

# Clar Sets and Maximum Forcing Numbers of Hexagonal Systems \*

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## Abstract

Let  $H$  be a hexagonal system with a perfect matching. Xu et al. discovered that the maximum forcing number of  $H$  equals its Clar number. In this article we obtain a result: for any resonant set  $K$  of a peri-condensed hexagonal system  $H$  consisting of disjoint hexagons not meeting the boundary of  $H$ , if the subgraph obtained from  $H$  by deleting  $K$  and the boundary of  $H$  has a perfect matching or is empty, then the Clar number of  $H$  is at least  $|K| + 2$ . This fact improves the previous corresponding result due to Zheng and Chen. Based on the result, we prove that for each perfect matching  $M$  of  $H$  with the maximum forcing number, there exists a Clar set consisting of disjoint  $M$ -alternating hexagons of  $H$ .

## 1 Introduction

A *hexagonal system*, also called benzenoid system, is a 2-connected finite plane graph whose every interior face is bounded by a regular hexagon of side length one [17]. It can also be formed by a cycle with its interior in the infinite hexagonal lattice on the plane (graphene) [4]. A *perfect matching* of a hexagonal system  $H$  is a set of disjoint edges covering all vertices of  $H$ . This concept coincides with that of a Kekulé structure in organic chemistry. Since a hexagonal system with at least one perfect matching may be viewed as the carbon-skeleton of a benzenoid hydrocarbon molecule, various topological

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properties of hexagonal systems have been extensively studied. The interested reader may refer to [2–4] with references therein.

A basic concept of Clar's aromatic sextet theory is that of Clar number, which can measure the stability of polycyclic benzenoid hydrocarbons [2]. According to Clar's theory, within a series of isometric benzenoid hydrocarbons, the one with larger Clar number is more stable [2].

Let  $M$  be a perfect matching of a graph  $G$ . A cycle  $C$  (resp. a path  $P$ ) of  $G$  is said to be  $M$ -alternating if the edges of  $C$  (resp.  $P$ ) appear alternately in and off  $M$ . For a subgraph  $F$  of  $G$ , let  $G - F$  denote the graph obtained from  $G$  by deleting all the vertices of  $F$  together with their incident edges.

Let  $H$  be a hexagonal system with a perfect matching. A set  $K$  of disjoint hexagons of  $H$  is called a *resonant set* (or *cover*) if there is a perfect matching  $M$  of  $H$  such that all hexagons in  $K$  are  $M$ -alternating. It is obvious that  $K$  is a resonant set of  $H$  if and only if  $H - K$  either has a perfect matching or is an empty graph. In particular,  $\emptyset$  is regarded as a perfect matching of an empty graph (no vertices). A resonant set is *maximum* if its cardinality is maximum. A maximum resonant set of  $H$  is also called a *Clar set* or *Clar formula*, and its size is called the *Clar number* of  $H$ , denoted by  $Cl(H)$ . For the relevant researches on the Clar number and Clar formula, please see [5, 7, 9, 12, 18, 19, 22].

In 1985, Zheng and Chen [26] gave an important property for a maximum resonant set of a hexagonal system as follows.

**Theorem 1.1.** [26] *Let  $H$  be a hexagonal system and  $K$  a maximum resonant set of  $H$ . Then  $H - K$  has a unique perfect matching.*

The proof of Theorem 1.1 is based on the following Lemma 1.2.

**Lemma 1.2.** [26] *Let  $H$  be a peri-condensed hexagonal system,  $K$  a resonant set of internal hexagons and  $\partial(H)$  the boundary of the exterior face of  $H$ . If  $H - K - \partial(H)$  has a perfect matching, then  $K$  is not a maximum resonant set.*

A hexagonal system  $H$  is said to be *fully benzenoid* if a maximum resonant set of  $H$  includes all vertices. Gutman and Salem showed [6] that a fully benzenoid has a unique maximum resonant set.

The *innate degree of freedom* of a Kekulé structure was defined by Randić and Klein [13] as the minimum number of double bonds which simultaneously belong to the given

kekulé structure and to no other one, nowadays it is named “forcing number” by Harary et al. [10].

Let  $M$  be a perfect matching of a graph  $G$ . A *forcing set*  $S$  of  $M$  is a subset of  $M$  such that  $S$  is contained in no other perfect matchings of  $G$ . The *forcing number* of  $M$ , denoted by  $f(G, M)$ , is the smallest cardinality over all forcing sets of  $M$ . The *maximum* (resp. *minimum*) *forcing number* of  $G$  is the maximum (resp. minimum) value of forcing numbers of all perfect matchings of  $G$ , denoted by  $F(G)$  (resp.  $f(G)$ ). For the relevant researches on the matching forcing problem, we refer to [1, 11, 23–25].

For planar bipartite graphs, Pachter and Kim revealed a minimax fact that connects the forcing number of a perfect matching and its alternating cycles as follows.

**Theorem 1.3.** [16] *Let  $M$  be a perfect matching of a plane bipartite graph  $G$ . Then  $f(G, M) = c(M)$ , where  $c(M)$  is the maximum number of disjoint  $M$ -alternating cycles of  $G$ .*

For a hexagonal system  $H$  with a perfect matching  $M$ , let  $h(M)$  denote the maximum number of disjoint  $M$ -alternating hexagons of  $H$ . Theorem 1.3 implies  $f(H, M) = c(M) \geq h(M)$ . Second equality does not hold always. Let us see an example in Fig. 1. The bold edges of Coronene form a perfect matching  $M'$  whose forcing number equals 2, but the graph has only one  $M'$ -alternating hexagon. However, Xu et al. [20] obtained the following result by finding a perfect matching  $M$  of  $H$  so that  $F(H) = f(H, M) = h(M)$ .

**Theorem 1.4.** [20] *Let  $H$  be a hexagonal system with perfect matchings. Then  $Cl(H) = F(H)$ .*

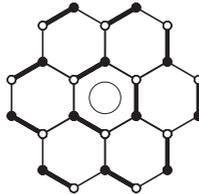


Figure 1: Coronene.

In this article, we show that for every perfect matching  $M$  of a hexagonal system  $H$  with the maximum forcing number, i.e.  $F(H) = f(H, M)$ , there exist  $F(H)$  disjoint  $M$ -alternating hexagons in  $H$ . That is,  $f(H, M) = h(M)$ . To prove this, we mainly improve

Lemma 1.2 to obtain Lemma 2.1 in Section 2. Based on this crucial lemma, in Section 3 we describe clearly structure properties for a maximum set of disjoint  $M$ -alternating cycles of  $H$  for any perfect matchings  $M$  with the maximum forcing number, then we give a proof of this main result.

## 2 A crucial lemma

In this section, all hexagonal systems considered are placed in the plane so that an edge-direction is vertical. A *peak* (resp. *valley*) of a hexagonal system is a vertex whose neighbors are below (resp. above) it. For convenience, the vertices of a hexagonal system are colored with white and black such that any pair of adjacent vertices receive different colors and the *peaks* are black.

Let  $H$  be a hexagonal system. The boundary of  $H$  means the boundary of the infinite face, denoted by  $\partial(H)$ . An edge on the boundary of  $H$  is a *boundary edge*. A hexagon of  $H$  is called an *external hexagon* if it contains a boundary edge and an *internal hexagon* otherwise.  $H$  is said to be *cata-condensed* if all vertices lie on its boundary and *peri-condensed* otherwise.

We state a crucial lemma as follows.

**Lemma 2.1.** *Let  $H$  be a peri-condensed hexagonal system and  $K$  a resonant set consisting of internal hexagons of  $H$ . Suppose  $H - K - \partial(H)$  has a perfect matching or is an empty graph. Then  $Cl(H) \geq |K| + 2$ .*

In order to prove the lemma, we need some further terminology and a known result.

Let  $M$  be a perfect matching of a hexagonal system  $H$ . An edge of  $H$  is called an  *$M$ -double edge* if it belongs to  $M$  and an  *$M$ -single edge* otherwise. An  $M$ -alternating cycle  $C$  of  $H$  is said to be *proper* if each edge of  $C$  in  $M$  goes from white end-vertex to black end-vertex along the clockwise direction of  $C$ .

The symmetric difference of two finite sets  $A$  and  $B$  is defined as  $A \oplus B := (A \cup B) - (A \cap B)$ . Given a perfect matching  $M$  of a hexagonal system  $H$ . If  $C$  is an  $M$ -alternating cycle (or hexagon) of  $H$ , then the symmetric difference  $M \oplus C$  is another perfect matching of  $H$  and  $C$  is an  $(M \oplus C)$ -alternating cycle of  $H$ . Here  $C$  may be viewed as its edge-set. Let  $P$  be a set of some hexagons of  $H$  and let  $F$  be a subgraph of  $H$ . The set of the common hexagons of  $P$  and  $F$  is denoted by  $P \cap F$ .

A hexagonal system  $H$  is called a *linear chain* if the centers of all hexagons lie on a straight line. Zhang et al. obtained the following result in [21, Theorem 4].

**Theorem 2.2.** [21] *A hexagonal system  $H$  has  $Cl(H) = 1$  if and only if  $H$  is a linear chain.*

For a cycle  $C$  of a hexagonal system  $H$ , let  $I[C]$  denote the subgraph of  $H$  formed by  $C$  together with its interior.

**Proof of Lemma 2.1.** By the assumption, we can choose a cycle  $C$  of  $H$  satisfying that

- (i) the graph  $I[C]$  is a peri-condensed hexagonal system, and
- (ii)  $C$  is disjoint with each member of  $K$  and  $H - K - C$  has a perfect matching, and  $I[C]$  contains as few hexagons as possible subject to (i) and (ii). Set  $H' := I[C]$  and  $K' := K \cap H'$ .

**Claim 1.** For any resonant set  $K_0$  of  $H'$ ,  $K_0 \cup (K \setminus K')$  is a resonant set of  $H$ .

*Proof.* Since  $H - K - C$  has a perfect matching,  $H$  has a perfect matching  $M_0$  such that each member in  $K \cup \{C\}$  is  $M_0$ -alternating. So the restriction of  $M_0$  on  $H - H'$  is a perfect matching of  $H - H'$ , denoted by  $M_c$ . Let  $M'_0$  be a perfect matching of  $H'$  such that each member in  $K_0$  is  $M'_0$ -alternating. Let  $M' := M'_0 \cup M_c$ . Then  $M'$  is a perfect matching of  $H$  such that each member in  $K_0 \cup (K \setminus K')$  is an  $M'$ -alternating hexagon. ■

From Claim 1 it suffices to prove that  $Cl(H') \geq |K'| + 2$ . If  $K' = \emptyset$ , by Theorem 2.2 we have that  $Cl(H') \geq |K'| + 2$ . From now on suppose that  $K' \neq \emptyset$ . Without loss of generality, let  $M$  be a perfect matching of  $H'$  such that the boundary  $C$  of  $H'$  and each member in  $K'$  are proper  $M$ -alternating cycles. We have the following claim.

**Claim 2.**  $H'$  has no external hexagons that are proper  $M$ -alternating.

*Proof.* Suppose to the contrary that an external hexagon  $h$  of  $H'$  is proper  $M$ -alternating. Then  $M \oplus h$  is a perfect matching of  $H'$ , and each component of  $C \oplus h$  is a proper  $(M \oplus h)$ -alternating cycle. Since any two proper  $M$ -alternating hexagons of  $H'$  are disjoint,  $h$  is disjoint with each member of  $K'$ . Since  $K' \neq \emptyset$ ,  $C \oplus h$  has a component as a cycle  $C'$  which satisfies the above conditions (i) and (ii). But  $I[C']$  has fewer hexagons than  $I[C]$ , contradicting the choice for  $C$ . Hence Claim 2 holds. ■

Along the boundary  $C$  of  $H'$ , we will find two substructures of  $H'$  in its left-top corner and left-bottom corner as Figs. 3 and 4, respectively, as follows.

A *b-chain* of hexagonal system  $H'$  is a maximal horizontal linear chain consisting of the consecutive external hexagons when traversing (counter)clockwise the boundary  $\partial(H')$ . A b-chain is called *high* (resp. *low*) if all hexagons adjacent to it are below (resp. above) it. For example, in Fig. 2  $D_0, D_1, D_2, G_1, G_2, \dots, G_9, G'_1, D_5, D_6$  and  $D_7$  are b-chains. In particular,  $D_0, D_1, D_2$  and  $G_1$  are high b-chains, while  $G'_1, D_5$  and  $D_6$  are low b-chains. But  $G_2, G_3, \dots, G_9$  and  $D_7$  are neither high nor low b-chains.

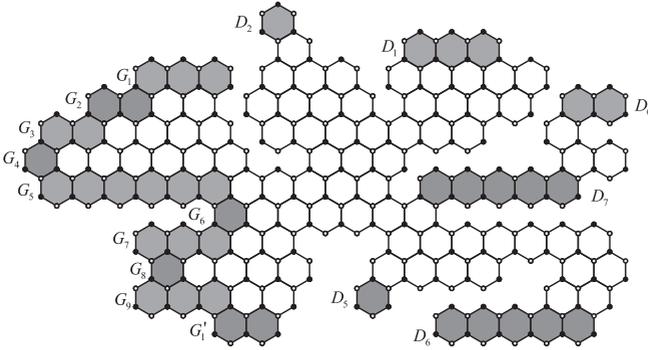


Figure 2: Various b-chains of a hexagonal system.

Choose a high b-chain and a low b-chain of  $H'$ . They are distinct. Otherwise  $H'$  itself is a linear chain, contradicting that  $H'$  is peri-condensed. From the high b-chain to the low b-chain along the boundary  $\partial(H')$  counterclockwise, we pass through a sequence of consecutive b-chains. In this process, let  $G_1$  be the last high b-chain and let  $G'_1$  be the first low b-chain after  $G_1$ . Clearly, there is no other high b-chain and low b-chain between  $G_1$  and  $G'_1$ . That is, those b-chains between  $G_1$  and  $G'_1$  descend monotonously.

From high b-chain  $G_1$  we have a sequence of consecutive b-chains  $G_1, G_2, \dots, G_m$  with the following properties: (1) for each  $1 \leq i < m$ ,  $G_{i+1}$  is next to  $G_i$ , and the left end hexagon of  $G_{i+1}$  lies on the lower left side of  $G_i$ , (2) either  $G_m$  is just the low b-chain  $G'_1$  or  $G_{m+1}$  is the b-chain next to  $G_m$  such that  $G_{m+1}$  has no hexagon lies on the lower left side of  $G_m$ . Let  $G$  be a hexagonal chain of  $H'$  consisting of b-chains  $G_1, G_2, \dots, G_m$ . Then  $G$  is a ladder-shape hexagonal chain.

Similarly, from low b-chain  $G'_1$  we have a sequence of consecutive b-chains  $G'_1, G'_2, \dots, G'_s$

with the following properties: (1) for each  $1 \leq j < s$ ,  $G'_j$  is next to  $G'_{j+1}$ , and the left end hexagon of  $G'_{j+1}$  lies on the higher left side of  $G'_j$ , (2) either  $G'_s$  is just the high b-chain  $G_1$  or  $G'_s$  is next to the b-chain  $G'_{s+1}$  such that  $G'_{s+1}$  has no hexagon lies on the higher left side of  $G'_m$ . Let  $G'$  be a hexagonal chain of  $H'$  consisting of b-chains  $G'_1, G'_2, \dots, G'_s$ .

For example, given a high b-chain  $D_1$  and a low b-chain  $D_5$  in Fig. 2, we can get two required hexagonal chains  $G = G_1 \cup G_2 \cup G_3 \cup G_4$  and  $G' = G_9 \cup G'_1$ .

**Claim 3.** Either  $G$  and  $G'$  are disjoint or the last b-chain  $G_m$  in  $G$  coincides with the first b-chain  $G'_s$  in  $G'$ .

To analyze the substructures  $G$  and  $G'$  of  $H'$ , as [26] we label the hexagons of  $G$  and some edges as follows (see Fig. 3): let  $S_{i,j}$ ,  $1 \leq i \leq m$  and  $1 \leq j \leq n(i)$ , be the hexagons of b-chain  $G_i$  as Fig. 3, neither  $A$  nor  $A'$  is contained in  $H'$ . Denote by  $e_{i,j}$  be the boundary edge of  $H'$  which is parallel to  $e_{1,1}$  and belongs to  $S_{i,j}$ ,  $1 \leq i \leq m$  and  $1 \leq j \leq n(i)$ , and denote the other boundary edges in  $S_{1,1}$  and  $S_{m,n(m)}$  by  $a, a', e_0, e'_0$  respectively, as shown in Fig. 3.

Since the boundary  $C$  of  $H'$  is a proper  $M$ -alternating cycle, all the edges  $e_0, e'_0, e_{i,j}$ ,  $1 \leq i \leq m$ ,  $1 \leq j \leq n(i)$ , are  $M$ -double edges. So we can draw a ladder-shape broke line segment  $L_1 = P_0 P_1 \cdots P_{q+1}$  ( $q \geq 1$ ) satisfying the following conditions.

**(A1)** The endpoints  $P_0$  and  $P_{q+1}$  of  $L_1$  are the midpoints of the edges  $a$  and  $a'$ , respectively.  $P_i$  ( $1 \leq i \leq q$ ) is the center of a hexagon  $S_i$  of  $H'$ ,  $P_i P_{i+1}$  ( $0 \leq i \leq q$ ) is orthogonal to one of the three edge directions, and  $P_{i+1}$  ( $0 \leq i \leq q$ ) lies on the lower left side or the left side of  $P_i$  according as  $i$  is even or odd (see Fig. 3).  $L_1$  only passes through hexagons of  $H'$ . Clearly, the graph consisting of the hexagons intersected by  $L_1$  is a hexagonal chain, denoted by  $H_1$ ;

**(A2)** All the edges intersected by  $L_1$  are  $M$ -single edges, all the  $M$ -double edges which are located in the region above  $L_1$  are parallel to  $e_{1,1}$  (see Fig. 3).

Note that there exists such a broke line segment such that it only passes through hexagons  $S_{i,j}$ ,  $1 \leq i \leq m$  and  $1 \leq j \leq n(i)$ . Among all those broke line segments, we can select one, also denoted by  $L_1$ , such that there are the maximum number of  $M$ -double edges above it.

Symmetrically we treat substructure  $G'$  of  $H'$  as follows. Let  $T_{i,j}$ ,  $1 \leq i \leq s$  and  $1 \leq j \leq t(i)$ , be the hexagons of b-chain  $G'_i$ , neither hexagon  $B$  nor hexagon  $B'$  is

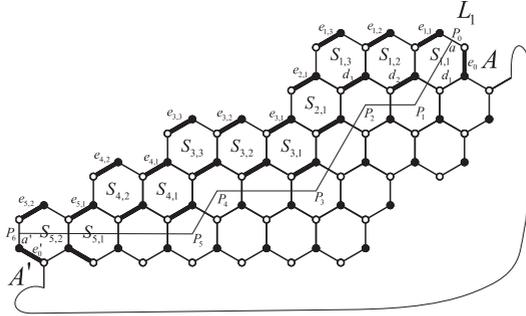


Figure 3: The hexagonal chain  $G$  on the left-top corner of  $H'$  (bold edges are  $M$ -double edges,  $m = 6$ ,  $n(1)=3$ ,  $n(2)=1$ ,  $n(3)=3$ ,  $n(4)=2$ ,  $n(5)=2$ . And  $A, A' \notin H'$ .)

contained in  $H'$  as Fig. 4. Let  $f_{k,\ell}$ ,  $1 \leq k \leq s$  and  $1 \leq \ell \leq t(k)$ , be a series of boundary edges on this structure as indicated in Fig. 4. Since the boundary of  $H'$  is a proper  $M$ -alternating cycle, we can see that all the edges  $f_0, f'_0, f_{k,\ell}$ ,  $1 \leq k \leq s$  and  $1 \leq \ell \leq t(k)$ , are  $M$ -double edges (see Fig. 4).

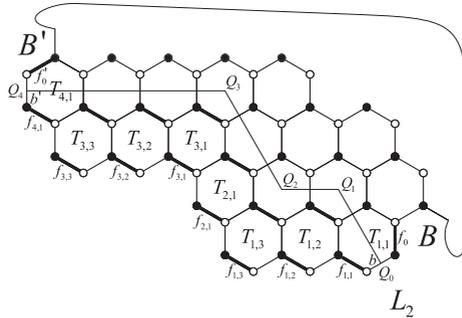


Figure 4: The hexagonal chain  $G'$  on the left-bottom corner of  $H'$  (bold edges are  $M$ -double edges,  $s = 4$ ,  $t(1)=3$ ,  $t(2)=1$ ,  $t(3)=3$ ,  $t(4)=1$ . And  $B, B' \notin H'$ .)

Like  $L_1$ , we also draw a ladder-shape broke line segment  $L_2 = Q_0Q_1 \cdots Q_{r+1}$  ( $r \geq 1$ ) as indicated in Fig. 4 so that the part below  $L_2$  has as many  $M$ -double edges parallel to  $f_{1,1}$  as possible. Let  $Q_i$  ( $1 \leq i \leq r$ ) be the center of a hexagon  $T_i$  of  $H'$ . Let  $H_2$  be the hexagonal chain consisting of the hexagons intersected by  $L_2$ .

Clearly, both  $L_1$  and  $L_2$  have an odd number of turning points. We now have the

following claim.

**Claim 4.** The boundary of  $H_1$  (resp.  $H_2$ ) is a proper  $M$ -alternating cycle and  $m \geq 2$  (resp.  $s \geq 2$ ).

*Proof.* We only consider  $H_1$  (the other case is almost the same). Let  $d_i$  be the edge of  $S_{1,i}$  opposite to  $e_{1,i}$ ,  $1 \leq i \leq n(1)$  (see Fig. 3). By Claim 2,  $S_{1,1}$  is not an  $M$ -alternating hexagon. It implies that all edges  $d_2, \dots, d_{n(1)}$  are  $M$ -double edges. Hence,  $S_{2,1}$  is a hexagon of  $H'$  and  $m \geq 2$ .

Let  $P_1$  be the path induced by those vertices of  $H_1$  which are just upon  $L_1$ . By the choice of  $L_1$ , we can see that  $P_1$  is an  $M$ -alternating path with two end edges in  $M$ . Let  $P_2$  be the path induced by those vertices of  $H_1$  which are just below  $L_1$ . It suffices to show that  $P_2$  is also an  $M$ -alternating path with two end edges in  $M$ .

Let  $w_1 (= e'_0), w_2, \dots, w_{\ell_2}$  be a series of parallel edges on the bottom of  $H_1$  and let  $h_1 (= e_0), h_2, \dots, h_{\ell_1}$  be a series of vertical edges of  $H_1$  on the right of  $P_0P_1$  (see Fig. 5).

For  $q = 1$ , by the condition (A2) and  $\{e_0, e'_0\} \subseteq M$ , it follows that  $h_1, h_2, \dots, h_{\ell_1}$  (resp.  $w_1, w_2, \dots, w_{\ell_2}$ ) are forced by  $e_0$  (resp.  $e'_0$ ) in turn and thus belong to  $M$  (see Fig. 5(a)). Therefore,  $P_2$  is an  $M$ -alternating path with two end edges in  $M$ .

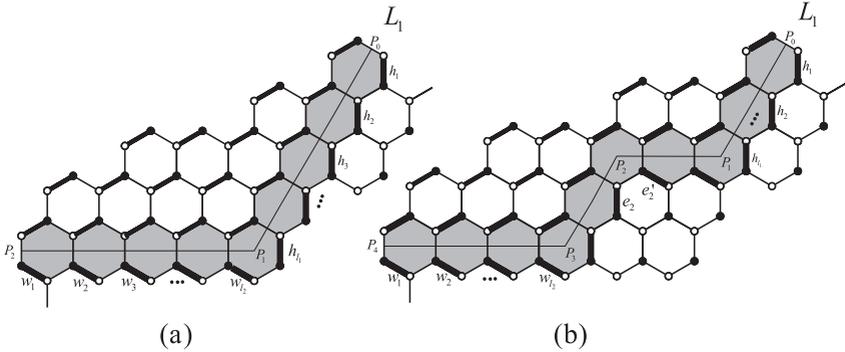


Figure 5: Illustration for Claim 4 in the proof of Lemma 2.1.

Let  $q \geq 3$ . For even  $i$ ,  $2 \leq i \leq q-1$ , let  $e''_i$  be the slant edge of  $S_i$  below  $L_1$ . Let  $e_i$  and  $e'_i$  be the two edges of  $H'$  which are adjacent to  $e''_i$  and below  $L_1$  (see Fig. 6(a)). Clearly,  $e_i$  is parallel to  $e_0$ , and  $e'_i$  is parallel to  $e'_0$ . We assert that  $e''_i \notin M$ . Otherwise,  $e''_i$  is an  $M$ -double edge. Since  $C$  is a proper  $M$ -alternating cycle,  $e''_i$  does not lie on the boundary

$C$  of  $H'$ . Thus  $S'_i$  is a hexagon of  $H'$  (see Fig. 6(b)). Moreover, we can switch from  $L_1$  to a new broke line segment  $L'_1$  which passes through  $S'_i$  and satisfies the conditions (A1–A2) (see Fig. 6(b)). But the part above  $L'_1$  has more  $M$ -double edges than above  $L_1$ , contradicting the choice for  $L_1$ . Thus the assertion is true. From condition (A2), we can see that  $\{e_0, e'_0, e_2, e'_2, \dots, e_{q-1}, e'_{q-1}\} \subseteq M$ . It follows that  $P_2$  is an  $M$ -alternating path with two end edges in  $M$  (see Fig. 5(b)). ■

For odd  $i$ , by Claim 4  $S_i$  ( $1 \leq i \leq q$ ) and  $T_i$  ( $1 \leq i \leq r$ ) are all proper  $M$ -alternating hexagons, and the other hexagons of  $H_1$  and  $H_2$  are not  $M$ -alternating. For convenience, let  $S_0 := S_{1,1}, S_{q+1} := S_{m,n(m)}, T_0 := T_{1,1}$  and  $T_{r+1} := T_{s,t(s)}$ . By Claim 2, we have that  $S_0 \neq S_1, S_{q+1} \neq S_q, T_0 \neq T_1$  and  $T_{r+1} \neq T_r$ . Further, by Claim 4 we can see that each hexagon in  $K'$  either belongs to  $H_1 \cup H_2$  or is disjoint with  $H_1 \cup H_2$ .

Let  $K_1 := \{S_0, S_2, \dots, S_{q+1}\}$  and  $K_2 := \{T_0, T_2, \dots, T_{r+1}\}$ . To complete the proof of the lemma, there are two cases to be considered.

**Case 1.**  $H_1$  and  $H_2$  are disjoint (see Figs. 3 and 4).

It is straightforward to verify that  $H_i - K_i$  has a perfect matching,  $i = 1, 2$ , so  $K_i$  is a resonant set of  $H_i$  and  $|K_i| \geq |H_i \cap K'| + 1$ .

Let  $K'' := (K_1 \cup K_2) \cup (K' - K' \cap H_1 - K' \cap H_2)$ . Similar to the proof of Claim 1, we have that  $K''$  is a resonant set of  $H'$  and  $|K''| \geq |K'| + 2$ . Thus  $Cl(H') \geq |K'| + 2$ .

**Case 2.**  $H_1$  intersects  $H_2$ .

By Claim 3 the last b-chain  $G_m$  in  $G$  coincides with the first b-chain  $G'_s$  in  $G'$ . Hence  $S_{q+1} = T_{r+1}$ . By Claim 4 both boundaries of  $H_1$  and  $H_2$  are proper  $M$ -alternating cycles. It follows that only segment  $P_q P_{q+1}$  of  $L_1$  is identical to segment  $Q_r Q_{r+1}$  of  $L_2$ . Hence  $H_1 \cup H_2$  is a cata-condensed hexagonal system with exactly one branch hexagon  $S_q (= T_r)$  as Fig. 7, and its boundary is also a proper  $M$ -alternating cycle. So  $H_1$  and  $H_2$  have exactly one common  $M$ -alternating hexagon. We also can see that  $K_1 \cup K_2$  is a resonant set of  $H_1 \cup H_2$ , and  $|K_1 \cup K_2| \geq |K' \cap (H_1 \cup H_2)| + 2$ . Let  $K'' := (K_1 \cup K_2) \cup (K' - K' \cap (H_1 \cup H_2))$ . By Claim 1, we have that  $K''$  is a resonant set of  $H'$  and  $|K''| \geq |K'| + 2$ . Thus  $Cl(H') \geq |K'| + 2$ .

Now the entire proof of the lemma is complete. ■

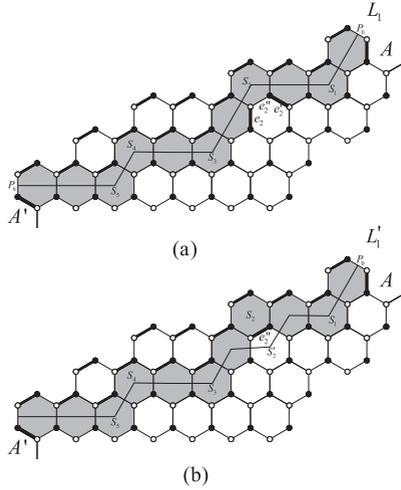


Figure 6: Illustration for Claim 4 in the proof of Lemma 2.1.

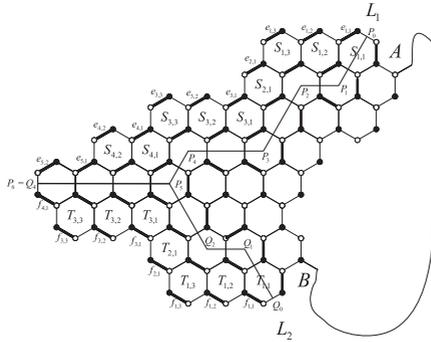


Figure 7: Illustration for Case 2 in the proof of Lemma 2.1.

### 3 Main results

We now state our main result as follows.

**Theorem 3.1.** *Let  $H$  be a hexagonal system with a perfect matching. For every perfect matching  $M$  of  $H$  such that  $f(H, M) = F(H)$ , there exist  $F(H)$  disjoint  $M$ -alternating hexagons of  $H$ .*

By Theorem 1.3, there are  $F(H)$  disjoint  $M$ -alternating cycles of  $H$ . It is well known that each  $M$ -alternating cycle of  $H$  has an  $M$ -alternating hexagon in its interior [24]. In order to prove the above theorem, we only need to prove the following lemma.

Let  $\mathcal{C}$  be a set of disjoint cycles of a hexagonal system  $H$ . A member of  $\mathcal{C}$  is called *minimal* if it contains no other members of  $\mathcal{C}$  in its interior.

**Lemma 3.2.** *Let  $H$  be a hexagonal system. Let  $M$  be a perfect matching of  $H$  with the maximum forcing number and let  $\mathcal{A}$  be a maximum set of disjoint  $M$ -alternating cycles of  $H$ . Then for any two members in  $\mathcal{A}$  their interiors are disjoint, and for any  $C \in \mathcal{A}$ ,  $I[C]$  is a linear chain.*

*Proof.* Let  $n := F(H) = f(H, M)$ . By Theorem 1.3,  $n = |\mathcal{A}|$ . Suppose to the contrary that there exist two cycles in  $\mathcal{A}$  so that their interiors have a containment relation. Then  $\mathcal{A}$  has a non-minimal member  $C_0$  and its interior contains only minimal members of  $\mathcal{A}$ .

Let  $\mathcal{A}_0$  denote the set of minimal members of  $\mathcal{A}$  whose interiors are contained in the interior of  $C_0$ . Then the restriction of  $M$  on  $I[C_0]$  is also a perfect matching of  $I[C_0]$ , denoted by  $M_c$ . Note that each  $M$ -alternating cycle has an  $M$ -alternating hexagon in its interior [24]. Then each cycle in  $\mathcal{A}_0$  can be replaced by an  $M$ -alternating hexagon, the set of these hexagons is a resonant set of  $I[C_0]$ , denoted by  $K$ . Clearly,  $K$  is disjoint with  $C_0$ ,  $|K| = \mathcal{A}_0$  and  $I[C_0] - C_0 - K$  has a perfect matching. By Lemma 2.1,  $I[C_0]$  has a resonant set  $S$  such that  $|S| \geq |K| + 2$ . Let  $M_0$  be a perfect matching of  $I[C_0]$  such that all hexagons in  $S$  are  $M_0$ -alternating. Let  $M_1 := (M \setminus M_c) \cup M_0$  and  $\mathcal{A}' := S \cup (\mathcal{A} - \{C_0\} - \mathcal{A}_0)$ . Then  $M_1$  is a perfect matching of  $H$  such that each member in  $\mathcal{A}'$  is an  $M_1$ -alternating cycle. Note that  $|\mathcal{A}'| \geq n + 1$ . By Theorem 1.3, we have that  $f(H, M_1) \geq n + 1$ . This contradicts that the maximum forcing number of  $H$  is  $n$ . Therefore, for any two members in  $\mathcal{A}$  their interiors are disjoint.

For any  $C \in \mathcal{A}$ , we assert that the Clar number of  $I[C]$  is 1. Otherwise,  $I[C]$  has a resonant set  $S'$  with  $|S'| \geq 2$ . Similar to the above discussion, we can obtain  $n + 1$  disjoint cycles which are  $M_2$ -alternating with respect to some perfect matching  $M_2$  of  $H$ . By Theorem 1.3, we have that  $F(H) \geq n + 1$ , a contradiction. Hence the assertion is true. By Theorem 2.2, for any  $C \in \mathcal{A}$ ,  $I[C]$  is a linear chain. ■

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