Some novel minimax results for perfect matchings of hexagonal systems *

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Abstract

The anti-forcing number of a perfect matching M of a graph G is the minimum number of edges of G whose deletion results in a subgraph with a unique perfect matching M, denoted by af(G, M). When G is a plane bipartite graph, Lei et al. established a minimax result: For any perfect matching M of G, af(G, M)equals the maximum number of M-alternating cycles of G where any two either are disjoint or intersect only at edges in M; For a hexagonal system, the maximum antiforcing number equals the fries number. In this paper we show that for every perfect matching M of a hexagonal system H with the maximum anti-forcing number or minus one, af(H, M) equals the number of M-alternating hexagons of H. Further we show that a hexagonal system H has a triphenylene as nice subgraph if and only af(H, M) always equals the number of M-alternating hexagons of H for every perfect matching M of H.

Keywords: Hexagonal system; Perfect matching; Anti-forcing number; Fries number; Triphenylene.

1 Introduction

All graphs considered in this paper are finite and simple connected graphs. Let G be a graph with vertex set V(G) and edge set E(G). A perfect matching M of G is a set of edges of G such that each vertex of G is incident with exactly one edge in M. This graph-theoretical concept coincides with a Kekulé structure of chemical molecules.

In 1987, Randić and Klein [14] proposed the *innate degree of freedom* of a Kekulé structure, i.e. the minimum number of double bonds which simultaneously belong to the given Kekulé structure and to no other one. This notion has arisen in the study of

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finding resonance structures of a given molecule in chemistry. Later, it is named "forcing number" by Harary et al. [13].

A forcing set S for a perfect matching M of a graph G is a subset of M which is not contained in 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). The maximum forcing number of G is the maximum value of forcing numbers of all perfect matchings of G, denoted by F(G). For further information on this topic, we refer the reader to a survey [4] and other references [2, 3, 10, 18, 20, 32, 27].

Let M be a perfect matching of a graph G. A cycle (resp. a path P) C of G is M-alternating if the edges of C (resp. P) appear alternately in M and $E(G)\backslash M$. It was revealed [2, 20] that a subset $S \subseteq M$ is a forcing set of M if and only if S contains at least one edge of each M-alternating cycle of G. This implies a simple inequality $f(G, M) \ge c(G, M)$, where c(G, M) denotes the maximum number of disjoint M-alternating cycles in G. In the case where G is a plane bipartite graph, Pachter and Kim [18] observed that these two numbers are always equal to each other.

Theorem 1.1. [18] Let G be a plane bipartite graph with a perfect matching M. Then

$$f(G, M) = c(G, M).$$

A more general result on bipartite graphs due to B. Guenin and R. Thomas is given as follows; see [11, Corollary 5.8].

Theorem 1.2. [11] Let G be a bipartite graph, and let M be a perfect matching in G. Then G has no matching minor isomorphic to $K_{3,3}$ or the Heawood graph if and only if f(G', M') = c(G', M') for every subgraph G' of G such that $M' = M \cap E(G')$ is a perfect matching in G'.

In 2007, the anti-forcing number of a graph was introduced by Vukičević and Trinajstić [25] as the smallest number of edges whose removal results in a subgraph with a unique perfect matching. In an early paper, Li [17] proposed a forcing single edge (i.e. anti-forcing edge) of a graph, which belongs to all but one perfect matching. For other researches on this topic, see Refs [4, 7, 26, 29].

More recently, by an analogous manner as the forcing number, Klein and Rosenfeld [15] and Lei et al. [16] independently defined the anti-forcing number of a single perfect matching in a graph. Let M be a perfect matching of a graph G. A subset $S \subseteq E(G) \setminus M$ is called an *anti-forcing set* of M if G - S has a unique perfect matching M, where G - S denotes the graph obtained from G by deleting all edges in S. The following lemma shows an equivalent condition.

Lemma 1.3. [16] Let G be a graph and M be a perfect matching of G. A subset S of $E(G)\setminus M$ is an anti-forcing set of M if and only if S contains at least one edge of every M-alternating cycle.

The minimum cardinality of anti-forcing sets of M is called the *anti-forcing number* of M, denoted by af(G, M). From these concepts, we can see that the anti-forcing number of a graph G is just the minimum value of anti-forcing numbers of all perfect matchings of G. The maximum anti-forcing number of G is the maximum value of anti-forcing numbers of all perfect matchings of G, denoted by Af(G). Two sharp upper bounds on maximum anti-forcing number and anti-forcing spectrum of a graph, we may refer to recent refs. [9, 23, 8].

Given a graph G with a perfect matching M, two M-alternating cycles of G are said to be *compatible* if they either are disjoint or intersect only at edges in M. A set \mathcal{A} of pairwise compatible M-alternating cycles of G is called a *compatible* M-alternating set. Let c'(G, M) denote the maximum cardinality of compatible M-alternating sets of G. We also have $af(G, M) \geq c'(G, M)$. For plane bipartite graphs G, Lei et al. [16] established the equality.

Theorem 1.4. [16] Let G be a plane bipartite graph with a perfect matching of M. Then

$$af(G,M) = c'(G,M).$$

A hexagonal system (or benzenoid) is a 2-connected finite plane graph such that every interior face is bounded by a regular hexagon of side length one [21]. It can also be formed by a cycle with its interior in the infinite hexagonal lattice on the plane (graphene) [6]. A hexagonal system with a perfect matching is regarded as a molecular graph (carbonskeleton) of a benzenoid hydrocarbon. Hence these kinds of graphs are called benzenoid systems and have been extensively investigated; We may refer to a detailed review [19] due to Randić.

Recently it was known [28, 16] that maximum forcing number and anti-forcing number of a hexagonal system are equal to the famous Clar number and Fries number respectively, which can measure the stability of polycyclic benzenoid hydrocarbons [1, 5, 12]. The same results hold for (4,6)-fullerene graphs [22].

Let H be a hexagonal system with a perfect matching. A subgraph H_0 of H is called nice if $H - V(H_0)$ has a perfect matching. A set of disjoint hexagons of H is called sextet pattern if they form a nice subgraph of H. The size of a maximum resonant set of H is the Clar number of H, denoted by Cl(H).

Theorem 1.5. [28] Let H be a hexagonal system with a perfect matching. Then F(H) = Cl(H).

Xu et al. [28] obtained the theorem by using Zheng and Chen's result [34] that if H - K has at least two different perfect matchings for a resonant set K of H, then $Cl(H) \ge |K| + 1$. By rising this bound by one, the present authors obtained a stronger result.

Theorem 1.6. [35] Let H be a hexagonal system with a perfect matching. For every perfect matching M of H with forcing number F(H), H has F(H) disjoint M-alternating hexagons.

However, Theorem 1.6 does not necessarily hold for perfect matchings of H with the forcing number F(H) - 1. For example, the Coronene (see Figure 1(a)) has the maximum forcing number 3. For the specific perfect matching of Coronene marked by the bold lines, it has forcing number two, but it has only one alternating hexagon.

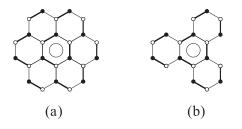


Figure 1: (a) Coronene, and (b) Triphenylene.

For a hexagonal system H with a perfect matching M, let fr(H, M) denote the number of all M-alternating hexagons in H. The maximum value of fr(H, M) over all perfect matchings M is just the *Fries number* of H, denoted by Fr(H). Since all M-alternating hexagons of H are compatible, Theorem 1.4 implies $af(H, M) = c'(H, M) \ge fr(H, M)$. The second equality does not hold in general. For example, the bold lines of Triphenylene in Figure 1(b) constitute a perfect matching with anti-forcing number two, whereas it has only one alternating hexagon. However, Lei et al. [16] obtained the following result by finding a perfect matching M with the equality.

Theorem 1.7. [16] Let H be a hexagonal system with a perfect matching. Then

$$Af(H) = Fr(H).$$

In this article, we show that af(H, M) = fr(H, M) always holds for every perfect matching M of a hexagonal system H with the maximum anti-forcing number or minus one.

Theorem 1.8. Let H be a hexagonal system with a perfect matching. Then for every perfect matching M of H with anti-forcing number Af(H) or Af(H) - 1, we have

$$af(H,M) = fr(H,M).$$
(1)

To prove this main result, in Section 2 we introduce some auxiliary terms relevant to our studies and give a crucial lemma that states that for a non-crossing compatible M-alternating set of H with two members whose interiors have a containment relation, the maximum anti-forcing number of H is larger than the cardinality by at least two. In Section 3, by using this lemma we obtain a stronger result: for any perfect matching M of H whose anti-forcing number reaches the maximum value or minus one, any two members in any given maximum non-crossing compatible M-alternating set of H have disjoint interiors and any member bounds a linear hexagonal chain, then give a proof of Theorem 1.8. In Section 4 we give a complete characterization to hexagonal systems Hthat always have Eq. (1) for each perfect matching M of H by forbidding a triphenylene as nice subgraph.

2 A crucial lemma

In what follows, we assume that all hexagonal systems are embedded in the plane such that some edges parallel to each other are vertical except for Figure 8. 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 two adjacent vertices receive different colors, and the *peaks* are colored black.

Let G be a plane bipartite graph with a perfect matching M, and let \mathcal{A} be a compatible M-alternating set of G. Two cycles in \mathcal{A} are said to be *non-crossing* if their interiors either are disjoint or have a containment relation. Further, we say \mathcal{A} is *non-crossing* if any two cycles in \mathcal{A} are non-crossing. The following useful lemma was described in the first claim of the proof of [16, Theorem 3.1].

Lemma 2.1. [16] Let H be a hexagonal system with a perfect matching M. Then for any compatible M-alternating set \mathcal{A} of H, H has a non-crossing compatible M-alternating set \mathcal{A}' with $|\mathcal{A}'| = |\mathcal{A}|$.

We now state a crucial lemma as follows.

Lemma 2.2. For a hexagonal system H with a perfect matching M_0 , let \mathcal{A}_0 be a noncrossing compatible M_0 -alternating set of H. Suppose \mathcal{A}_0 has a pair of members so that their interiors have a containment relation. Then $Af(H) \geq |\mathcal{A}_0| + 2$.

In order to prove this lemma, we need some further terminology. Let M be a perfect matching of H. An edge of H is called an M-double edge if it belongs to M, and an M-single edge otherwise. M-double edges are often indicated by bold or double edges in figures. An M-alternating cycle C of H is said to be proper (resp. improper) if each M-double edge in C goes from white end to black end (resp. from black end to white end) along the clockwise direction of C. The boundary of the infinite face of H is called the boundary of H, 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.

A hexagonal system H is *cata-condensed* if all vertices of H lie on $\partial(H)$. A hexagon of a cata-condensed hexagonal system is a *branch* if it has three adjacent hexagons. For example, the graph showed in Figure 1(b) is a cata-condensed hexagonal system with exactly one branch. A cata-condensed hexagonal system without branch is a *hexagonal chain*. In particular, it is a *linear chain* if the centers of all hexagons lie on a straight line. A maximal linear chain of a hexagonal chain is called a *segment*.

The symmetric difference of finite sets A_1 and A_2 is defined as $A_1 \oplus A_2 := (A_1 \cup A_2) \setminus (A_1 \cap A_2)$. This operation can be defined among many finite sets in a natural way and is associative and commutative. If C is an M-alternating cycle of H, then $M \oplus C$ is also a perfect matching of H and C is an $(M \oplus C)$ -alternating cycle of H, where C may be regarded as its edge-set.

For a cycle C of a hexagonal system H, let I[C] denote the subgraph of H formed by C together with its interior, and let h(C) be the number of hexagons in I[C].

Proof of Lemma 2.2. By the assumption, we can choose a perfect matching M of H and a non-crossing compatible M-alternating set \mathcal{A} of H so that the following three conditions hold.

(i) $|\mathcal{A}| = |\mathcal{A}_0|,$

(ii) \mathcal{A} has a pair of members so that their interiors have a containment relation,

(iii) $h(\mathcal{A}) := \sum_{C \in \mathcal{A}} h(C)$ is as small as possible subject to (i) and (ii).

Since \mathcal{A} is non-crossing, we have that for any two cycles in \mathcal{A} their interiors either are disjoint or one contains the other one. Hence the cycles in \mathcal{A} form a *poset* according to the containment relation of their interiors. Since each *M*-alternating cycle has an *M*-alternating hexagon in its interior (cf. [32]), we immediately have the following claim.

Claim 1. Every minimal member of \mathcal{A} is a hexagon.

By the choice of \mathcal{A} , we can see that \mathcal{A} has at least one non-hexagon member. Let C be a minimal non-hexagon member of \mathcal{A} . Then C is an M-alternating cycle whose interior contains only minimal members of \mathcal{A} . By Claim 1 C contains at least one hexagon as a member of \mathcal{A} in its interior. Set H' := I[C]. So it follows that H' is not a linear hexagonal chain.

Claim 2. For any *M*-alternating hexagon h in H', either $h \in \mathcal{A}$ or at least one of the three *M*-double edges of h does not belong to C.

Proof. If h belongs to \mathcal{A} , then the claim holds. If not, suppose to the contrary that the three M-double edges of h belong to C. Then $M \oplus h$ is a perfect matching of H, and all (one to three) components of $C \oplus h$ are $(M \oplus h)$ -alternating cycles. We can see that every minimal member of \mathcal{A} in H' is disjoint with h. By the choice of $C, C \oplus h$ has a component as a cycle C' which is not a hexagon and contains a minimal member of \mathcal{A} in its interior. Since each vertex of H has degree 2 or 3, each M-double edge of H is contained in at most two cycles of \mathcal{A} . This implies that $\mathcal{A} \setminus \{C\}$ has at most one member intersecting h. If such a member exists, denote it by C'' and let $\mathcal{A}' := (\mathcal{A} \cup \{h, C'\}) - \{C, C''\}$; otherwise, let $\mathcal{A}' := (\mathcal{A} \cup \{C'\}) - \{C\}$. Then \mathcal{A}' is a compatible $(M \oplus h)$ -alternating set of H satisfying Conditions (i) and (ii). But $h(\mathcal{A}') < h(\mathcal{A})$, contradicting the choice for \mathcal{A} . Hence Claim \mathbb{C}

Now we focus our attention on hexagonal system H' with the boundary C as some preliminaries. Without loss of generality, suppose that C is a proper M-alternating cycle (for the other case, analogous arguments are implemented on right-top and right-bottom corners of H').

We apply an approach and notion appeared in Ref. [35]. Along the boundary C of H', we will find two substructures of H' in its left-top corner and left-bottom corner as Figures 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 Figure 2 (taken from [35]), D_0 , D_1 , D_2 , G_1 , G_2 , ..., 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, \ldots, G_9 and D_7 are neither high nor low b-chains.

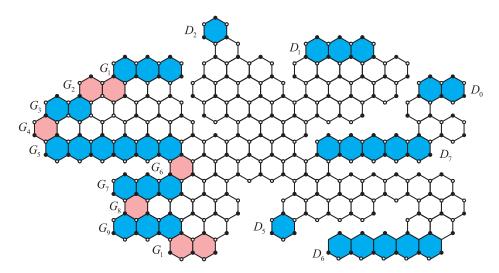


Figure 2: Various b-chains of a hexagonal system, taken from [35].

Given a high b-chain and a low b-chain of H', they are distinct, otherwise H' itself is a linear chain, contradicting the choice of C. When traversing the b-chains along the boundary $\partial(H')$ counterclockwise from the high b-chain to the low b-chain, let G_1 be the last high b-chain and let G'_1 be the first low b-chain after G_1 . Then the 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, \ldots, G_m , $m \geq 1$, 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 a b-chain next to G_m such that G_{m+1} has no hexagon lying on the lower left side of G_m . Let G be the subgraph of H' consisting of b-chains $G_1, G_2, \ldots, G_{m-1}$ and the hexagons of G_m lying on the lower left side of G_{m-1} . Then G is a ladder-shape hexagonal chain.

Similarly, from low b-chain G'_1 we have a sequence of consecutive b-chains $G'_1, G'_2, \ldots, G'_{s}$, $s \geq 1$, with the following properties: (1) for each $1 \leq j < s$, G'_{j+1} is next to G'_j , and the left end hexagon of G'_{j+1} lies on the upper left side of G'_j , (2) either G'_s is just the high b-chain G_1 or G'_{s+1} is next to the b-chain G'_s such that G'_{s+1} has no hexagon lying on the upper left side of G'_s . Let G' be the subgraph of H' consisting of b-chains $G'_1, G'_2, \ldots, G'_{s-1}$ and the hexagons of G'_s lying on the higher left side of G'_{s-1} . So G' is an inverted ladder-shaped hexagonal chain.

For example, given a high b-chain D_1 and a low b-chain D_5 in Figure 2, we can get

two required hexagonal chains $G = G_1 \cup G_2 \cup G_3 \cup G_4$ and $G' = G_9 \cup G'_1$. The following claim is obvious.

Claim 3. Either G and G' are disjoint or they intersect only in the b-chain $G_m = G'_s$.

To analyze the substructure G of H', we label some edges of G as follows (see Figure 3): let $e_{1,1}$ be the slant M-double edge of the right end hexagon of G_1 which belongs to C and contains a peak of H'. Neither A nor A' is contained in H'. Denote by $e_{i,j}$, $1 \le i \le m$ and $1 \le j \le n(i)$, the *j*-th edge of G_i that is parallel to $e_{1,1}$ and on the boundary C of H', and denote the specific edges in G_1 and G_m by a, a' and e_0, e'_0 respectively.

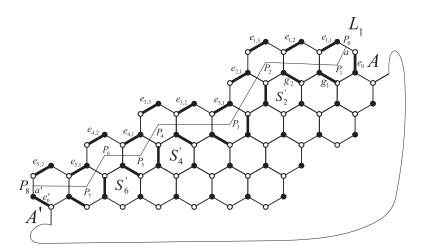


Figure 3: Hexagonal chain G on the left-top corner of H' (bold edges are M-double edges, m = 5, n(1)=3, n(2)=1, n(3)=3, n(4)=2, n(5)=2 and $A, A' \notin H'$) and the corresponding broken line segment L_1 .

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. In order to simplify our discussions, we draw a ladder-shape broken line segment $L_1 = P_0P_1 \cdots P_{q+1}(q \geq 1)$ (see Figure 3) satisfying: (1) L_1 only passes through hexagons of G, (2) the endpoints P_0 and P_{q+1} are the midpoints of the edges a and a' respectively, (3) L_1 passes through the centers of all hexagons of G, and (4) each P_i ($1 \leq i \leq q$) is a turning point, which is the center of a hexagon S_i of G. Then each line segment P_iP_{i+1} ($0 \leq i \leq q$) is orthogonal to an edge direction, 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.

Similarly we treat substructure G' of H' as follows (see Figure 4). Let $f_{k,\ell}$, $1 \le k \le s$ and $1 \le \ell \le t(k)$, and f_0, f'_0, b, b' be a series of boundary edges on this structure as indicated in Figure 4. Neither hexagon B nor hexagon B' is contained in H'. Since the boundary of H' is a proper M-alternating cycle, we can see that all the edges $f_0, f'_0, f_{k,\ell},$ $1 \le k \le s$ and $1 \le \ell \le t(k)$, are M-double edges.

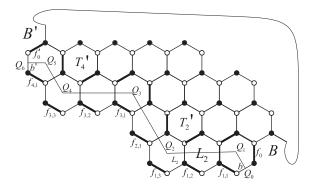


Figure 4: Hexagonal chain G' on the left-bottom corner of H' (bold edges are M-double edges, s = 4, t(1)=3, t(2)=1, t(3)=3, t(4)=1 and $B, B' \notin H'$) and the corresponding broken line segment L_2 .

Like L_1 , we also draw a ladder-shape broken line segment $L_2 = Q_0Q_1 \cdots Q_{r+1} (r \ge 1)$ as indicated in Figure 4 so that L_2 only passes through hexagons of G' and each turning point Q_i $(1 \le i \le r)$ is the center of a hexagon T_i of G'. It is obvious that both L_i , i = 1, 2, have an odd number of turning points. By Claim 3, we immediately obtain the following claim.

Claim 4. Either the broken line segments L_1 and L_2 are disjoint or the last segment $P_q P_{q+1}$ of L_1 is identical to the last segment $Q_r Q_{r+1}$ of L_2 .

Since the boundary of H' is a proper *M*-alternating cycle, we have that all the edges of *H* intersected by L_i , i = 1, 2, are *M*-single edges. We now have the following claim.

Claim 5. (a) The boundary of G (resp. G') is a proper M-alternating cycle, and (b) n(1) = 1 or 2 (resp. t(1) = 1 or 2), and $m \ge 2$ (resp. $s \ge 2$).

Proof. We only consider G (the other case is almost the same). Let Z_1 be the path induced by those vertices of G which are just upon L_1 . Let Z_2 be the path induced by those vertices of G which are just below L_1 . Since the boundary C of H' is a proper M-alternating cycle, Z_1 is an M-alternating path with two end edges in M.

To prove statement (a), it suffices to show that Z_2 is also an *M*-alternating path with two end edges in *M*. Let $w_1(=e'_0), w_2, \ldots, w_{\ell_2}$ be all parallel edges of *G* below P_qP_{q+1} and let $h_1(=e_0), h_2, \ldots, h_{\ell_1}$ be all vertical edges of *G* on the right of P_0P_1 (see Figure 5). Note that all the edges intersected by L_1 are *M*-single edges. It follows from $\{e_0, e'_0\} \subseteq M$ that $h_1, h_2, \ldots, h_{\ell_1}$ (resp. $w_1, w_2, \ldots, w_{\ell_2}$) are forced by e_0 (resp. e'_0) in turn to belong to *M*.

If q = 1, Z_2 is an *M*-alternating path with two end edges in *M*. Let $q \ge 3$. For each even $i, 2 \le i \le q - 1$, let e''_i be the slant edge of S_i in Z_2 . Let e_i and e'_i be the two edges of Z_2 adjacent to e''_i (see Figure 5(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, $e''_i \in M$, and e''_i does not lie on the boundary *C* of *H'* since *C* is a proper *M*-alternating cycle. So *H'* has a hexagon S'_i containing e_i, e'_i and e''_i . Let $C' := C \oplus S_i$ and let $\mathcal{A}' := (\mathcal{A} \cup \{C'\}) - \{C\}$ (see Figure 5(b)). Then \mathcal{A}' is a compatible *M*-alternating set of *H* satisfying conditions (i) and (ii). But $h(\mathcal{A}') = h(\mathcal{A}) - 1$, contradicting the choice of \mathcal{A} . So the assertion is true. Note that all the edges intersected by L_1 are *M*-single edges. We have $\{e_0, e'_0, e_2, e'_2, \ldots, e_{q-1}, e'_{q-1}\} \subseteq M$. So it follows that Z_2 is an *M*-alternating path with two end edges in *M* (see Figure 3). Hence statement (a) holds.

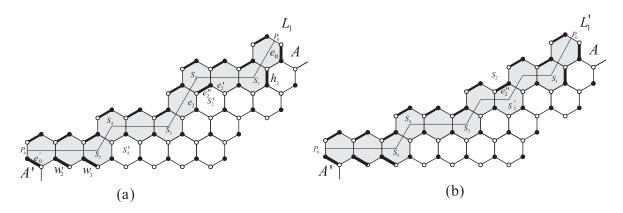


Figure 5: Illustration for Claim 5 in the proof of Lemma 2.2.

Next we prove statement (b). Suppose to the contrary that $n(1) \geq 3$. Let $S_{1,1}$ and $S_{1,2}$ be the first and second hexagons of high b-chain G_1 from right to left. Then P_1 is the center of $S_{1,1} = S_1$. For i = 1, 2, let g_i be the edge of $S_{1,i}$ parallel to a and below L_1 (see Figure 3). By statement (a), we have $g_1, g_2 \in M$. Therefore, S_1 is a proper M-alternating hexagon, but not in \mathcal{A} . By Claim 2, $g_1 \notin C$. Since the boundary C of H' is an M-alternating cycle, g_1 has no end-vertices in C. This implies that S_1 has three consecutively adjacent hexagons in H'. We can see that none of members of \mathcal{A} except C intersect S_1 . Let $M' := M \oplus S_1$ and $\mathcal{A}' := (\mathcal{A} \cup \{C \oplus S_1\}) - \{C\}$. Then M' is a perfect matching of H, and \mathcal{A}' is a compatible M'-alternating set satisfying conditions (i) and (ii). But $h(\mathcal{A}') < h(\mathcal{A})$, contradicting the choice for \mathcal{A} . Hence n(1) = 1 or 2.

Suppose to the contrary that m = 1. By statement (a), we can see that $g_1 \in M$ and g_1 is an edge of S_1 . We have that S_1 is a proper *M*-alternating hexagon, but not in \mathcal{A} . By analogous arguments as above, we arrive in a similar contradiction no matter n(1) = 1 or 2. Hence $m \geq 2$ and statement (b) holds.

Claim 5 implies that for all odd integers i and j, S_i $(1 \le i \le q)$ and T_j $(1 \le j \le r)$ are proper *M*-alternating hexagons, and the other hexagons of *G* and *G'* are not *M*-alternating.

For each even $i, 2 \leq i \leq q-1$, let S'_i denote the hexagon (in the hexagonal lattice, but not necessarily contained in H) adjacent to S_i and below L_1 (see Figure 3). Similarly, for each even $j, 2 \leq j \leq r-1$, let T'_j denote the hexagon adjacent to T_j and above L_2 (see Figure 4).

By the above discussions to H', we now go back to the discussion to H and will get our result. We now get a new perfect matching M' of H from M by rotating all M-alternating

hexagons of G and G' as follows (see Figure 6),

$$M' := M \oplus S_1 \oplus S_3 \oplus \cdots \oplus S_q \oplus T_1 \oplus T_3 \oplus \cdots \oplus T_r.$$

Let \mathcal{B} be the set of M'-alternating hexagons in $G \cup G'$ and let $\mathcal{B}' = \{S'_2, S'_4, \ldots, S'_{q-1}\}$ $\cup \{T'_2, T'_4, \ldots, T'_{r-1}\}$. Then $\mathcal{B} \supseteq \{S_1, S_3, \ldots, S_q, T_1, T_3, \ldots, T_r\}$. We can have the following system of cycles of H,

$$\mathcal{A}' := (\mathcal{A} \cup \mathcal{B}) \setminus (\mathcal{B}' \cup \{C\}).$$

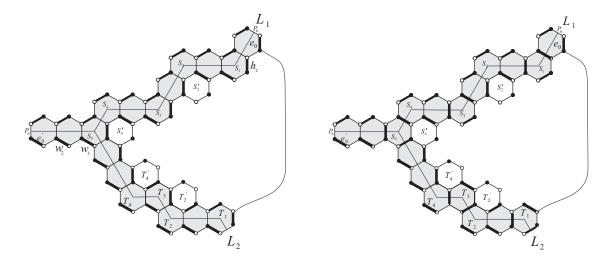


Figure 6: Illustration for Claim 6: The gray hexagons form $G \cup G'$, and perfect matchings M and M' of H have restrictions on $G \cup G'$ as left and right respectively.

Claim 6. \mathcal{A}' is an M'-alternating compatible set and $|\mathcal{A}'| \ge |\mathcal{A}| + 2$.

Proof. Given any member C' in \mathcal{A}' . Then $C' \in \mathcal{A}$ or \mathcal{B} . First we want to show that C' is an M'-alternating cycle. If C' does not intersect anyone of $S_1, S_3, \ldots, S_q, T_1, T_3, \ldots, T_r$, then $C' \in \mathcal{A}$ and C' is both M- and M'-alternating cycle. If $C' = S_i$ or T_j for odd $1 \leq i \leq q$ and odd $1 \leq j \leq r$, then $C' \in \mathcal{B}$ and C' is both M- and M'-alternating cycle. The remaining case is that C' intersects some S_i or T_j for odd $1 \leq i \leq q$ and odd $1 \leq j \leq r$, say the former S_i , but $C' \neq S_i$. We assert that $C' \in \mathcal{B}$, which implies that C' is an M'-alternating hexagon. Suppose to the contrary that $C' \in \mathcal{A} \setminus \mathcal{B}$. Then C' is an M-alternating hexagon not in G since each member of \mathcal{A} lying in the interior of C is a hexagon. So $C' = S'_{i-1}$ for $i \geq 3$ or $C' = S'_{i+1}$ for $i \leq q-2$, a contradiction. Otherwise, C' lies outside C since C and C' are non-crossing. Since C and C' are compatible M-alternating cycles, C' passes through only either the right vertical edge e_0 of S_1 for $n(1) \geq 2$ or e'_0 of S_q for n(m) = 1 and G and G' being disjoint. In such either case, three M-double edges of S_1 or S_q belong to C, contradicting Claim 2, so the assertion holds.

Next we show that \mathcal{A}' is an M'-alternating compatible set. For the members of \mathcal{A}' lying in the interior of C, they are M'-alternating hexagons and thus compatible.

For the members C' of \mathcal{A}' lying in the exterior of C, C' is disjoint with everyone of $S_1, S_3, \ldots, S_q, T_1, T_3, \ldots, T_r$. Otherwise, $C' \in \mathcal{B}$ by the above assertion, contradicting that C' lies on the exterior of C. So such members C' are M-alternating cycles in \mathcal{A} and compatible. Suppose that C' intersects some member h of \mathcal{A}' inside C. By the Jordan Curve Theorem we know that $C' \cap h \subset C$. That is, each edge of $C' \cap h$ belong to C. Since M and M' have the same restriction on $C' \cap h$ and C' and C are compatible M-alternating cycles, each edge of $C' \cap h$ belong to M, thus to M', so C' and h are compatible M'-alternating cycles.

Finally we show the remaining inequality. For each odd i with $1 \leq i \leq q-2$, the hexagons between S_i and S_{i+2} in G are not M-alternating, but at least one and at most two of them are M'-alternating hexagons, which correspond to S'_{i+1} . Similarly for each odd j with $1 \leq i \leq r-2$, the hexagons between T_i and T_{i+2} in G' are not M-alternating, but at least one and at most two of them are M'-alternating hexagons, which correspond to T'_{i+1} . Next we consider the end segments of hexagonal chains G and G'. If $n(1) \geq 2$, then S_1 is the right end-hexagon of G_1 , and $S_1 \notin \mathcal{A}$ since S_1 and C are not compatible M-alternating cycles. But, $S_1 \in \mathcal{B}$. Otherwise, G_1 is a single hexagon other than S_1 , the upper end segment of G has a unique M-hexagon and two M'-alternating hexagons, S_1 and its neighbor. Similarly we have that the last row G_m of G has more members of \mathcal{B} than \mathcal{A} by at least one. In analogous arguments as above we also have that the first segment and last row of G' each has more members of \mathcal{A} than \mathcal{B} by at least one. Note that if both last rows of G and G' are identical, then their extra members together count one, and C is moved out \mathcal{A} . So we have that $|\mathcal{A}'| \geq |\mathcal{A}| + 2$.

By Theorem 1.3 and Claim 6, we have $Af(H) \ge af(H, M') = c'(H, M') \ge |\mathcal{A}'| \ge |\mathcal{A}| + 2 = |\mathcal{A}_0| + 2$, that is, $Af(H) \ge |\mathcal{A}_0| + 2$. Now the entire proof of the lemma is complete.

3 Minimax results for large anti-forcing numbers

We can describe a minimax result stronger than Theorem 1.8 as follows.

Theorem 3.1. For a hexagonal system H, let M be a perfect matching of H with af(H, M) = Af(H) or Af(H) - 1, and let \mathcal{A} be a maximum non-crossing compatible M-alternating set of H. Then (1) any two members in \mathcal{A} have disjoint interiors, and (2) for any $C \in \mathcal{A}$, I[C] is a linear chain.

From Statement (1) of Theorem 3.1, which is implied by Lemma 2.2, we immediately obtain our main result.

Proof of Theorem 1.8. Let \mathcal{A} be a maximum non-crossing compatible M-alternating set of H. Then by Theorem 1.4 and Lemma 2.1, we have $af(H, M) = |\mathcal{A}|$. By Theorem 3.1(1), we know that for any two cycles in \mathcal{A} their interiors are disjoint. It was shown in

[33] that for each $C \in \mathcal{A}$, H has an M-alternating hexagon h in I[C]. All such cycles C in \mathcal{A} are replaced with M-alternating hexagons h of I[C] to get a set K of M-alternating hexagons with $|K| = |\mathcal{A}|$. So we have $fr(H, M) \ge |K| = af(H, M)$. On the other hand, $af(H, M) \ge fr(H, M)$ since K is also a compatible M-alternating set. Both inequalities imply the result.

In order to prove Theorem 3.1(2), the characterization for hexagonal systems H with af(H) = 1 due to Li [17] are presented here. It is clear that H has an anti-forcing edge if and only if af(H) = 1.

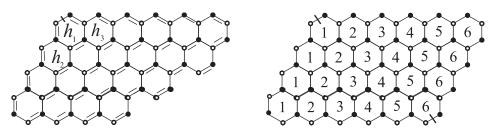


Figure 7: Truncated parallelograms H(6, 6, 5, 4) and H(6, 6, 6, 6): anti-forcing edges are marked.

For integers $n_1 \ge n_2 \ge \ldots \ge n_k$, $k \ge 1$, let $H(n_1, n_2, \ldots, n_k)$ be a hexagonal system with k horizontal rows of $n_1 \ge n_2 \ge \ldots \ge n_k$ hexagons and first hexagon of each row being immediately below and to the right of the first one in the previous row, and we call it *truncated parallelogram* [6]; For example, see Figure 7. In particular, $H(r, r, \ldots, r)$ with $k \ge 2$ is parallelogram, both $H(1, 1, \ldots, 1)$ with $k \ge 1$ and H(r) with $r \ge 1$ are linear chains.

Theorem 3.2. [17] Let H be a hexagonal system. Then af(H) = 1 if and only if H is a truncated parallelogram.

Proof of Theorem 3.1. (1) By Theorem 1.4 and Lemma 2.1, we have $af(H, M) = |\mathcal{A}|$. Suppose to the contrary that statement (1) does not hold. Then by Lemma 2.2 we have $Af(H) \ge |\mathcal{A}| + 2 = af(H, M) + 2 \ge Af(H) + 1$, a contradiction. So statement (1) holds.

(2) Let $n := af(H, M) = |\mathcal{A}|$ and let $\mathcal{A} =: \{C_1, C_2, \ldots, C_n\}$. Choose an anti-forcing set S of M with |S| = n. Let $S_i := S \cap E(C_i)$, $i = 1, 2, \ldots, n$. By Lemma 1.3 we have $S_i \neq \emptyset$ for each i. Since \mathcal{A} is a compatible M-alternating set, $S_i \cap S_j = \emptyset$ for any $1 \le i < j \le n$. So we can assume that $S := \{e_1, e_2, \ldots, e_n\}$ with $e_i \in E(C_i)$ for all $1 \le i \le n$. For any $1 \le i \le n$, since C_i is an M-alternating cycle of H, the restriction M_i of M on $I[C_i]$ is a perfect matching of $I[C_i]$. By Theorem 3.1(1), we can see that only edge e_i of S lies in $I[C_i], 1 \le i \le n$. So all M_i -alternating cycles in $I[C_i]$ pass through edge $e_i, 1 \le i \le n$. By Lemma 1.3, we have that $\{e_i\}$ is an anti-forcing set of $M_i, 1 \le i \le n$. That is, e_i is an anti-forcing edge of $I[C_i]$. By Theorem 3.2, each $I[C_i]$ is a truncated parallelogram.

If some $I[C_i]$ is not a linear chain, i.e. $I[C_i]$ has at least two rows and at least two columns of hexagons, then $I[C_i]$ has a unique perfect matching M_i not containing edge e_i (see Figure 7 (left)). Let h_1 be the hexagon of $I[C_i]$ with edge e_i , and let h_2 and h_3 be the two hexagons of I[C] adjacent to h_1 in the first column and the first row respectively. It was pointed out in [17] that h_1 is only M_1 -alternating hexagon in $I[C_1]$. So $M' := M \oplus h_1$ is a perfect matching of H, and h_1, h_2 and h_3 are M'-alternating hexagons. We can see that $\mathcal{A}' := \mathcal{A} \cup \{h_1, h_2, h_3\} - \{C\}$ is a compatible M'-alternating set of H. Hence $Af(H) \ge af(H, M') \ge |\mathcal{A}'| = |\mathcal{A}| + 2 \ge Af(H) + 1$, a contradiction. Hence each $I[C_i]$ is a linear chain and statement (2) holds. \Box

4 Minimax result for all perfect matchings

It is natural to ask whether Theorem 1.8 holds for all perfect matchings M of a hexagonal system H. A counterexample can show that the minimax relation does not necessarily hold for a perfect matching of a hexagonal system H with the third maximum anti-forcing number Af(H) - 2.

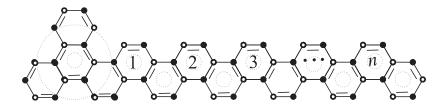


Figure 8: A hexagonal system R_n with a perfect matching M.

Let R_n be a hexagonal system with 2n + 4 hexagons and a perfect matching M as shown in Figure 8 (the edges in M are indicated by double edges). Then R_n contains one triphenylene whose central hexagon is denoted h. Let $M' = M \oplus h$. Then all hexagons of R_n are M'-alternating. So the Fries number of R_n is the number of hexagons in R_n (see also [13]). By Theorem 1.7, we have $Af(R_n) = Af(R_n, M') = Fr(R_n) = 2n + 4$.

However we can confirm that $af(R_n, M) = Af(H) - 2 > fr(H, M)$. By counting *M*-alternating hexagons in R_n , we have that fr(H, M) = 2n + 1. On the other hand, we can find a compatible *M*-alternating set of size 2n + 2. So $af(R_n, M) \ge 2n + 2 >$ fr(H, M). By a direct check or Theorem 1.8, we have $af(R_n, M) \le Af(R_n) - 2$. So $af(R_n, M) = Af(H) - 2$.

We can see that the above counterexample contains a triphenylene as nice subgraph. In fact we can give a characterization for a hexagonal system H to have the mini-max relation af(H, M) = fr(H, M) by forbidding triphenylene as nice subgraph (see Theorem 4.3).

To the end we present some concepts and known results. Let H be a hexagonal system with a perfect matching. Let r(H) and k(H) be the numbers of sextet patterns and Kekulé structures of H respectively. **Theorem 4.1** ([30, 24]). Let H be a hexagonal system with a perfect matching. Then $r(H) \leq k(H)$, and the following statements are equivalent. (i) r(H) = k(H),

(ii) H has a coronene as a nice subgraph, and

(iii) H has two disjoint cycles R and C so that R lies in the interior of C and $R \cup C$ is a nice subgraph of G.

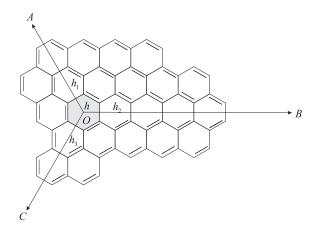


Figure 9: A hexagonal system with a unique M-alternating hexagon for a perfect matching M marked by double lines.

Let H be a hexagonal system with a hexagon h. Draw three rays OA, OB and OC from the center O of h so that they pass through the centers of three disjoint edges of h respectively, which divide the plane into three areas AOB, BOC and COA. Such three regional coordinate system is denoted by O - ABC. Zhang et al. [31] ever gave the following fact.

Lemma 4.2. A hexagonal system H has a perfect matching M with a unique M-alternating hexagon h if and only if it has the coordinate system O - ABC so that O is the center of h,rays OA, OB and OC do not intersect edges in M and all edges of M in anyone of areas AOB, BOC and COA are parallel to each other.

Theorem 4.3. Let H be a hexagonal system with a perfect matching. Then H has no triphenylenes as nice subgraph if and only if for each perfect matching M of H, af(H, M) = fr(H, M).

Proof. We first prove the sufficiency. Suppose to the contrary that H contains a triphenylene as a nice subgraph. Let M' be a perfect matching of the triphenylene as shown in Figure 1(b). Because the triphenylene is a nice subgraph of H, M' can be extended to a perfect matching M of H. So $M' \subseteq M$. Let C be the boundary of the triphenylene. It is easy to see that C is an M-alternating cycle of H and C is compatible with each M-alternating hexagon of H. By Theorem 1.4, we have $af(H, M) \geq fr(H, M) + 1 > fr(H, M)$, a contradiction. Hence the sufficiency holds. We now prove the necessity. Suppose to the contrary that H has a perfect matching M_0 so that $af(H, M_0) > fries(H, M_0)$. Let \mathcal{A} be a maximum non-crossing compatible M_0 -alternating set of H. By Theorem 1.4 and Lemma 2.1 we have $af(H, M_0) = |\mathcal{A}|$ and there are two cycles in \mathcal{A} so that their interiors have a containment relation; Otherwise, since there is an M_0 -alternating hexagon in the interior of each M_0 -alternating cycle [33], H has at least $af(H, M_0) = M_0$ -alternating hexagons, that is, $af(H, M_0) \leq fr(H, M_0)$, a contradiction. So we can select two cycles C_1 and C_2 in H to meet the following conditions:

(i) $I[C_1] \subseteq I[C_2]$,

(ii) H has a perfect matching M so that C_1 and C_2 are compatible M-alternating cycles, and

(iii) $h(C_1) + h(C_2)$ is as small as possible subject to Conditions (i) and (ii) (recall that $h(C_i)$ is the number of hexagons inside C_i).

If $I[C_2]$ has an *M*-alternating hexagon *h* which is disjoint with C_2 , then $h \cup C_2$ is a nice subgraph of *H*. By Theorem 4.1, *H* contains a coronene as a nice subgraph. So *H* also contains triphenylene as a nice subgraph.

From now on suppose that all the *M*-alternating hexagons in $I[C_2]$ intersect C_2 . Obviously, if C_2 is a proper (resp. improper) *M*-alternating cycle, then each of the *M*-alternating hexagons in $I[C_2]$ is also proper (resp. improper). Without loss of generality, suppose that the C_2 and *M*-alternating hexagons in $I[C_2]$ are proper. Take an *M*-alternating hexagon *h* inside C_1 . Since C_1 and C_2 are compatible *M*-alternating, *h* is compatible with C_2 . We can show the following fact.

Claim. h is the only *M*-alternating hexagon in $I[C_2]$.

Proof. Suppose to the contrary that h' is an M-alternating hexagon of $I[C_2]$ different from h. Then h' and h are disjoint because any two proper M-alternating hexagons do not intersect. Let $M' := M \oplus h'$ and $C'_2 := C_2 \oplus h'$. Then M' is a perfect matching of H, and each component of $C_2 \oplus h'$ is an M'-alternating cycle. Take a component C'_2 of $C_2 \oplus h'$ so that h lies inside C'_2 . Then h and C'_2 are also compatible M'-alternating cycles. It is clear that the cycles C'_2 and h satisfy the above conditions (i) and (ii). But $h(C'_2) + 1 < h(C_2) + h(C_1)$, a contradiction with the minimality of $h(C_2) + h(C_1)$. \Box

Note that the restriction of M on $I[C_2]$ is a perfect matching of $I[C_2]$. From the Claim and Lemma 4.2, from center O of h we establish coordinate system O - ABC so that OA, OB and OC do not pass through M-edges in $I[C_2]$, and all M-double edges of $I[C_2]$ in anyone of areas AOB, BOC and COA are parallel to each other (see Figure 9). Because h and C_2 are two compatible M-alternating cycles, every M-single edge of h is not on C_2 . This shows that h has three adjacent hexagons h_1, h_2 , and h_3 in $I[C_2]$ which intersect OA, OB, and OC respectively. Further, hexagons h, h_1, h_2 and h_3 form a triphenylene whose boundary is M-alternating cycle. So the triphenylene is a nice subgraph of H, a contradiction. So $af(H, M_0) = fr(H, M_0)$ and the necessity holds.

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