

Spectrum of Matching Forcing Numbers of a Hexagonal System with a Forcing Edge*

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Abstract

The forcing number of a Kekulé structure of a hexagonal system is the smallest number of double bonds that determine the entire Kekulé structure. It is known that the maximum forcing number equals the Clar number for any hexagonal systems. In this paper by applying Z -transformation graph (or resonance graph) we show that the forcing numbers of all Kekulé structures of a hexagonal system H with a forcing edge form either the integer interval from 1 to the Clar number of H or with only the gap 2.

1 Introduction

A *perfect matching* (or *Kekulé structure*) of a graph G is a set of disjoint edges which cover all vertices of G . A *forcing set* S of a perfect matching M of G is a subset of M such that S is contained in no other perfect matchings of G . The *forcing number* of M is the smallest cardinality over all forcing sets of M , denoted by $f(G, M)$. An edge of G is called a *forcing edge* if it is contained in exactly one perfect matching of G . The *minimum* (resp. *maximum*) *forcing number* of G is the minimum (resp. maximum) value of forcing numbers of all perfect matchings of G , denoted by $f(G)$ (resp. $F(G)$).

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The concept of the forcing number of a perfect matching of a graph was originally introduced by Harary et al. [8]. The same idea appeared in earlier chemical literatures due to Klein and Randić [11, 14] under the name of the *innate degree of freedom* of a Kekulé structure, which plays an important role in the resonance theory in chemistry. The minimum forcing number of a graph has been extensively studied [1–3, 12, 18, 25]. Adams et al. [1] showed that determining smallest forcing set of a perfect matching of a bipartite graph with maximum degree three is an NP-complete problem. Afshani et al. [2] proved that the smallest forcing number problem of graphs is NP-complete for bipartite graphs with maximum degree four.

Let M be a perfect matching of a graph G . A cycle C of G is called an M -alternating cycle if the edges of C appear alternately in M and $E(G) \setminus M$, where $E(G)$ is the edge set of G . For planar bipartite graphs, Pachter and Kim proved the following minimax theorem.

Theorem 1.1 [12]. Let M be a perfect matching in a planar bipartite graph G . Then $f(G, M) = c(M)$, where $c(M)$ is the maximum number of disjoint M -alternating cycles of G .

Adams et al. [1] defined the *forcing spectrum* of a graph G as:

$$\text{Spec}(G) = \{f(G, M) \mid M \text{ is a perfect matching of } G\}.$$

Forcing spectra of some special fullerene graphs C_{20} , C_{60} , C_{70} and C_{72} have been computed as to be continuous [15–17, 25]. Jiang and Zhang [9] proved that the forcing spectrum of tubular BN-fullerene graph with cyclic edge-connectivity three is an integer interval.

A *hexagonal system* (or *benzenoid system*) is a finite 2-connected plane graph in which each interior face is surrounded by a regular hexagon of side length one. Hexagonal systems as carbon-skeleton of benzenoid hydrocarbons are studied extensively [5]. A hexagonal system is called *forced* if it has a forcing edge. Such graphs have been characterized independently by Hansen and Zheng [6], and Zhang and Li [21].

In this paper our aim is to determine the forcing spectra of forced hexagonal systems. Some relevant aspects of forced hexagonal systems are reviewed in the next section. In Section 3, we show that for forced hexagonal systems, “ M -alternating cycles” in Theorem 1.1 can be replaced by “ M -alternating hexagons”. That is, in this special case we obtain

a stronger minimax theorem: the forcing number of any perfect matching M is equal to the maximum number of disjoint M -alternating hexagons.

In Section 4, we take Z -transformation graph (or resonance graph in literature [10, 13]) as a tool to determine the forcing spectrum of a forced hexagonal system. The Z -transformation graph $Z(H)$ of a hexagonal system H is the graph whose vertices are the perfect matchings of H and two vertices are adjacent provided the corresponding perfect matchings M and M' differ in just one hexagon [20, 24, 26], that is, their symmetric difference $M\Delta M' = (M - M') \cup (M' - M)$ forms a hexagon of H . Z -transformation graph has ever been used to solve the forcing edge problem of hexagonal systems [21]. We always find a special path P in the Z -transformation graph of a forced hexagonal system H such that one end-vertex corresponds to a perfect matching whose forcing number is 1, 2 or 3 and the other end-vertex corresponds to a perfect matching that has the maximum forcing number of H , and any two adjacent vertices in P correspond to two perfect matchings whose forcing numbers have the difference at most one. This implies that the forcing spectrum of H is a continuous integer interval from 1 to the Clar number $cl(H)$ or with only the gap 2.

2 Structures and properties of forced hexagonal systems

In this section we review the structures of forced hexagonal systems. Suppose that all hexagonal systems considered are drawn in the plane such that some edges are vertical. Let H be a hexagonal system with a specific hexagon s_0 of the center O . We establish a 3-coordinate system $O - ABC$ on H such that O is the origin and the three axes are perpendicular to three disjoint edges of s_0 respectively. The coordinate system $O - ABC$ divides the plane into three areas AOB , BOC and COA . For a point W in the plane, we define its coordinates with respect to $O - ABC$. If W lies in the area AOB (for other cases we can do similarly), draw two lines through W such that one is parallel to axis OB and intersects axis OA at the point W_A , and the other is parallel to axis OA and intersects axis OB at the point W_B . The lengths of OW_A and OW_B are defined as the coordinates of W on axes OA and OB respectively, and the coordinate of W on axis OC is defined as zero. If the lengths of OW_A and OW_B are denoted by x and y respectively, then the coordinate of W with respect to $O - ABC$ is written as $(x, y, 0)$.

The *inner dual graph* $T(H)$ of H is the graph whose vertices are centers of hexagons of H and two centers are joined by an edge in $T(H)$ if the corresponding two hexagons have a common edge. Clearly, $T(H)$ is a plane graph. The periphery of $T(H)$ is defined as the boundary of its exterior face (a closed walk). If $T(H)$ intersects OA and OB at just one path respectively, the part of the periphery of $T(H)$ in area AOB and between OA and OB is a path $W_1W_2 \cdots W_m$ and the coordinates $(x_i, y_i, 0)$ of W_i ($i = 1, 2, \dots, m$) satisfy $x_1 \geq x_2 \geq \cdots \geq x_m$ and $y_1 \leq y_2 \leq \cdots \leq y_m$; or $x_1 \leq x_2 \leq \cdots \leq x_m$ and $y_1 \geq y_2 \geq \cdots \geq y_m$, then the periphery of $T(H)$ is called to be *monotone* in area AOB . If the periphery of $T(H)$ is monotone in all three areas, then $T(H)$ is said to be monotone with respect to the coordinate system $O - ABC$. If there is no hexagon of H in some area, then this area is called an *empty* area.

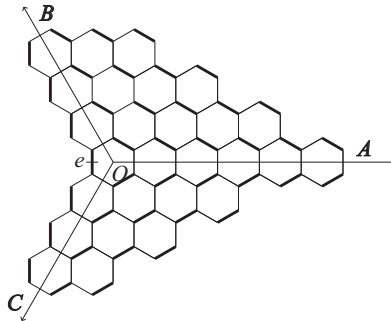


Figure 1. The coordinate system of a forced hexagonal system H with the 3-divisible perfect matching M_0 (bold edges) and a forcing edge e (marked by a short bar).

Zhang et al. proved [20] that $Z(H)$ has a vertex of degree one if and only if there is a coordinate system $O - ABC$ of H such that $T(H)$ is monotone with respect to $O - ABC$. In particular, the following characterization of forced hexagonal systems was presented.

Theorem 2.1 [6, 21]. A hexagonal system H is forced if and only if there is a coordinate system $O - ABC$ of H such that $T(H)$ is monotone with respect to $O - ABC$ and at least one area of AOB , BOC and COA is empty.

For convenience, from now on we always place a forced hexagonal system H on the plane with its coordinate system $O - ABC$ as is shown in Fig. 1: axis OA is horizontal and directs to the right, OB is upward and OC is downward, and BOC is empty. In fact, H has a perfect matching M_0 (see the bold edges) such that each edge of M_0 does not

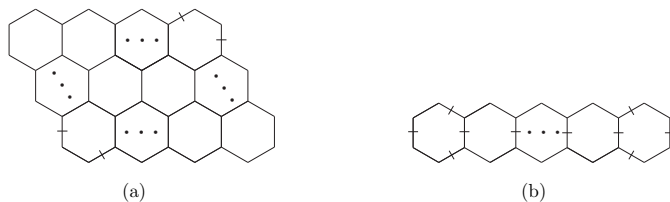


Figure 2. Distribution of forcing edges in parallelogram (a) and linear chain (b) (marked by short bars).

intersect any axis and two edges of M_0 lie in the same area if and only if they are parallel each other. Then the hexagon with the center O is the unique M_0 -alternating hexagon and M_0 is said to be β -divisible with respect to $O - ABC$. So the distribution of forcing edges of a forced hexagonal system can be determined completely by Zhang and Li [21]. In fact, the edge of the hexagon with the center O in area BOC belongs to M_0 and must be forced (see Fig. 1). Further, if the other area AOB or AOC is empty, the edge of the hexagon with the center O in the corresponding area is also forced. In particular, linear hexagonal chains with h hexagons have $h + 5$ forcing edges, and non-degenerated parallelogram hexagonal systems have four forcing edges (see Fig. 2).

Any forced hexagonal system is a constructing benzenoid system [22] or t -tier strip benzenoid system [23]. From Theorem 2 in [22] or Lemma 1 in [23], we have the following property.

Property 2.2. Let M be a perfect matching of a forced hexagonal system H . Then M contains exactly one vertical edge of each row of H .

Suppose H is a forced hexagonal system consisting of t rows of linear hexagonal chains, denoted by B_1, \dots, B_t , from top to bottom. Let M be a perfect matching of H . An edge is called M -matched if M contains it. By Property 2.2, there is only one M -matched vertical edge of B_i . Suppose that the M -matched vertical edge of B_i is denoted by e_i , $i = 1, 2, \dots, t$. If we count the vertical edges of B_i from left to right, and e_i is the b_i -th vertical edge of B_i , then there arises an integer sequence (b_1, b_2, \dots, b_t) with respect to M . Suppose B_k ($1 \leq k \leq t$) intersects axis OA . Then e_k is the M -matched vertical edge of B_k . We define the right area of e_k as is shown in Fig. 3. By using these notations, we have the following result.

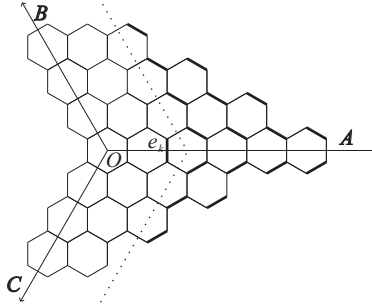


Figure 3. M -matched edges (bold edges) in the right area of e_k (right of the two dashed rays).

Property 2.3. $b_1 \leq b_2 \leq \dots \leq b_k \geq b_{k+1} \geq \dots \geq b_t$. Moreover, all M -matched edges in the right area of e_k are uniquely determined.

Proof. Any forced hexagonal system is a constructing benzenoid system, Theorem 2 in ref [22] implies that $b_1 \leq b_2 \leq \dots \leq b_k \geq b_{k+1} \geq \dots \geq b_t$. M -matched edges in the right area of e_k are uniquely determined since there are no M -matched vertical edges in the right area of e_k . □

3 A minimax theorem

Let H be a hexagonal system with a perfect matching M . For a cycle C of H , let $I[C]$ be the subgraph of H consisting of C together with its interior.

Lemma 3.1. Let H be a forced hexagonal system with a perfect matching M . For any two disjoint M -alternating cycles C_1 and C_2 of H , $I[C_1]$ and $I[C_2]$ have no common vertex.

Proof. To the contrary, suppose that $I[C_1]$ and $I[C_2]$ have a common vertex. Note that $I[C_1]$ and $I[C_2]$ have no common vertex on their boundaries since C_1 and C_2 are two disjoint M -alternating cycles. Without loss of generality, we suppose that $I[C_1]$ is contained in $I[C_2]$. C_1 must contain an M -matched vertical edge f of H since C_1 is an M -alternating cycle of H . Suppose H consists of t rows of linear hexagonal chains and f lies in the k -th ($1 \leq k \leq t$) row. Since $I[C_1]$ is contained in $I[C_2]$ and C_2 is an M -alternating cycle, C_2 must contain an M -matched vertical edge f' in the k -th row. Since $f \neq f'$, there are two M -matched vertical edges in the k -th row, which contradicts Property 2.2. □

Let M be a perfect matching of a hexagonal system H . Recall that $c(M)$ denotes the maximum number of disjoint M -alternating cycles of H . Let $h(M)$ denote the maximum number of disjoint M -alternating hexagons of H . A set F of disjoint M -alternating hexagons of H is called an M -resonant set, further a *maximum M -resonant set* if $|F| = h(M)$. In general we have $f(H, M) = c(M) \geq h(M)$. The following minimax result says that for forced hexagonal systems the equality always holds.

Theorem 3.2. Let M be a perfect matching of a forced hexagonal system H . Then $f(H, M) = h(M)$.

Proof. Let F denote a maximum set of disjoint M -alternating cycles of H . By Theorem 1.1, we have that $f(H, M) = c(M) = |F|$. If each member of F is a hexagon of H , then F is an M -resonant set and thus $h(M) \geq c(M) = |F|$. Since $c(M) \geq h(M)$, the equality holds. Otherwise, there is an M -alternating cycle C in F that is not a hexagon of H . Since C is an M -alternating cycle, the restriction of M to $I[C]$ forms a perfect matching of $I[C]$. Note that $I[C]$ is a hexagonal system, by Lemma 5 in [20], there is an M -alternating hexagon s in $I[C]$. According to Lemma 3.1, C and s must have a common M -matched vertical edge, and each cycle in $F \setminus \{C\}$ does not intersect s . Let $F' = (F \setminus \{C\}) \cup \{s\}$. Then F' is also a maximum set of disjoint M -alternating cycles of H , and the number of hexagons in F' is one more than the number of hexagons in F . Repeating this procedure, we can get an M -resonant set F^* such that $|F^*| = |F|$. So we have that $f(H, M) = |F^*| = h(M)$ as the beginning of this proof. \square

A *sextet pattern* of a hexagonal system H is an M -resonant set for a perfect matching M of H . A *Clar formula* of H is a sextet pattern of H with the maximum number of hexagons. The *Clar number* $cl(H)$ of H is the number of hexagons in a Clar formula [4, 7]. Hence $cl(H)$ equals the maximal value of $h(M)$ over all perfect matchings M of H .

Recall that $F(H)$ denotes the maximum forcing number of H . Our minimax theorem implies the following result.

Corollary 3.3. Let H be a forced hexagonal system. Then $F(H) = cl(H)$.

Remark 3.4. Theorem 3.2 does not hold for general hexagonal systems. However, Xu et al. [19] recently showed that Corollary 3.3 holds for any hexagonal systems.

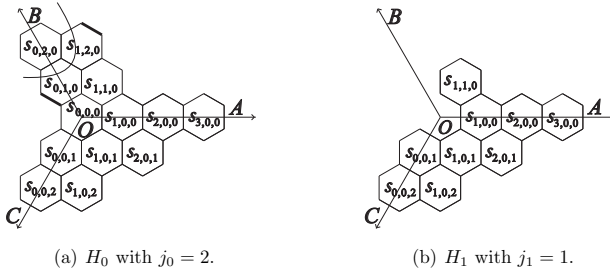


Figure 4. $H_1 = H_0 \ominus s_{0,2,0}$.

4 Forcing spectra of forced hexagonal systems

In this section we study the forcing spectra of forced hexagonal systems. Let H be a forced hexagonal system. As in Section 2, a coordinate system $O - ABC$ of H has been established so that $T(H)$ is monotone with respect to it and the area BOC is empty. Suppose that the distance between two centers of any two adjacent hexagons (two hexagons are adjacent if they have a common edge) of H is one. Then the center of each hexagon of H can be denoted by an integer triple (i, j, k) , where i, j and k are the three coordinates on axes OA, OB and OC respectively. If (i, j, k) is the coordinate of the center of a hexagon of H , then this hexagon is denoted by $s_{i,j,k}$. For example, the coordinate of the origin O is $(0, 0, 0)$, the corresponding hexagon is denoted by $s_{0,0,0}$.

Let $a := \max\{i | s_{i,0,0} \text{ is a hexagon of } H\}$, $b := \max\{j | s_{0,j,0} \text{ is a hexagon of } H\}$, and $c := \max\{k | s_{0,0,k} \text{ is a hexagon of } H\}$. For a hexagon s of H , let $H - s$ denote the subgraph obtained from H by deleting all vertices of s together with their incident edges. In the following we now describe a procedure to construct a Clar formula of H due to Zhang and Li [22].

For convenience, let $H_0 := H$ and $j_0 := b$. Let H_1 be the the subgraph obtained from $H_0 - s_{0,j_0,0}$ by deleting all unambiguously matched vertices together with their incident edges. We define this operation as $H_1 = H_0 \ominus s_{0,j_0,0}$ (an example is given in Fig. 4). Let $j_1 = \max\{j | s_{1,j,0} \text{ is a hexagon of } H_1\}$. Do the same operation, we can get $H_2 = H_1 \ominus s_{1,j_1,0}$. Repeating this procedure until to generate H_m, j_m and $s_{m,j_m,0}$, such that H_m intersects axis OA , but $H_m \ominus s_{m,j_m,0}$ does not. If $j_m > 0$, let $H'_1 = H_m \ominus s_{m,j_m,0}$; otherwise $H'_1 = H_m \ominus s_{a,0,0}$. Note that H'_1 does not intersect axis OA . If H'_1 is not an empty graph, let $i_1 = \max\{i | s_{i,0,1} \text{ is a hexagon of } H'_1\}$. Do the same operation, $H'_2 = H'_1 \ominus s_{i_1,0,1}$ is

obtained. Repeating this operation until to generate H'_n and $s_{i_n,0,n}$ such that $H'_n \ominus s_{i_n,0,n}$ is empty.

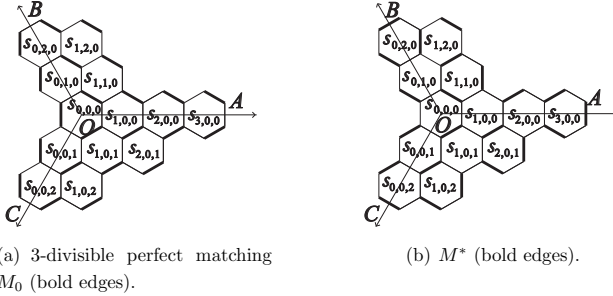


Figure 5. $M^* = M_0 \triangle s_{0,0,0} \triangle s_{0,1,0} \triangle s_{0,2,0} \triangle s_{1,0,0} \triangle s_{1,1,0} \triangle s_{2,0,0} \triangle s_{3,0,0} \triangle s_{0,0,1} \triangle s_{1,0,1} \triangle s_{2,0,1} \triangle s_{0,0,2} \triangle s_{1,0,2}$, $K^* = \{s_{0,2,0}, s_{1,1,0}, s_{3,0,0}, s_{2,0,1}, s_{1,0,2}\}$, $f(H, M^*) = 5$.

Let $K^* = \{s_{0,j_0,0}, s_{1,j_1,0}, \dots, s_{m-1,j_{m-1},0}, s_{m,j_m,0}, s_{i_1,0,1}, s_{i_2,0,2}, \dots, s_{i_n,0,n}\}$ (if $j_m = 0$, $s_{m,j_m,0}$ is replaced by $s_{a,0,0}$). Note that if $j_k > 0$ ($0 \leq k \leq m$), $s_{k,j_k,0}$ in K^* is the top-left hexagon of hexagonal system H_k , and the left vertical edge of $s_{k,j_k,0}$ has the end-vertices of degree 2 in H_k . If $j_m = 0$, then $s_{a,0,0}$ is the top-right hexagon of H_m , and the right vertical edge of $s_{a,0,0}$ has the end-vertices of degree 2 in H_m . For the hexagon $s_{i_k,0,k}$ ($1 \leq k \leq n$) of K^* , $s_{i_k,0,k}$ is the top-right hexagon of H'_k and the degrees of the two endpoints of the right vertical edge of $s_{i_k,0,k}$ both are two in H'_k . Zhang and Li proved the following result.

Lemma 4.1 [22]. K^* is a Clar formula of H .

Let M_0 be the 3-divisible perfect matching of H with respect to $O - ABC$ (see Fig. 5(a)). Let $M^* = M_0 \triangle s_{0,0,0} \triangle s_{0,1,0} \triangle \dots \triangle s_{0,j_0,0} \triangle s_{1,0,0} \triangle s_{1,1,0} \triangle \dots \triangle s_{1,j_1,0} \triangle \dots \triangle s_{m,j_m,0} \triangle s_{0,0,1} \triangle \dots \triangle s_{i_1,0,1} \triangle s_{0,0,2} \triangle \dots \triangle s_{i_2,0,2} \triangle \dots \triangle s_{i_n,0,n}$. Here, if $j_m = 0$ and $m < a$, then $s_{m,j_m,0}$ is replaced by $s_{m,0,0} \triangle s_{m+1,0,0} \triangle \dots \triangle s_{a,0,0}$. An example is given in Fig. 5, where $m = 2$, $j_2 = 0$, $a = 3$, and $s_{2,j_2,0}$ is replaced by $s_{2,0,0} \triangle s_{3,0,0}$. We can see that M^* is a perfect matching of H and each hexagon in K^* is M^* -alternating.

By Lemma 4.1 and Corollary 3.3 we have

Lemma 4.2. $F(H) = c(M^*) = h(M^*) = cl(H)$.

For convenience, let such hexagon sequence be denoted by $(h_0, h_1, \dots, h_{r-1})$, where $h_0 = s_{0,0,0}$, $h_{r-1} = s_{i_n,0,n}$ and $M^* = M_0 \triangle h_0 \triangle h_1 \triangle \dots \triangle h_{r-1}$. Let $M_{i+1} = M_i \triangle h_i$, $i =$

$0, \dots, r - 1$. Then we find a path $M_1 M_2 \dots M_r$ in $Z(H)$, where $M_1 = M_0 \triangle h_0$ and $M_r = M^*$.



Figure 6. Illustration for the proof of Lemma 4.3: possible hexagons s_1, \dots, s_6 around h_i , and M_i -matched edges (bold) and M_{i+1} -matched edges (dashed) of h_i .

Lemma 4.3. $|f(H, M_{i+1}) - f(H, M_i)| \leq 1$ for all $i = 1, 2, \dots, r - 1$.

Proof. By Theorem 3.2, we only need to compute the difference between $h(M_i)$ and $h(M_{i+1})$. Note that $M_{i+1} = M_i \triangle h_i$, $h_i \neq h_0$ and at most six hexagons in H are adjacent to h_i (see Fig. 6). h_i is an M_i -alternating hexagon such that the left vertical edge e_l belongs to M_i , and h_i is also an M_{i+1} -alternating hexagon such that the right vertical edge e_r belongs to M_{i+1} . Let d be the maximum number of disjoint M_i -alternating hexagons in $H - h_i$, F be a maximum M_i -resonant set of H and F' be a maximum M_{i+1} -resonant set of H . It is obvious that s_1, s_3 and s_5 are not in F and s_2, s_4 and s_6 are not in F' (see Fig. 6).

Claim 1. $d + 1 \leq |F| \leq d + 2$ and $d + 1 \leq |F'| \leq d + 2$.

Proof. First, we prove the lower bounds. Let K be a set of disjoint M_i -alternating hexagons of $H - h_i$ with the cardinality d . Then K is also an M_{i+1} -resonant set since M_i and M_{i+1} differ only in h_i . Further, $K \cup \{h_i\}$ is an M_i -resonant set and M_{i+1} -resonant set of H . Note that F is a maximum M_i -resonant set of H . Hence $|K \cup \{h_i\}| = d + 1 \leq |F|$. Similarly, we have $d + 1 \leq |F'|$. For the upper bounds, we consider the following three cases.

Case 1: h_i intersects axis OB or h_i is a hexagon in area AOB . We first consider F . Since the two vertical edges of s_2 lie to the right of e_l , by Property 2.3, none of the two vertical edges of s_2 is M_i -matched edge. So s_2 is not M_i -alternating. Note that s_4 and s_6 are two possible M_i -alternating hexagons in F , and F contains at most d disjoint M_i -alternating hexagons of $H - h_i$. Hence $|F| \leq d + 2$. For F' , since the two vertical edges of s_5 lie to the left of e_r , by Property 2.3 s_5 is not M_{i+1} -alternating. Note that s_1 and

s_3 are two possible M_{i+1} -alternating hexagons in F' , and F' contains at most d disjoint M_{i+1} -alternating hexagons of $H - h_i$. Hence $|F'| \leq d + 2$.

Case 2: h_i intersects axis OC or h_i is a hexagon in area COA . For F , since the two vertical edges of s_4 lie to the right of e_l , by Property 2.3 s_4 is not M_i -alternating. Note that s_2 and s_6 are two possible M_i -alternating hexagons in F , and F contains at most d disjoint M_i -alternating hexagons of $H - h_i$. Hence $|F| \leq d + 2$. For F' , the two vertical edges of s_1 lie to the left of e_r , so s_1 is not M_{i+1} -alternating by Property 2.3. Note that s_3 and s_5 are two possible M_{i+1} -alternating hexagons, and F' contains at most d disjoint M_{i+1} -alternating hexagons of $H - h_i$. So $|F'| \leq d + 2$.

Case 3: h_i intersects axis OA . For F , the two vertical edges of s_2 and the two vertical edges of s_4 all lie to the right of e_l , so none of s_2 and s_4 is M_i -alternating by Property 2.3. But s_6 is a possible M_i -alternating hexagon. Note that F contains at most d disjoint M_i -alternating hexagons of $H - h_i$. Hence $|F| \leq d + 1$.

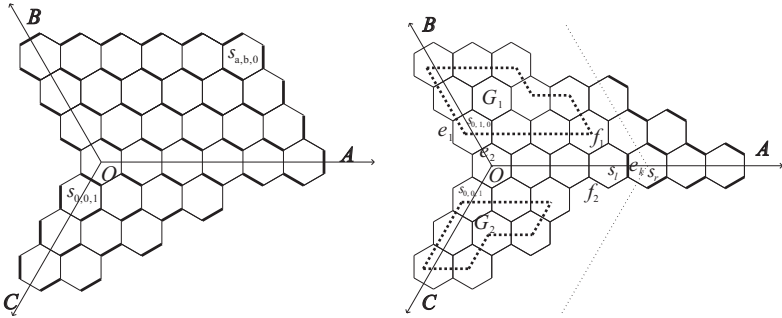
Now we prove that $|F'| \leq d + 2$. If $s_{0,0,1}$ is not a hexagon of H , then there is no hexagon of H under the axis OA by Theorem 2.1. So s_5 is not a hexagon of H , that is, $s_5 \notin F'$. Suppose $s_{0,0,1}$ is a hexagon of H . According to the above notations, $M_{i+1} = M_0 \triangle h_0 \triangle h_1 \dots \triangle h_i$. Since h_i intersects axis OA , each h_j ($1 \leq j \leq i$) does not intersect axis OC and does not lie in area COA . So $s_{0,0,1}$ is the unique M_{i+1} -alternating hexagon under axis OA since all M_{i+1} -matched vertical edges under axis OA lie on the boundary of H and in area BOC . Since $h_i \neq h_0$, $s_5 \neq s_{0,0,1}$. So s_5 is not an M_{i+1} -alternating hexagon of H , that is, $s_5 \notin F'$. Note that s_1 and s_3 are two possible M_{i+1} -alternating hexagons of F' , and F' contains at most d disjoint M_{i+1} -alternating hexagons of $H - h_i$. Hence $|F'| \leq d + 2$. □

By Theorem 3.2, $|F| = h(M_i) = f(H, M_i)$ and $|F'| = h(M_{i+1}) = f(H, M_{i+1})$. According to Claim 1, we have $d + 1 \leq f(H, M_i) \leq d + 2$ and $d + 1 \leq f(H, M_{i+1}) \leq d + 2$, which implies $|f(H, M_{i+1}) - f(H, M_i)| \leq 1$. □

As an immediate consequence of Lemma 4.3, we obtain the following corollary.

Corollary 4.4. The integer interval $[f(H, M_1), cl(H)]$ is a subset of $\text{Spec}(H)$.

Proof. $f(H, M_i) \in \text{Spec}(H)$ for all $i = 1, 2, \dots, r$ since M_i is a perfect matching of H . Note that $M_r = M^*$ and $F(H) = f(H, M^*) = h(M^*) = cl(H)$ by Lemma 4.2. By Lemma 4.3, the integer interval $[f(H, M_1), cl(H)]$ is a subset of $\text{Spec}(H)$. □



(a) The case that $abc \neq 0$ and H contains $s_{a,b,0}$. (b) The case that $abc \neq 0$ and H does not contain any one of $s_{a,b,0}$ and $s_{a,0,c}$.

Figure 7. Illustrations for the proof of Theorem 4.5, bold edges are M -matched.

Now we give the following main result.

Theorem 4.5. If $abc \neq 0$ and H does not contain any one of $s_{a,b,0}$ and $s_{a,0,c}$, then $\text{Spec}(H) = [1, cl(H)] \setminus \{2\}$. Otherwise, $\text{Spec}(H) = [1, cl(H)]$.

Proof. It is obvious that $f(H, M_0) = 1$. By Corollary 3.3, $cl(H) = F(H)$. By Corollary 4.4, $[f(H, M_1), F(H)] \subseteq \text{Spec}(H)$. If $abc = 0$, then $f(H, M_1) = 1$ or $f(H, M_1) = 2$. Hence $\text{Spec}(H) = [1, cl(H)]$.

So suppose that $abc \neq 0$. Then $f(H, M_1) = 3$, and $\{1, 3, 4, \dots, cl(H)\} \subseteq \text{Spec}(H)$. So we only need to determine whether $2 \in \text{Spec}(H)$ or not. If H contains $s_{a,b,0}$, then there is a perfect matching M of H such that only $s_{a,b,0}$ and $s_{0,0,1}$ are M -alternating hexagons of H (see Fig. 7(a)). By Theorem 3.2, $f(H, M) = h(M) = 2$. If H contains $s_{a,0,c}$, symmetrically we can find a perfect matching M' of H such that only $s_{a,0,c}$ and $s_{0,1,0}$ are M' -alternating hexagons of H , so $f(H, M') = 2$.

For the case $abc \neq 0$ and H contains neither $s_{a,b,0}$ nor $s_{a,0,c}$, we will prove that $2 \notin \text{Spec}(H)$. Suppose to the contrary that H has a perfect matching M with $f(H, M) = 2$. Let e_k be the M -matched vertical edge in the k -th row of H (intersecting axis OA). Then e_k is not a forcing edge of H since $f(H, M) = 2$. So e_k can intersect axis OA . Let H' be the subgraph obtained from H by deleting the two end-vertices of e_k and all vertices in the right area of e_k together with their incident edges, and removing those vertical edges in the k -th row of H . By Properties 2.2 and 2.3 the restriction of M on H' is still a perfect matching of H' . If H' has a pendent edge, it must be an M -matched edge. Delete

its end-vertices and their incident edges from H' . Do the same operations repeatedly until there is no vertices with degree one in the resulting graph. The resulting graph is a disjoint union of two forced hexagonal systems G_1 and G_2 , where G_1 contains $s_{0,1,0}$ and G_2 contains $s_{0,0,1}$, and the left vertical edge of $s_{0,1,0}$ is a forcing edge of G_1 and the left vertical edge of $s_{0,0,1}$ is a forcing edge of G_2 as pointed out in Section 2 (see Fig. 7(b)).

Let F_1 and F_2 be the restrictions of M on G_1 and G_2 respectively. Then F_1 and F_2 are perfect matchings of G_1 and G_2 respectively. We claim that $f(G_1, F_1) = 1$ and $f(G_2, F_2) = 1$. By Theorem 3.2, $f(G_1, F_1) = h(F_1) \geq 1$ and $f(G_2, F_2) = h(F_2) \geq 1$. If one of $f(G_1, F_1)$ and $f(G_2, F_2)$ is more than one, then $h(F_1) + h(F_2)$ is more than two, which implies that there are at least three disjoint M -alternating hexagons of H . By Theorem 3.2, we have $f(H, M) \geq 3$, contradicting that $h(M) = f(H, M) = 2$. So the claim holds. Hence G_1 (resp. G_2) has exactly one M -alternating hexagon s_1 (resp. s_2), which contains a forcing edge of G_1 (resp. G_2).

The hexagons to the left and right side of e_k and with common edge e_k are denoted by s_l and s_r respectively. Note that s_r may be not contained in H (see Fig. 7(b)). If s_r is a hexagon of H , by Property 2.3 s_r is an M -alternating hexagon. Hence s_1, s_2 and s_r are three disjoint M -alternating hexagons. This contradicts that $f(H, M) = 2$. So suppose that s_r is not a hexagon of H . Then e_k is on the boundary of H , the coordinate of the center of s_l on axis OA is a , and $a \neq 0$. Now we show that the two edges f_1 and f_2 of s_l (see Fig. 7(b)) both are M -matched, that is, s_l is an M -alternating hexagon. If f_1 lies on the boundary of H , then f_1 is M -matched since f_1 is a pendent edge in graph H' . Note that G_1 does not contain f_1 , so s_1 and s_l are disjoint. If f_1 does not lie on the boundary of H , then f_1 is on the boundary of G_1 . Since $abc \neq 0$ and H does not contain $s_{a,b,0}$, G_1 is neither a linear hexagonal chain nor a parallelogram hexagonal system. It is known that only e_1 and e_2 are forcing edges of G_1 from Section 2 (see Fig. 7(b)). Since $f(G_1, F_1) = 1$, $e_1, e_2 \in F_1$. So $s_{0,1,0}$ is the unique F_1 -alternating hexagon of G_1 , that is, $s_1 = s_{0,1,0}$. Note that f_1 is parallel to e_2 . So f_1 is F_1 -matched and thus M -matched. Hence f_1 is always M -matched and s_1 and s_l are disjoint. Similarly, we can prove that f_2 is M -matched, and s_2 and s_l are disjoint. So s_1, s_2 and s_l are three disjoint M -alternating hexagons, contradicting that $f(H, M) = 2$. □

References

- [1] P. Adams, M. Mahdian, E. S. Mahmoodian, On the forced matching numbers of bipartite graphs, *Discr. Math.* **281** (2004) 1–12.
- [2] P. Afshani, H. Hatami, E. S. Mahmoodian, On the spectrum of the forced matching number of graphs, *Australas. J. Comb.* **30** (2004) 147–160.
- [3] Z. Che, Z. Chen, Forcing on perfect matchings – A survey, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 93–136.
- [4] E. Clar, *The Aromatic Sextet*, Wiley, London, 1972.
- [5] S. J. Cyvin, I. Gutman, *Kekulé Structures in Benzenoid Hydrocarbons*, Springer, Berlin, 1988.
- [6] P. Hansen, M. Zheng, Bonds fixed by fixing bonds, *J. Chem. Inf. Comput. Sci.* **34** (1994) 297–304.
- [7] P. Hansen, M. Zheng, Upper bounds for the Clar number of a benzenoid hydrocarbon, *J. Chem. Soc. Faraday Trans.* **88** (1992) 1621–1625.
- [8] F. Harary, D. J. Klein, T. P. Živković, Graphical properties of polyhexes: perfect matching vector and forcing, *J. Math. Chem.* **6** (1991) 295–306.
- [9] X. Jiang, H. Zhang, On forcing matching number of boron-nitrogen fullerene graphs, *Discr. Appl. Math.* **159** (2011) 1581–1593.
- [10] S. Klavžar, P. Žigert, G. Brinkmann, Resonance graphs of catacondensed even ring systems are median, *Discr. Math.* **253** (2002) 35–43.
- [11] D. J. Klein, M. Randić, Innate degree of freedom of a graph, *J. Comput. Chem.* **8** (1987) 516–521.
- [12] L. Pachter, P. Kim, Forcing matchings on square grids, *Discr. Math.* **190** (1998) 287–294.
- [13] M. Randić, Resonance in catacondensed benzenoid hydrocarbons, *Int. J. Quantum Chem.* **63** (1997) 585–600.
- [14] M. Randić, D. J. Klein, Kekulé valence structures revisited. Innate degrees of freedom of π -electron couplings, in: N. Trinajstić (Ed.), *Mathematical and Computational Concepts in Chemistry*, Wiley, New York, 1985, pp. 274–282.
- [15] M. Randić, D. Vukičević, Kekulé structures of fullerene C_{70} , *Croat. Chem. Acta* **79** (2006) 471–481.

- [16] D. Vukičević, I. Gutman, M. Randić, On instability of fullerene C_{72} , *Croat. Chem. Acta* **79** (2006) 429–436.
- [17] D. Vukičević, M. Randić, On Kekulé structures of buckminsterfullerene, *Chem. Phys. Lett.* **401** (2005) 446–450.
- [18] H. Wang, D. Ye, H. Zhang, The forcing number of toroidal polyhexes, *J. Math. Chem.* **43** (2008) 457–475.
- [19] L. Xu, H. Bian, F. Zhang, Maximum forcing number of hexagonal systems, *MATCH Commun. Math. Comput. Chem.* **70** (2013) 493–500.
- [20] F. Zhang, X. Guo, R. Chen, Z -transformation graphs of perfect matchings of hexagonal systems, *Discr. Math.* **72** (1988) 405–415.
- [21] F. Zhang, X. Li, Hexagonal systems with forcing edges, *Discr. Math.* **140** (1995) 253–263.
- [22] F. Zhang and X. Li, Clar formula of a class of hexagonal system, *MATCH Commun. Math. Comput. Chem.* **24** (1989) 333–347.
- [23] H. Zhang, The Clar formulas of regular t -tier strip benzenoid systems, *Syst. Sci. Math. Sci.* **8** (1995) 327–337.
- [24] H. Zhang, Z -transformation graphs of perfect matchings of plane bipartite graphs: A survey, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 457–476.
- [25] H. Zhang, D. Ye, W. C. Shiu, Forcing matching numbers of fullerene graphs, *Discr. Appl. Math.* **158** (2010) 573–582.
- [26] H. Zhang, F. Zhang, Plane elementary bipartite graphs, *Discr. Appl. Math.* **105** (2000) 291–311.