $T\left[f_{1}\right]$ and $T\left[f_{2}\right]$ have no common hexagons. If no face in $T\left[f_{2}\right]$ adjoins one of $h_{1}, h_{3}$ and $h_{5}$, let $M_{3}:=M^{0} \oplus h_{1} \oplus h_{3} \oplus h_{5} \oplus h_{1}^{\prime} \oplus h_{3}^{\prime} \oplus h_{5}^{\prime}$; otherwise, let $M_{3}:=M^{0} \oplus h_{0} \oplus h_{2} \oplus h_{4} \oplus h_{1}^{\prime} \oplus h_{3}^{\prime} \oplus h_{5}^{\prime}$. 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 $\mathrm{C}_{70}$.

Lemma 3.3. $C_{70}$ is 2-resonant.
Proof: $\mathrm{C}_{70}$ 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 $h^{\prime}$ in $\mathrm{C}_{70}$. If $h, h^{\prime} \notin\left\{h_{1}, h_{3}, h_{5}, h_{7}, h_{9}\right\}$, then $h$ and $h^{\prime}$ are simultaneously $M_{1}$-alternating. If $h, h^{\prime} \notin\left\{h_{11}, h_{12}, h_{13}, h_{14}, h_{15}\right\}$, then $h$ and $h^{\prime}$ are simultaneously $M_{3}$-alternating. So suppose $h \in\left\{h_{1}, h_{3}, h_{5}, h_{7}, h_{9}\right\}$ and $h^{\prime} \in\left\{h_{11}, h_{12}, h_{13}, h_{14}, h_{15}\right\}$. By symmetry, we may assume $h=h_{1}$. If $h^{\prime} \in\left\{h_{12}, h_{15}\right\}$, we may let $h^{\prime}=h_{12}$ by the symmetry of $h_{12}$ and $h_{15}$. Then both $h$ and $h^{\prime}$ are $M_{2}$-alternating. Finally, if $h^{\prime} \in\left\{h_{13}, h_{14}\right\}$, then $h$ and $h^{\prime}$ are simultaneously $M_{4}$-alternating, where $M_{4}:=M_{1} \oplus h_{2} \oplus h_{10}$. Hence $\mathrm{C}_{70}$ is 2-resonant.


Figure 3: $\mathrm{C}_{70}$ 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 $|V(F)| \leq 12 \times 5=60$ 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, $\gamma\left(R_{5}\right)=3$.

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 $\partial B$. If $0<|W| \leq 4$, then $T=F-(V(B) \backslash W)$ 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 $\gamma(B) \geq 3$;
(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 $h_{i+1}(1 \leq i \leq 3)$ 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 $F-\left\{h_{2}, h_{4}, f_{2}\right\}$ has an isolated vertex; that is impossible. Hence both $f_{2}$ and $f_{3}$ must be pentagons and thus belong to $B$ since $B$ is maximal. Let $f_{4}\left(\neq f_{1}\right)$ be the face adjacent to both $f_{2}$ and $f_{3}$. Then $f_{4}$ is a pentagon; otherwise, $F-\left\{h_{1}, h_{4}, f_{4}\right\}$ 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 $F-\left\{h_{1}, h_{4}, f_{5}\right\}$ would be $K_{1,3}$, which has no perfect matchings. Thus $G:=\cup_{i=0}^{5} f_{i} \subseteq B$ 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 $G^{\prime}:=G \cup\left(\cup_{i=1}^{8} h_{i}\right)$.

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 $F-\left\{h_{1}, h_{4}, h_{7}\right\}$ would have an odd component with seven vertices (see Figure 8(b)). If $h_{8}$ is a pentagon, then $G^{\prime}$ 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 $G^{\prime}$ contains four 2-degree
vertices $w_{1}, w_{2}, w_{3}$ and $w_{4}$ (see Figure $8(\mathrm{~d})$ ). By Lemma 4.2(3), there are at most four faces of $F$ outside $G^{\prime}$. These faces must be all pentagons since the fragment $G^{\prime}$ 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.

(a)

(b)

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 $G^{\prime}$ as shown in Figure 9 (a) are distinct and disjoint. Then $G^{\prime \prime}:=G^{\prime} \cup h_{9} \cup h_{10}$ 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 $F-\left\{h_{3}, h_{8}, h_{9}\right\}$ 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 $G^{\prime \prime}$ 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 $G^{\prime \prime}$ 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 $f_{3}\left(\neq f_{0}\right)$ 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 $F-\left\{h_{1}, h_{3}, f_{4}\right\}$ 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 $F-\left\{h_{2}, h_{4}, h_{5}\right\}$ 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 $\left\{h_{1}, h_{3}, h_{6}\right\}$ is not a resonant pattern since $F-\left\{h_{1}, h_{3}, h_{6}\right\}$ 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, $\left\{h_{2}, h_{4}, h_{7}\right\}$ is not a resonant pattern (see Figure 10(c)). Now, we have a fragment $G:=\left(\cup_{i=0}^{4} f_{i}\right) \cup\left(\cup_{j=1}^{7} h_{j}\right)$ 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 $\left\{f_{i} \mid i \in \mathbb{Z}_{l}\right\}$ be a cyclic sequence of $l$ faces (polygons) of a fullerene graph $F$ such that two consecutive faces $f_{i}$ and $f_{i+1}\left(i \in \mathbb{Z}_{l}\right)$ intersect only at an edge, denoted by $e_{i}$, and two non-consecutive faces $f_{i}$ and $f_{j}$ are disjoint. The subgraph $R:=\cup_{i \in \mathbb{Z}_{l}} f_{i}$ is called a polygonal ring of $F$ if $\left\{e_{i} \mid i \in \mathbb{Z}_{l}\right\}$ 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 $\left(i \in \mathbb{Z}_{l(R)}\right)$ (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 $s^{\prime}(R)=6$.

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 $C^{\prime}$ are the boundaries of the central interior face and exterior face, respectively, and $C$ and $C^{\prime}$ have $s(R)$ and $s^{\prime}(R)$ 2-degree vertices, respectively, with $s(R) \leq s^{\prime}(R)$. We call $C$ and $C^{\prime}$ the inner cycle and the outer cycle of $R$, respectively. Then $s^{\prime}(R)+s(R)=l(R)$, $s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor$, and $s(R) \neq 1$ and $s^{\prime}(R) \neq 1$.

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

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

By Euler's formula $|V(G)|-|E(G)|+|F(G)|=1$, where $|F(G)|\left(=n_{5}(R)+n_{6}(R)\right)$ is the number of the interior faces of $G$, we have

$$
\begin{equation*}
n_{5}(R)+n_{6}(R)=\frac{1}{2}(s(R)+r(R)+2) \tag{1}
\end{equation*}
$$

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

$$
\begin{equation*}
\left.5 n_{5}(R)+6 n_{6}(R)=2 s(R)+3 r(R)+l(R)\right) . \tag{2}
\end{equation*}
$$

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

$$
\begin{equation*}
n_{5}(R)=6+s(R)-l(R), \tag{3}
\end{equation*}
$$

and

$$
\begin{equation*}
n_{6}(R)=l(R)+\frac{1}{2}(r(R)-s(R))-5 \tag{4}
\end{equation*}
$$

Equation (4) implies that $r(R) \equiv s(R)(\bmod 2)$.
For a fullerene graph $F$, let

$$
\begin{equation*}
\psi_{l}(F):=\min \{s(R) \mid R \text { is a pentagonal ring of } F \text { with length } l\} . \tag{5}
\end{equation*}
$$

For example, $\psi_{5}\left(F_{20}\right)=0$ and $\psi_{6}\left(F_{24}\right)=0$. Further, let

$$
\begin{equation*}
\tau(F):=\min \{l(R) \mid R \text { is a pentagonal ring of } F\} \tag{6}
\end{equation*}
$$

For example, $\tau\left(F_{20}\right)=5$ and $\tau\left(F_{24}\right)=6$.
Lemma 4.5. For any fullerene graph $F$ with a pentagonal ring, $5 \leq \tau(F) \leq 12$.
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 $s(R)=s^{\prime}(R)=2$ 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 $C^{\prime}$ be the inner cycle and the outer cycle of $R$, respectively. Then either
(1) $C$ or $C^{\prime}$ is the boundary of a face, or
(2) both $C$ and $C^{\prime}$ 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 $s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor=3$. 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 $\psi_{11}(F)=s(R) \geq 5$. On the other hand, $\psi_{11}(F)=s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor=5$. 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 $|h| \geq 7$, 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 $C$ form a polygonal ring $R^{\prime}$ with $C$ as the outer cycle. Since $|C|=16$, the inner cycle of $R^{\prime}$ bounds a face $f^{\prime}$ of $F$ by Lemma 4.6. Note $s(R) \equiv r(R)(\bmod 2)$. So $f^{\prime}$ 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 $R^{\prime}$ with length $l\left(R^{\prime}\right)=10$ (see Figure 13(b)). Then $11=\tau(F) \leq l\left(R^{\prime}\right)=10$, 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 ( $k \geq 3$ ) 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 Theorem4.4 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 $\mathrm{C}_{60}$ 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 $h_{1}, h_{2}, \ldots, h_{8}$ 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 $h^{\prime}$ and $h^{\prime \prime}$ such that $h^{\prime}$ is adjacent to both $h_{7}$ and $h_{8}$. By Lemma 2.3, $h^{\prime}$ is disjoint from $h_{2}$ and $h_{5}$. If $h^{\prime}$ is a hexagon, then $\mathcal{H}=\left\{h^{\prime}, h_{2}, h_{5}\right\}$ 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 $h^{\prime}$ must be a pentagon. By the symmetry of $G_{0}, h^{\prime \prime}$ 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 $15(\mathrm{c})$ ). By Lemma $4.2(3), F$ is isomorphic to the graph (d) in Figure 15, that is $F_{36}^{1}$ in Figure 14 .

Conversely, each of fullerene graphs $\mathrm{C}_{60}$ 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 $\mathrm{C}_{60}$ and $F_{36}^{1}$ are $k$-resonant for any integer $k \geq 1$ 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圆). 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.

(a)

(b)

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 $C^{\prime}$ 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 $1 \neq s(R) \leq\left\lfloor\frac{6}{2}\right\rfloor=3$. 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 $C^{\prime}$. 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 $k \geq 3$.


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 $C^{\prime}$ 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, $2 \leq \psi_{8}(F)=s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor=4$.

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 $R^{\prime}$ with length eight and $s\left(R^{\prime}\right)=2$, 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 $R^{\prime}$ with length eight and $s\left(R^{\prime}\right)=2$; see Figure 19. So $3=\psi_{8}(F) \leq s\left(R^{\prime}\right)=2$ 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.
$h^{\prime}$ and $h^{\prime \prime}$ within $C$. Let $h_{1}$ and $h_{2}$ be the two faces outside $C^{\prime}$ 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 $C^{\prime}$ as shown in Figure 20 (a) and let $S:=\{v\}$ and $\mathcal{H}:=\left\{h_{1}, h_{2}, h^{\prime}\right\}$. 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, $\mathcal{H}:=\left\{h_{2}, h_{4}, h^{\prime \prime}\right\}$ is not resonant since $F-\mathcal{H}$ has an isolated vertex $v$ (see Figure 20 (b)), also contradicting that $F$ is 3-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. $\square$

(a)

(b)

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 $k \geq 3$.

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 $C^{\prime}$ 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 $f^{\prime}$ within $C$ satisfy $|f|+\left|f^{\prime}\right|=|C|+2=13$. Hence $F$ has a face of size larger than 6 , a contradiction. So $3 \leq \psi_{9}(F)=s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor=4$. 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 $R^{\prime}$ with length 9 and $s\left(R^{\prime}\right)=3$, 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 Lemma4.2(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 $h_{1}^{\prime}, h_{2}^{\prime}, \ldots, h_{6}^{\prime}$ be the six faces adjoining $R$ clockwise along $C^{\prime}$ such that $h_{1}^{\prime}$ is adjacent to $f_{0}, f_{1}$ and $f_{2}$ (see Figure 23(a)). If at least two of $h_{1}^{\prime}, h_{3}^{\prime}$ and $h_{5}^{\prime}$ are hexagons, say $h_{1}^{\prime}$ and $h_{5}^{\prime}$, then $h_{1}^{\prime}, h_{5}^{\prime}$ 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 $h_{1}^{\prime}, h_{3}^{\prime}$ and $h_{5}^{\prime}$ is a hexagon, then by Lemma $4.2(3), F$ has a face with size seven, a contradiction. So all of $h_{1}^{\prime}, h_{3}^{\prime}$ and $h_{5}^{\prime}$ 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 $k \geq 3$. 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 $\left\{h_{1}, h_{4}^{\prime}\right\}$ and $\left\{h_{1}, h_{6}^{\prime}\right\}$. Let $M$ be the perfect matching of $F_{32}$ consisting of the double edges illustrated in Figure 21, Clearly, $h_{1}, h_{4}^{\prime}$ and $h_{6}^{\prime}$ are all $M$-alternating. Hence both $\left\{h_{1}, h_{4}^{\prime}\right\}$ and $\left\{h_{1}, h_{6}^{\prime}\right\}$ 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, $\psi_{10}(F) \geq 2$. 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 $\left|h_{0}\right|+\left|h_{1}\right|=l(R)+s(R)+2=14$ since the edge within $C$ is counted twice in $\left|h_{0}\right|+\left|h_{1}\right|$. 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 $\sum_{i \in \mathbb{Z}_{3}}\left|h_{i}\right|=l(R)+s(R)+6=19$. So at least one of $h_{0}, h_{1}$ and $h_{2}$ has size no less than seven, a contradiction, too. So $4 \leq \psi_{10}(F)=s(R) \leq\left\lfloor\frac{l(R)}{2}\right\rfloor=5$.

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 $\left(R-\left\{f_{3}, f_{4}\right\}\right) \cup f$ with length 9 , contradicting $\tau(F)=10$. So suppose $f$ is a hexagon. Then $\mathcal{H}:=\left\{f, h_{1}, h_{3}\right\}$ 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 $h_{1}^{\prime}, h_{2}^{\prime}, \cdots h_{6}^{\prime}$ be the faces adjoining $R$ in clockwise order along its boundary such that $h_{1}^{\prime} \cap f_{1} \neq \emptyset$ (see Figure 25(b)). By Lemmas 2.3 and 4.6, they are pairwise distinct. If both $h_{4}^{\prime}$ and $h_{6}^{\prime}$ are hexagons, then $\mathcal{H}:=\left\{h_{4}, h_{4}^{\prime}, h_{6}^{\prime}\right\}$ is not a resonant pattern since $F-\mathcal{H}$ has an isolated vertex $v$, contradicting that $F$ is 3 -resonant. So one of $h_{4}^{\prime}$ and $h_{6}^{\prime}$ is a pentagon, say $h_{6}^{\prime}$. By the symmetry, one of $h_{1}^{\prime}$ and $h_{3}^{\prime}$ is a pentagon. If $h_{1}^{\prime}$ is a pentagon, then $F$ would have a pentagonal ring of length nine, contradicting $\tau(F)=10$. So $h_{3}^{\prime}$ is a pentagon, and both $h_{1}^{\prime}$ and $h_{4}^{\prime}$ 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 $R^{\prime}$ with length 10 and $s\left(R^{\prime}\right)=4$. Hence $s\left(R^{\prime}\right)=4<\psi_{10}(F) \leq s\left(R^{\prime}\right)$, 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 $f_{2}, \ldots, f_{5}$ ). If $f$ is a pentagon, then $F$ contains a pentagonal ring with length 9 (the pentagonal ring $\left(R-\left\{f_{3}, f_{4}\right\}\right) \cup f$ 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 $C$ would have one common neighbor within $C$, a contradiction. Then the five faces adjacent to $R$ within $C$ form a ring $R^{\prime}$ of $F$ with $C$ as its outer cycle. Note that the edges of $R^{\prime}$ connecting its outer cycle and inner cycle form a cyclic 5 -edge-cut of $F$. Since $|C|=15$, the inner cycle of $R^{\prime}$ bounds a face $f^{\prime}$ of $F$ by Lemma 4.6. So $f^{\prime}$ 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 $k \geq 3$. 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 $k \geq 1$. For $F_{36}^{2}$, let $G_{1}:=h_{1} \cup h_{2} \cup h_{3} \cup h_{4}$ and $G_{2}:=h_{1}^{\prime} \cup h_{2}^{\prime} \cup h_{4}^{\prime} \cup h_{5}^{\prime}$. 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 $k \geq 3$.


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), $s(R)=6$ and $n_{6}(R)=4+\frac{1}{2} r(R)$. 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 $r:=$ $r(R) \geq 2$. 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, $3 r-2 m=6$.

If $G$ is not connected, then $G$ is a forest since $F$ is cyclically 5-edge connected. Then $m=r-\omega$, where $\omega \geq 2$ is the number of components of $G$. So $3 r-2(r-\omega)=6$, and $r=6-2 \omega \leq 2$. Therefore $r=2$ and $G$ consists of two isolated vertices, denoted by $u, v$. We may assume that $N(u)=\left\{v_{0}, v_{1}, v_{2}\right\}$ and $N(v)=\left\{v_{3}, v_{4}, v_{5}\right\}$. 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 $v_{2} v_{3} \notin E(f)$ and $v_{5} v_{0} \notin E(f)$. Therefore $|f| \geq 8$, a contradiction.

So suppose that $G$ is connected. Let $\partial G$ 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 $3 r-2(r-1+x)=6$, and $r=4+2 x$. 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 $|\partial G|+6 x=2 m=2 r-2+2 x=2(4+2 x)-2+2 x=6+6 x$. 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).

$G_{2}$

$G_{3}$


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 $|\partial G|=6, \partial G$ 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 $f_{0}^{\prime}, f_{1}^{\prime}, f_{2}^{\prime}, f_{3}^{\prime}$ be the hexagons marked in $F_{48}$ (see Figure 27), and let $M_{1}:=M_{0} \oplus f_{1} \oplus f_{2} \oplus f_{3}, M_{2}:=M_{0} \oplus f_{1}^{\prime} \oplus f_{2}^{\prime} \oplus f_{3}^{\prime}$ and $M_{3}:=M_{0} \oplus f_{1} \oplus f_{2} \oplus f_{3} \oplus f_{1}^{\prime} \oplus f_{2}^{\prime} \oplus f_{3}^{\prime}$. Let $\mathcal{H}$ be any set of mutually disjoint hexagons of $F_{48}$. If $h_{0}, h_{0}^{\prime} \notin \mathcal{H}$, then every hexagon of $\mathcal{H}$ is $M_{0}$-alternating. If $h_{0}^{\prime} \notin \mathcal{H}$ but $h_{0} \in \mathcal{H}$, then every hexagon of $\mathcal{H}$ is $M_{1}$-alternating. If $h_{0} \notin \mathcal{H}$ but $h_{0}^{\prime} \in \mathcal{H}$, then every hexagon of $\mathcal{H}$ is $M_{2}$-alternating. If $\left\{h_{0}, h_{0}^{\prime}\right\} \subseteq \mathcal{H}$, then $\mathcal{H}=\left\{h_{0}, h_{0}^{\prime}\right\}$ and both $h_{0}$ and $h_{0}^{\prime}$ are $M_{3}$-alternating. Thus $F_{48}$ is $k$-resonant for $k \geq 3$.

Summarizing the above results (Lemmas 5.175.6), 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 $k \geq 1$.

From Theorem 5.7, we arrive immediately at the 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:

$$
\begin{equation*}
B_{G}(x)=\sum_{i=0}^{C(G)} \sigma(G, i) x^{i} \tag{7}
\end{equation*}
$$

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 $\mathrm{C}_{60}$ is computed [24] as

$$
\begin{equation*}
B_{\mathrm{C} 60}(x)=5 x^{8}+320 x^{7}+1240 x^{6}+1912 x^{5}+1510 x^{4}+660 x^{3}+160 x^{2}+20 x+1 . \tag{8}
\end{equation*}
$$

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.

$$
\begin{align*}
& B_{F_{20}}(x)=1 \\
& B_{F_{24}}(x)=(x+1)^{2}=x^{2}+2 x+1, \\
& B_{F_{28}}(x)=(2 x+1)^{2}=4 x^{2}+4 x+1, \\
& B_{F_{32}}(x)=(3 x+1)^{2}=9 x^{2}+6 x+1, \\
& B_{F_{36}}(x)=2 x^{4}+16 x^{3}+20 x^{2}+8 x+1,  \tag{9}\\
& B_{F_{36}^{2}}(x)=\left(x^{2}+4 x+1\right)^{2}=x^{4}+8 x^{3}+18 x^{2}+8 x+1, \\
& B_{F_{40}}(x)=\left(5 x^{2}+5 x+1\right)^{2}=25 x^{4}+50 x^{3}+35 x^{2}+10 x+1, \text { and } \\
& B_{F_{48}}(x)=\left(2 x^{3}+9 x^{2}+7 x+1\right)^{2}=4 x^{6}+36 x^{5}+109 x^{4}+130 x^{3}+67 x^{2}+14 x+1 .
\end{align*}
$$

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