2-resonance of plane bipartite graphs and its applications to boron–nitrogen fullerenes

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A set \( \mathcal{H} \) of disjoint faces of a plane bipartite graph \( G \) is a resonant pattern if \( G \) has a perfect matching \( M \) such that the boundary of each face in \( \mathcal{H} \) is an \( M \)-alternating cycle. An elementary result was obtained [Discrete Appl. Math. 105 (2000) 291–311]: a plane bipartite graph is 1-extendable if and only if every face forms a resonant pattern. In this paper we show that for a 2-extendable plane bipartite graph, any pair of disjoint faces form a resonant pattern, and the converse does not necessarily hold. As an application, we show that all boron–nitrogen (B–N) fullerene graphs are 2-resonant, and construct all the 3-resonant B–N fullerene graphs, which are all \( k \)-resonant for any positive integer \( k \). Here a B–N fullerene graph is a plane cubic graph with only square and hexagonal faces, and a B–N fullerene graph is \( k \)-resonant if any \( i \) (\( 0 \leq i \leq k \)) disjoint faces form a resonant pattern. Finally, the cell polynomials of 3-resonant B–N fullerene graphs are computed.

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1. Introduction

Let \( G \) be a graph with vertex set \( V(G) \) and edge set \( E(G) \). A set of edges \( M \) of \( G \) is a matching if no two edges of \( M \) have a common vertex. Furthermore, a matching \( M \) is perfect if each vertex of \( G \) is incident with an edge of \( M \). A connected graph \( G \) is \( n \)-extendable (|\( V(G) \)| > \( 2n + 2 \)) if any matching of \( n \) edges is contained in a perfect matching of \( G \). The concept for \( n \)-extendable graphs was introduced by Plummer [16,15]. It is well-known that an \( n \)-extendable graph is \((n + 1)\)-connected and \((n − 1)\)-extendable for \( n \geq 1 \).

For a plane graph \( G \) with a perfect matching \( M \), a cycle \( C \) of \( G \) is said to be \( M \)-alternating (or \( M \)-conjugated) if the edges of \( C \) appear alternately in and off \( M \). A face \( F \) of \( G \) is \( M \)-resonant if its boundary is an \( M \)-alternating cycle. We also say \( F \) is resonant in \( G \). A set \( \mathcal{H} \) of disjoint faces of \( G \) is a resonant pattern if \( G \) has a perfect matching \( M \) such that the faces in \( \mathcal{H} \) are all \( M \)-resonant.

The resonance of faces of a plane bipartite graph is closely related to 1-extendable property. It was revealed that [33] each face (including the infinite one) of a plane bipartite graph \( G \) is resonant if and only if \( G \) is 1-extendable. For the case of benzenoids and coronoids, please see [30,34]. In this paper we mainly obtain that if a plane bipartite graph \( G \) is 2-extendable, then any two disjoint faces of \( G \) form a resonant pattern. This main result will be proved in Section 2. However, the converse does not hold in general. For plane bipartite graphs, this result has no further generalizations since no planar graphs are 3-extendable [17]. By applying this result, we present a complete characterization for \( k \)-resonance of boron–nitrogen fullerenes (or B–N fullerene graphs). B–N fullerene graphs are cubic plane graphs with only square and hexagonal faces. By a simple calculation using Euler’s formula [28], we have that there are exactly 6 square faces and others hexagonal. A B–N fullerene graph \( B \) is \( k \)-resonant (\( k ≥ 1 \)) if any \( i \) (\( 0 ≤ i ≤ k \)) disjoint faces of \( B \) form a resonant pattern.

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Ever since B–N nanotubes was first synthesized in 1995 [2], the structural properties and isomer stabilities of B–N nanotubes and B–N fullerenes were investigated from both chemical and mathematical points of view [5,14,23,24,27]. The concept of resonance originates from Clar’s aromatic sextet theory [3] and Randić’s conjugated circuit model. For interested readers, please see also [18–22]. The k-resonance was first proposed by Zheng [35] for benzenoid systems. Then the k-resonance of many other molecular graphs were investigated extensively [6,12,13,25,26,29,31,35]. But 2-resonance for benzenoid systems, open-ended nanotubes and carbon fullerenes remains open.

Here is a natural motivation for us to consider the k-resonance of B–N fullerene graphs. Doslić showed that the cyclic edge connectivity of a B–N fullerene graph is 3 or 4. In Section 3 of this paper we show that a B–N fullerene graph with the cyclic edge connectivity 3, a B–N nanotube, is k-resonant for any positive integer k. Then we show that a B–N fullerene graph with the cyclic edge connectivity 4 is 2-extendable, and thus it is 2-resonant by our previous main result. In short we have that every B–N fullerene graph is 2-resonant. This is an unexpected result. Furthermore, we construct all the five 3-resonant B–N fullerene graphs in addition to B–N nanotubes. Like benzenoid systems [35], coronoid systems [1], open-end nanotubes [31], toroidal polyhexes [25,32], Klein-bottle polyhexes [26] and fullerene graphs [29], we also show that the 3-resonant B–N fullerene graphs are also k-resonant for any k ≥ 3. Hence, any set of disjoint faces of them form a resonant pattern. In the fourth section, we compute the cell polynomials of 3-resonant B–N fullerene graphs.

2. Face resonance of 2-extendable plane bipartite graphs

The following theorem establishes a relation between 1-extendability and face resonance for plane bipartite graphs.

**Theorem 2.1** ([33]). Let G be a plane bipartite graph. Then each face of G is resonant if and only if G is 1-extendable.

For n-extendable graphs, Plummer showed that

**Theorem 2.2** ([16]). If G is an n-extendable graph, then G is also (n − 1)-extendable.

Let M1 and M2 be two matchings of a graph G. The symmetric difference of M1 and M2 is defined as M1 ⊕ M2 := (M1 ∪ M2) \ (M1 ∩ M2). If M1 and M2 are two perfect matchings of G, then M1 ⊕ M2 is the union of disjoint cycles. M1-edge means an edge that belongs to M1. Let P be a path of G and a, b be two vertices of P. We denote the subpath of P from a to b by aPb. The following lemma is implicated in the proof of Theorem 2.1 in [33]. We outline it again for convenience.

**Lemma 2.3.** Let G be a plane bipartite graph with a perfect matching M. Let F be any facial cycle of G with a perfect matching I. If e ∈ I \ M, then each M-alternating cycle containing e does not contain any edge of I ∩ M.

**Proof.** Label counterclockwise the vertices of F by v1, v2, ..., v2n. Color properly the vertices of G with white and black such that v2i+1 is black and v2(i+1) is white for 0 ≤ i ≤ n − 1. Suppose that I := {v1v2, v3v4, ..., v2n−1v2n} and e = v1v2 ∈ I \ M. Let C be an M-alternating cycle containing e. We assert that C does not pass through any edge of I ∩ M. Otherwise, let e′ = v2i−1v2i (i ≥ 2) be the first edge entering I ∩ M when traversing C from v1 to v2 through e. Since F bounds a face, along M-alternating cycle C we must first enter v2i−1 and then reach v2i through e′. Let P(v2, v2i−1) be a path of C from v2 to v2i−1. Then P(v2, v2i−1) is an M-alternating path starting at an edge in M and ending at an edge off M. Thus P is of even length, and its two ends v2 and v2i−1 should have the same color. That is impossible. □

Then we state our main result as follows, which gives a sufficient condition for 2-resonance of plane bipartite graphs.

**Theorem 2.4.** If G is a 2-extendable plane bipartite graph, then any pair of disjoint faces of G form a resonant pattern.

**Proof.** Let G be a 2-extendable plane bipartite graph. For any two disjoint faces f1 and f2 of G, we want to show that there is a perfect matching M in G such that both F1 and F2 are M-alternating cycles, where F1 and F2 denote the boundaries of f1 and f2 respectively.

Label counterclockwise the vertices of F1 by v1, v2, ..., v2n, where 2n = |V(F2)|. Color properly the vertices of G with white and black such that v2i+1 is black and v2(i+1) is white for 0 ≤ i ≤ n − 1. Then I := {v1v2, v3v4, ..., v2n−1v2n} is a perfect matching of F2. By Theorems 2.1 and 2.2, F1 is resonant. Choose a perfect matching M0 of G such that F1 is M0-alternating and M0 contains as many edges of I as possible. Let I1 = I ∩ M0. If I1 = I, then both F1 and F2 are M0-alternating, and we are done. Hence it suffices to show that I1 = I.

Without loss of generality, suppose both f1 and f2 are finite faces and F1 is improperly M0-alternating cycle, i.e. each M0-edge in F1 goes counterclockwise from white end-vertex to black end-vertex along F1.

Suppose on the contrary that I1 = I and e1 = v1v2 ∉ I1. For a cycle C of G passing through edge e1, let C(s, t) denote the path on C from s to t along the direction of C from v2 to v1 through e1, where s and t are two vertices of C. Then we have the following claim.

**Claim 1.** For any M0-alternating cycle C containing e1, E(C) ∩ E(F1) ≠ ∅.

**Proof.** Suppose to the contrary that E(C) ∩ E(F1) = ∅ for some M0-alternating cycle C containing e1. By Lemma 2.3, E(C) ∩ I1 = ∅. Then M0 ⊕ C, a perfect matching of G still alternating on F1, has at least one more edge in I than M0. This is a contradiction to the choice of M0. □
By Theorem 2.2, G is also 1-extendable. Then G has a perfect matching, say $M_1$, such that $e_1 \in M_1$. Since $e_1 \not\in M_0$, let $C_1$ be a cycle in the symmetric difference $M_0 \oplus M_1$ containing $e_1$. Then $C_1$ is an $M_0$ and $M_1$-alternating cycle. By Claim 1, $E(C_1) \cap E(F_1) \neq \emptyset$.

Let $v$ be the first vertex entering $F_1$ when traversing $C_1$ from $v_1$ to $v_2$ through $e_1$ and $u$ the one when traversing $C_1$ from $v_1$ in the opposite direction (see Fig. 1). Let $P_{v, v_2} := C_1(v, v_2)$ and $P_{v_1, u} := C_1(v_1, u)$. Since $P_{v, v_2}$ is an $M_1$ and $M_0$-alternating path starting at an edge in $M_1$ and ending at an edge in $M_0$, $P_{v, v_2}$ is of even length. Thus $v$ is white (the same color with $v_2$). Similarly, $u$ is black (the same color with $v_1$). Let $P_{u, v}$ be the path on $F_1$ from $u$ to $v$ along the clockwise direction of $F_1$. Then $C_1 \cap F_1 \subseteq P_{u, v}$.

Choose such a perfect matching $M_1$ of $G$ containing $e_1$, such that $P_{u, v}$ is shortest. Without loss of generality, suppose that both $f_1$ and $f_2$ lie in the exterior of $C_1$ (see Fig. 1).

Let $e_2 = uv'$ be an end edge of $P_{u, v}$. Then $e_2 \in M_0$. Since $G$ is 2-extendable, it has a perfect matching containing both $e_1$ and $e_2$. Then $e_1$ belongs to the symmetric difference of $M_0$ and any of such perfect matchings but $e_2$ does not. Let $M_2$ be a perfect matching containing $e_1$ and $e_2$, such that the cycle, denoted by $C_2$, in $M_0 \oplus M_2$ containing $e_1$ intersects $F_1$ in at least one edge as possible. By Claim 1, $E(C_2) \cap E(F_1) \neq \emptyset$.

Similarly, let $w$ be the first vertex entering $F_1$ when traversing $C_2$ from $v_1$ to $v_2$ through $e_1$ and $y$ the one when traversing $C_2$ from $v_1$ in the opposite direction. As before, $y$ is black and $w$ is white. Let $P_{y, w}$ be the path on $F_1$ from $y$ to $w$ along the clockwise direction. Then $C_2 \cap F_1 \subseteq P_{y, w}$. We have the following claim.

**Claim 2.** $y, w \in V(P_{u, v})$.

**Proof.** Suppose on the contrary that $y \not\in V(P_{u, v})$. We traverse $C_2$ from $v_2$ to $v_1$ through $e_2$, then let $x$ be the last vertex leaving $C_1$ before reaching $y$. Note that in this direction, each $M_0$-edge on $C_2$ goes from the black end-vertex to the white one, and each component of $C_1 \cap C_2$ is an $M_0$-alternating path from black vertex to white one. Hence $x$ is white. Since $y \not\in V(P_{u, v})$, we must go outside $C_1$ to reach $y$. Hence $x$ lies either on $P_{v_1, u}$ or on $P_{v_2, v}$.

**Case 1.** $x \in V(P_{v_1, u})$ (see Fig. 1(a)).

Since $y$ is black, the $M_0$-edge incident to $y$ lies on the $y - u$ path on $F_1$ along the clockwise direction. On the other hand, $M_0$-alternating cycles cannot intersect themselves. Thus we must enter $xP_{v_1, u}u$ in order to reach $v_2$ from $y$. Hence, $C_2$ intersects $C_1$ at some other vertices on $xP_{v_1, u}u$ before reaching $v_2$. Let $x'$ be such a vertex that is nearest to $x$ on $xP_{v_1, u}u$. Then $x'$ is black and thus is an entering vertex of $C_1$ while traversing. Then $xP_{v_1, u}x'$ and $C_2(x, x')$ form a cycle $C_0$, which does not contain $e_1$.

Let $M'_2 := M_0 \oplus E(C_2) \oplus E(C_0)$. Since $C_2$ is an $M_0$ and $M_2$-alternating cycle, $M_0 \oplus E(C_2)$ is a perfect matching of $G$ and $C_2(x, x')$ is an $M_0 \oplus E(C_2)$-alternating path for which its end-edges belong to $M_0 \oplus E(C_2)$. Since $xP_{v_1, u}x'$ intersects $C_2$ only at its end-vertices, it is an $M_0 \oplus E(C_2)$-alternating path for which both of its end-edges are not in $M_0 \oplus E(C_2)$. Hence $C_0$ is an $M_0 \oplus E(C_2)$-alternating matching of $G$.

Then $\{e_1, e_2\} \subseteq M'_2$. Further $M'_2 \oplus M_0 = E(C_2) \oplus E(C_0)$ forms the edge set of a cycle $C'_2$, obtained from $C_2$ by replacing $C_2(x, x')$ with $xP_{v_1, u}x'$. Then $e_1 \in E(C'_2)$. Since $E(C_2(x, x')) \cap E(F_1) \neq \emptyset$ and $E(xP_{v_1, u}x') \cap E(F_1) = \emptyset$, $C'_2$ has at least one less edge of $F_1$ than $C_2$. This contradicts the choice of $M_2$.

**Case 2.** $x \in V(P_{v_2, v})$ (see Fig. 1(b)).

In this case, we must enter $xP_{v_2, v}v_2$ in order to reach $v_2$ from $y$ while traversing $C_2$ in the specific direction. Like before, let $x'$ (black) be the nearest entering vertex to $x$ on $xP_{v_2, v}v_2$ before reaching $v_2$ from $y$. Then, by the same argument as in Case 1, $xP_{v_2, v}x'$ and $C_2(x, x')$ form a cycle $C_0$ and $M_0 \oplus E(C_2)$ is a perfect matching of $G$ such that $C_0$ is $M_0 \oplus E(C_2)$-alternating. Then $M'_2 := M_0 \oplus E(C_2) \oplus E(C_0)$ is a perfect matching of $G$ and $\{e_1, e_2\} \subseteq M'_2$. Hence $M'_2 \oplus M_0 = E(C_2) \oplus E(C_0)$ forms the edge set of a cycle $C'_2$, obtained from $C_2$ by replacing $C_2(x, x')$ with $xP_{v_2, v}x'$. Since $E(C_2(x, x')) \cap E(F_1) \neq \emptyset$ and $E(xP_{v_2, v}x') \cap E(F_1) = \emptyset$, $C'_2$ has at least one less edge of $F_1$ than $C_2$. This contradicts the choice of $M_2$. Thus $y \in V(P_{u, v})$. □
Every B–N fullerene graph is a 3-connected graph. Theorem 2.4 shows that $P_6$ is the cycle in bold and $C_6$ is obtained from $C_4$ by replacing $C_4(x, x')$ with $xP_{v_1,u}x'$. (Fig. 2)

Claim 3. $P_{y,w} \subset P_{u,v}$.

Proof. Since $y, w \in V(P_{u,v})$, either $P_{y,w} \subset P_{u,v}$ or $P'_{y,w} \subset P_{y,w}$, where $P'_{y,w}$ is the path on $F_1$ from $u$ to $v$ along the counterclockwise direction of $F_1$.

Suppose that $P'_{y,w} \subset P_{y,w}$. Then $w$ lies on $uP_{v_1,u}y$; see Fig. 2. We still traverse $C_2$ from $v_2$ to $v_1$ through $e_1$. It follows that the last vertex, say $x$, leaving $C_1$ before reaching $y$ must lie on $P_{v_1,u}$. Since $P'_{y,w} \subset P_{y,w}$, $C_2(y, w)$ must pass through $xP_{v_1,u}u$ in order to reach $w$ from $y$. Thus $C_2$ intersects $C_1$ at some other vertices on $xP_{v_1,u}$ besides $x$ before reaching $v_2$. Like before, let $x'$ be the nearest such one to $x$ on $xP_{v_1,u}$. Then $xP_{v_1,u}x'$ and $C_2(x, x')$ form a cycle $C_0$, and $M_0 \oplus E(C_2)$ is a perfect matching of $G$ such that $C_0$ is an $M_0 \oplus E(C_2)$-alternating cycle. Then $M_2 := M_0 \oplus E(C_2) \oplus E(C_0)$ is a perfect matching of $G$ and $\{e_1, e_2\} \subset M_2$. Hence $M' \oplus M_0 = E(C_2) \oplus E(C_0)$ forms the edge set of a cycle $C_2$ obtained from $C_2$ by replacing $C_2(x, x')$ with $xP_{v_1,u}x'$. Since $E(C_2(x, x')) \cap E(F_1) \neq \emptyset$ and $E(xP_{v_1,u}x') \cap E(F_1) = \emptyset$, $C_2$ has at least one less edge of $F_1$ than $C_2$. This contradicts the choice of $M_2$. Hence $P_{y,w} \subset P_{u,v}$. Since $e_2 \in E(P_{u,v})$ but $e_2 \notin E(P_{y,w})$, $P_{y,w} \subset P_{u,v}$. The proof of the Claim is finished. \phantom{x}

Claim 3 shows that $P_{y,w} \subset P_{u,v}$ for a perfect matching $M_2$ of $G$ containing $e_1$. This contradicts the choice of $M_1$. Hence $I_1 = I_2$. \phantom{x}

Note that the converse of the theorem does not hold. For example, two 3-connected plane bipartite graphs displayed in Fig. 3 are not 2-extendable, but any at most two disjoint faces form a resonant pattern.

3. 2-resonance of B–N fullerenes

As an application of Theorem 2.4, we consider the 2-resonance of B–N fullerene graphs in this section. First, we present some further information on B–N fullerene graphs.

A $(k, 6)$-cage is a 3-regular, 3-connected plane graph whose faces are only $k$-gons and hexagons. Recall that B–N fullerene graphs are 3-regular plane graphs whose faces are only squares and hexagons. We have the following relation.

Lemma 3.1. Every B–N fullerene graph is a $(4, 6)$-cage.

Proof. It suffices to show that each B–N fullerene graph is 3-connected. Since every face of a B–N fullerene graph is bounded by a cycle, it is 2-edge connected. Suppose on the contrary that a B–N fullerene graph $B$ is not 3-connected. Since each 3-regular graph has an equal vertex and edge-connectivity, $B$ has an edge-cut of size 2, which always consists of two disjoint edges. We choose an edge-cut of size 2, say $C = \{e_1, e_2\}$, such that one of the two components of $B - C$ does not contain any edge-cut with size two of $B$. Let $H_1$ be this component and $H_2$ the other component.

Fig. 3. Non-2-extendable 3-connected plane bipartite graphs any two disjoint faces of which form a resonant pattern: $\{e_1, e_2\}$ cannot be extended to a perfect matching.
Fig. 4. A (4,6)-cage $T_3$.

Let $C_1$ and $C_2$ be the boundaries of the faces of $H_1$ and $H_2$ that are not faces of $B$, respectively. Then there are exactly two vertices of degree 2 on each of $C_1$ and $C_2$ and the others of degree 3. Let $F_1$ and $F_2$ be the two faces of $B$ whose boundaries contain both $e_1$ and $e_2$, respectively. Then the total size of $F_1$ and $F_2$ equals $\|C_1\| + \|C_2\| + 4$, where $\|C_i\|$ denotes the length of $C_i$ for $i = 1, 2$. Since the size of $F_i$ $(i = 1, 2)$ is no more than 6, $\|C_1\| + \|C_2\| \leq 8$. Since $B$ is simple and bipartite, both $C_1$ and $C_2$ are cycles of length 4. Hence $\|C_1\| = \|C_2\| = 4$. Then the two edges from the two 3-degree vertices on $C_1$ to the other vertices of $H_1$ form an edge-cut with size two of $B$. This contradicts the choice of $C$ and $H_1$. Hence $B$ is 3-connected. □

A graph $G$ is cyclically $k$-edge connected if $G$ cannot be separated into two components, each of which contains a cycle, by deleting fewer than $k$ edges. Denote by $c\lambda_+(G)$ the largest integer $k$ such that $G$ is cyclically $k$-edge connected, and call this number the cyclical edge-connectivity of $G$.

Let $T_n$ denote the $(4, 6)$-cage consisting of $n$ concentric layers of hexagons, capped on each end by a cap formed by three squares (indicated in Fig. 4). Let $\mathcal{T} = \{T_n | n \geq 1\}$ be the family of all such $(4, 6)$-cages $T_n$.

Došlić [4] computed the cyclical edge-connectivity of $(4, 6)$-cages.

Lemma 3.2 ([4]). Let $G$ be a $(4, 6)$-cage. If $G \in \mathcal{T}$, then $c\lambda_+(G) = 3$; otherwise, $c\lambda_+(G) = 4$.

The following theorem due to Holton and Plummer implies the 2-extendability of cyclically 4-edge connected B–N fullerene graphs.

Theorem 3.3 ([8]). If $G$ is an $(n + 1)$-regular, $(n + 1)$-connected bipartite graph with cyclic connectivity at least $n^2$, then $G$ must be $n$-extendable.

Corollary 3.4. Cyclically 4-edge connected B–N fullerene graphs are 2-extendable.

Combining Theorem 2.4 and the above corollary, we have the following result.

Corollary 3.5. Cyclically 4-edge connected B–N fullerene graphs are 2-resonant.

Now we turn to the $k$-resonance of B–N fullerene graphs in $\mathcal{T}$.

We define some notations for $T_n$ $(n \geq 1)$ first. Let $H_0$, $H_1$, \ldots, $H_{n+1}$ be all the layers of $T_n$, where $H_0$ and $H_{n+1}$ are its two caps and hexagonal layer $H_i$ is adjacent to $H_{i-1}$ and $H_{i+1}$ for $1 \leq i \leq n$. For $1 \leq i \leq n + 1$, we set $L_i := H_{i-1} \cap H_i$. Then $L_0$ and $L_{n+2}$ denote the common vertices of the squares of $H_0$ and $H_{n+1}$, respectively; and $L_1$ is a cycle of length 6, $1 \leq i \leq n + 1$. Note that $H_i$ $(0 \leq i \leq n + 1)$ has three pairwise adjacent faces, each of which is adjacent to two faces in every adjacent layer of $H_i$. Then we label the faces of $T_n$ as follows: Give the labels $h_0^1$, $h_0^2$, $h_0^3$ to the three squares of $H_0$ arbitrarily. Suppose that the labels of the faces in $H_0, \ldots, H_i(i \geq 0)$ are given. Then label the only face of $H_{i+1}$ not adjacent to $h_j^i$ with $h_{i+1}^j$ for $j = 1, 2, 3$.

Lemma 3.6. Every $T_n$ $(n \geq 1)$ in $\mathcal{T}$ is $k$-resonant for any $k \geq 1$.

Proof. It suffices to show that $T_n - F$ has a perfect matching for any given set of disjoint faces $F$ of $T_n$. Then we claim that for each $0 \leq i \leq n$, there is a matching $M_i$ of $T_n - F$ such that for each $0 \leq j \leq i$, each vertex of $L_j$ is covered either by $F$ or by $M_i$ and either one of $h_1^j, h_2^j$ and $h_3^j$ belongs to $F$ or a unique vertex of $L_j$ matches to a vertex of $L_{j+1}$ in $M_i$. We use induction on $i$ to prove the claim. Note that at most one face of $H_i$ belongs to $F$ for $0 \leq i \leq n + 1$.

For the 0th step, if one of $h_0^1$, $h_0^2$ and $h_0^3$ belongs to $F$, then $M_0 := \emptyset$ satisfies the claim; see Fig. 5(a). Otherwise, at least one neighbor of $L_0$ on $L_1$ is not in $V(F)$. Let $e$ be the edge connecting $L_0$ and this neighbor. Then $M_0 := \{e\}$ satisfies the claim.

Suppose the claim is true for $i$, $0 \leq i \leq n$ and $M_i$ has been already constructed by the inductive procedure. We consider the case $i + 1$. By the induction hypothesis, two cases are distinguished.
Case 1. One of $h_1^i$, $h_2^i$, and $h_3^i$, say $h_1^i$, belongs to $F$ (see Fig. 5).

Then the three vertices on $L_{i+1}$ belong to $h_1^i$ are covered by $F$ and the other three vertices form a path $u s t$, which lie on $h_1^i$. If $h_1^i$ belongs to $F$, then $M_{i+1} := M_i$ satisfies the claim; see Fig. 5(a). Otherwise, let $e_1$ denote the edge connecting $u$ to its neighbor on $L_{i+2}$ and $e_2 := st$ since one of the end-vertices $u$ and $t$, say $u$, has the neighbor in $L_{i+2}$ uncovered by $F$. Then $M_{i+1} := M_i \cup \{e_1, e_2\}$ satisfies the claim; see Fig. 5(b).

Case 2. $h_1^i$, $h_2^i$, and $h_3^i$ are not in $F$ and $v_i v_{i+1} \in M_n$, where $v_i \in V(L_i)$, $v_{i+1} \in V(L_{i+1})$ (see Fig. 6).

If one face of $H_{i+1}$, say $h_1^i$, whose boundary does not contain $v_{i+1}$, belongs to $F$, then there are two adjacent vertices on $L_{i+1}$, named $w_1$ and $w_2$, uncovered by $F$ and $M_i$. Then $M_{i+1} := M_i \cup \{w_1 w_2\}$ satisfies the claim; see Fig. 6(a). Otherwise, $L_{i+1} - v_{i+1}$ is a 4-length path $w_1 - w_2 - \cdots - w_5$, each vertex of which is not covered by $F$ and $M_i$. Let $w_1'$ and $w_5'$ be the neighbors of $w_1$ and $w_5$ on $L_{i+2}$, respectively. At least one of them, say $w_1'$, does not belong to $V(F)$. Then $M_{i+1} := M_i \cup \{w_1 w_1', w_2 w_3, w_4 w_5\}$ satisfies the claim; see Fig. 6(b).

Hence the claim holds. Further the claim implies that $M_{i+1}$ is a perfect matching of $T_n - F$. Hence, $T_n$ is $k$-resonant for any $k \geq 1$. □

Combining Corollary 3.5 and Lemma 3.6, we have a main result as follows.

**Theorem 3.7.** Every B–N fullerene graph is 2-resonant.
Let $G$ be a 2-connected 3-regular plane bipartite graph. If all the vertices of $G$ are covered by a set of disjoint faces of size 4, then $G$ is $k$-resonant for any $k \geq 1$.

**Proof.** It suffices to show that for any given set $S$ of disjoint faces of $G$, $G - S$ has a perfect matching. Let $R$ be a set of disjoint faces of size 4 of $G$ that covers all the vertices of $G$. Let $S':=\{f \in R: \text{ either } f \in S \text{ or } f \text{ is adjacent to some faces of } S\}$. Then $S' \subseteq R$ and each face in $R \setminus S'$ is disjoint from every face in $S$. Hence $G - S'$ has a perfect matching $M$. Since each face of $R$ adjacent to faces of $S$ shares one or two disjoint edges with them, $S' - S$ is a set of disjoint edges, denoted by $M'$. Since $V(S) \subseteq V(S')$, $M \cup M'$ is a perfect matching of $G - S$. □

**Lemma 4.2.** Let $G$ be a 3-regular plane graph. If $G$ is cyclically 4-edge connected, then there are no three faces which are pairwise adjacent but do not share a common vertex, nor two faces which share more than one disjoint edges in $G$.

**Proof.** If the conditions of the lemma hold, $G$ always has a cyclical edge cut with size less than 4 (for example, see Fig. 7). □

**Example 4.3.** Let $B$ be a cyclically 4-edge connected $B-N$ fullerene graph. If $B$ is $k$-resonant ($k \geq 3$), then each vertex of $B$ lies on a square and thus $|V(B)| \leq 24$.

**Proof.** Let $B$ be a cyclically 4-edge connected $B-N$ fullerene graph that is $k$-resonant for integer $k \geq 3$. Suppose on the contrary that there is a vertex $v$ of $B$ that does not lie on any square. Let $v_1$, $v_2$ and $v_3$ be the three neighbors of $v$. Let $e_i = v v_i$ and $f_i$, $i = 1, 2, 3$, denote the face of $B$ whose boundary contains the edges in $\{e_1, e_2, e_3\} \setminus \{e_i\}$. By the hypothesis, $f_1$, $f_2$ and $f_3$ are hexagons.

Let $h_1$, $h_2$ and $h_3$ be other faces different from $f_1$, $f_2$ and $f_3$ such that $v_1$ lies on the boundary of $h_i$ for $i = 1, 2, 3$ (see Fig. 8). Then by Lemma 4.2 (a) and (b), $h_1$, $h_2$ and $h_3$ are mutually disjoint and distinct.

Then $B - (h_1 \cup h_2 \cup h_3)$ leaves an isolated vertex $v$. This contradicts the 3-resonance of $B$. Hence, each vertex of $B$ is covered by a square. There are six faces of size 4 in $B$. Hence, $|V(B)| \leq 24$. □

A fragment $H$ of a $B-N$ fullerene graph $B$ is a subgraph of $B$ consisting of a cycle $C$ together with its interiors (or exteriors). A fragment $H$ of $B$ is said to be a square fragment if every face inside $C$ (or outside $C$) is a square. The size of a square fragment $H$ is the number of squares of $H$ inside $C$ (or outside $C$). A face of $B$ adjacent to $H$ but not in $H$ is called a neighboring face of $H$. Let $H$ be a square fragment. We call $H$ a maximal square fragment if all its neighboring faces are hexagonal.

**Theorem 4.4.** A cyclically 4-edge connected $B-N$ fullerene graph $B$ is $k$-resonant ($k \geq 3$) if and only if $B$ is one of $B_1, B_2, B_3, B_4$ and $B_5$ in Fig. 9.
Theorem 4.4

Let $B$ be a $k$-resonant ($k \geq 3$) B–N fullerene graph. If $B$ has three squares $f_1$, $f_2$ and $f_3$ that are pairwise adjacent and share a vertex (see Fig. 10), then we can show that $B$ is isomorphic to the cube, $B_3$. Let $H$ be a subgraph of $B$ consisting of squares $f_1$, $f_2$ and $f_3$, and let $e_1$, $e_2$ and $e_3$ be the three edges going out $H$. Since $B$ is 3-regular, $|V(B)|$ is even. Furthermore both $H$ and $B - H$ have an odd number of vertices. Suppose that $|V(B - H)|$ is no less than three, then $|E(B - H)| = \frac{3|V(B - H)| - 3}{2} \geq |V(B - H)|$. Hence $B - H$ has a cycle. This implies that $\{e_1, e_2, e_3\}$ is a cyclical 3-edge cut, contradicting that $B$ is cyclically 4-edge connected. Hence $B - H$ contains exactly one vertex and $e_1$, $e_2$ and $e_3$ are incident to the same vertex outside $H$. Thus $B$ is the cube $B_3$ (see Fig. 9). If $B$ has a closed square chain $H \cong C_{2n} \times K_2$, then $n$ is 2 or 3. For the former, $B$ is the cube; for the latter, $B$ is isomorphic to $B_5$ (see Fig. 9). Conversely, since two disjoint squares of a cube cover all the vertices and three disjoint squares of $B_5$ cover all the vertices, by Lemma 4.1 $B_3$ and $B_5$ are $k$-resonant for any $k \geq 1$.

For all other cases, each square of $B$ is contained in a maximal square fragment that is an open square chain $(P_n \times K_2)$. Let $v_1, v_2, v_3, v_4$ be the four 2-degree vertices on a maximal square fragment $H$. We distinguish five cases to consider.

Case 1. Each maximal square fragment of $B$ has size 1. Then by Lemma 4.3 all the vertices of $B$ are covered by a set of disjoint squares.

Let $v_1, v_2, v_3$ and $v_4$ be the four vertices of a square $f_i$ of $B$ and $w_i$ be the neighbor of $v_i$ out of $f_i$ for $i = 1, 2, 3, 4$. Then the four faces $h_1, h_2, h_3$ and $h_4$ adjacent to $f_i$ are all hexagons. By Lemma 4.2, $h_1$ and $h_3$ are disjoint and so do $h_2$ and $h_4$. Then $w_1, w_2, w_3$ and $w_4$ are covered by four other squares, say $f_2, f_3, f_4$ and $f_5$ (see Fig. 10). Then the four vertices on $f_2, f_3, f_4$ and $f_5$ but not on $h_1, h_2, h_3$ or $h_4$ have their third neighbors, say $w'_2, w'_3, w'_4$ and $w'_5$. Since $h_5, h_6, h_7$ and $h_8$ are hexagons, $B$ is isomorphic to $B_1$ (see Fig. 11). Conversely, by Lemma 4.1, $B_1$ is $k$-resonant for all $k \geq 3$.

Case 2. $H$ has size 2.

Let $f_1$ and $f_2$ be the two squares of $H$ (see Fig. 12). Then for each $i (1 \leq i \leq 4)$, let $w_i$ be the neighbor of $v_i$ out of $H$. Then faces $h_1, h_2, h_3$ and $h_4$ around $H$ are all hexagons since $H$ is maximal. By Lemma 4.2, $h_1$ and $h_3$ are distinct and disjoint and so do $h_2$ and $h_4$.

Let $u_1$ be the common neighbor of $w_1$ and $w_2$ and $u_2$ the common neighbor of $w_3$ and $w_4$. Then $w_1$ and $w_2$ are covered by two other squares, respectively, say $f_3$ and $f_4$, which share an edge incident to $u_1$. Similarly, the two squares $f_5$ and $f_6$ covering $w_3$ and $w_4$, respectively, share an edge incident to $u_2$. Thus $B$ is isomorphic to $B_2$. One can verify that $B_2$ is $k$-resonant for each $k \geq 3$. 

Proof. Let $B$ be a $k$-resonant ($k \geq 3$) B–N fullerene graph.
Case 3. $H$ has size 3.

Let $H$ have three squares $f_1, f_2, f_3$ such that $f_i$ and $f_j$ ($1 \leq i < j \leq 3$) are adjacent if and only if $j = i + 1$. Let $w_i$ be the third neighbor of $v_i$ for $i = 1, 2, 3, 4$ (see Fig. 13). Since the four neighboring faces of $H$ are all hexagons, $w_1$ is adjacent to $w_2$ and $w_3$ to $w_4$. Since $w_i$ ($i = 1, 2, 3, 4$) are covered by other squares, $B$ is isomorphic to $B_4$. Conversely, $B_4$ has 4 disjoint squares covering all the vertices of $B_4$. Hence it is $k$-resonant for any $k \geq 3$.

Case 4. $H$ has size four.

Let $H$ be a square chain with four squares $f_1, f_2, f_3$ and $f_4$ (see Fig. 14). Then $v_1$ and $v_2$ have the same neighbor $w_1$, and $v_3$ and $v_4$ have the same neighbor $w_2$. Since the face with the path $w_1v_1v_4w_2$ in its boundary is a hexagon, $w_1$ is not adjacent to $w_2$. Hence $\{w_1, w_2\}$ is a cut set of size 2, contradicting the 3-connectedness of $B$–N fullerene graphs.

Case 5. $H$ has size five or six.
If $H$ consists of five squares (see Fig. 15 (left)), then $v_1$ is adjacent to $v_2$ and $v_3$ to $v_4$. Hence $H$ is not a maximal square fragment. This is a contradiction. If $H$ consists of six squares (see Fig. 15 (right)), then the neighboring face $h'$ of $H$ containing $v_1$ and $v_2$ has size more than six. It is impossible. □

By Lemma 3.6 and Theorem 4.4, the $k$-resonance ($k \geq 3$) of B–N fullerene graphs can be characterized as follows:

**Theorem 4.5.** A B–N fullerene graph $B$ is $k$-resonant ($k \geq 3$) if and only if $B \in \mathcal{T}$ or $B$ is one of $B_1, B_2, B_3, B_4, B_5$.

**Corollary 4.6.** A B–N fullerene graph is $k$-resonant ($k \geq 3$) if and only if it is 3-resonant.

## 5. Cell polynomials of 3-resonant B–N fullerene graphs

The cell polynomial (also known as the “resonant ring polynomial” or “R-polynomial”) proposed by Gutman and John [7,10,11] for counting resonant patterns of polycyclic conjugated hydrocarbon extends Hosoya and Yamaguchi’s sextet polynomial [9]. The cell polynomial of a B–N fullerene graph $B$ can be expressed as

$$\rho(B; x, y) = \sum_{0 \leq i < C_1, 0 \leq j < C_2} r(B; i, j)x^iy^j,$$

where $r(B; i, j)$ denotes the number of resonant patterns of $B$ with $i$ squares and $j$ hexagons, and $C_1$ (resp. $C_2$) is the maximum number of squares (resp. hexagons) in all the resonant patterns.

As we have shown, any set of disjoint faces of a 3-resonant B–N fullerene graph form a resonant pattern. The cell polynomials of the five B–N fullerene graphs $B_1$ to $B_5$ in Theorem 4.4 are computed as follows.

$$\rho(B_1; x, y) = x^6 + 6x^5 + 15x^4 + 8x^3y^2 + 20x^3y + 20x^2y + 24xy + 12x^2 + 12xy + 8y^3 + 15x^2 + 24xy + 16y^2 + 6x + 8y + 1;$$

$$\rho(B_2; x, y) = 2x^3y + 3x^3 + 6x^2y + y^3 + 12x^2 + 12xy + 4y^2 + 6x + 5y + 1;$$

$$\rho(B_3; x, y) = 3x^2 + 6x + 1;$$

$$\rho(B_4; x, y) = x^4 + 4x^3 + 2xy^2 + 11x^2 + 8xy + 2y^2 + 6x + 4y + 1;$$

$$\rho(B_5; x, y) = 2x^3 + 9x^2 + y^2 + 6 + 2y + 1.$$

Then we compute the cell polynomial for $T_n$ ($n \geq 1$) by the transferred matrix method. Since $T_0 \cong B_3$,

$$\rho(T_0; x, y) = 3x^2 + 6x + 1.$$

Remember that in $T_n$, $H_0$ is one of the cap consisting of three pairwise adjacent squares and $H_1$ is the hexagon layer adjacent to $H_0$. In $\rho(T_n; x, y)$, we denote the part of the polynomial, corresponding to the resonant patterns that contain none of the faces of $H_0$ or $H_1$, by $a_{00}^n$; the part corresponding to the resonant patterns that contain one face of $H_0$ but none of $H_1$ by $a_{10}^n$, the part corresponding to the resonant patterns that contain none of the faces of $H_0$ but one of $H_1$ by $a_{01}^n$; and the part corresponding to the resonant patterns that contain one face of $H_0$ and one of $H_1$ by $a_{11}^n$. Then

$$\rho(T_n; x, y) = a_{00}^n + a_{10}^n + a_{01}^n + a_{11}^n.$$

For example, in $\rho(T_0; x, y)$, $a_{00}^0 = 1$, $a_{10}^0 = 3x$, $a_{01}^0 = 3x$, $a_{11}^0 = 3x^2$.

Note that for a given face $f$ of $H_1$ in $T_n$, $H_{i+1}$ (or $H_{i-1}$) has only one face disjoint from $f$. Hence, if one face of $H_1$ belongs to a resonant pattern $F$ in $T_n$ and there is a face of $H_{i+1}$ (or $H_{i-1}$) also belongs to $F$, then the face of $H_{i+1}$ (or $H_{i-1}$) belonging to $F$ is uniquely determined by the one in $H_1$.

Moreover, $T_{n+1}$ ($n \geq 0$) can be viewed as the graph obtained from $T_n$ by extending a layer of hexagons between $H_0$ and $H_1$ in it. Hence, $a_{00}^n$ can be deduced from $a_{00}^0$ and $a_{01}^0$ as

$$a_{00}^1 = a_{00}^0 + a_{01}^0.$$

And similarly, $a_{10}^1$, $a_{01}^1$, and $a_{11}^1$ can be deduced as follows:

$$a_{01}^1 = 3a_{00}^0y + a_{01}^0y; \quad a_{10}^1 = a_{10}^0 + 3a_{11}^0; \quad a_{11}^1 = a_{10}^0y + a_{11}^0y.$$

Fig. 15. The illustration for Case 5 in the proof of Theorem 4.4.
that is, \((a_{00}, a_{01}, a_{10}, a_{11}) = (a_{00}^0, a_{01}^0, a_{10}^0, a_{11}^0)T\), where

\[
T = \begin{bmatrix} 1 & 3y & 0 & 0 \\ 1 & y & 0 & 0 \\ 0 & 0 & 1 & y \\ 0 & 0 & 3 & y \end{bmatrix}.
\]

Set \(A_0 = (a_{00}^0, a_{01}^0, a_{10}^0, a_{11}^0) = (1, 3x, 3x, 3x^2)\). Then

\[\rho(T_1; x, y) = a_{10}^0 + a_{01}^0 + a_{10}^1 + a_{11}^1 = A_0 TL,\]

where \(L = (1, 1, 1, 1)^T\).

In fact, for any \(n \geq 1\), the recursive relation is valid. That is \((a_{00}^n, a_{01}^n, a_{10}^n, a_{11}^n) = (a_{00}^{n-1}, a_{01}^{n-1}, a_{10}^{n-1}, a_{11}^{n-1})T = A_0 T^n\). Hence,

\[\rho(T_n; x, y) = A_0 T^nL.\]

For example,

\[\rho(T_1; x, y) = 3x^2y + 9x^2 + 6xy + 6x + 3y + 1,\]

and

\[\rho(T_2; x, y) = 3x^2y^2 + 18x^2y + 6xy^2 + 9x^2 + 3y^2 + 2xy + 6x + 6y + 1.\]

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