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The Minimum Forcing and Anti–Forcing Numbers of Convex Hexagonal Systems*

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Abstract

A convex hexagonal system (CHS) is a hexagonal system whose inner dual has the convex polygonal boundary. The minimum forcing number of a graph G is the smallest cardinality of a matching of G contained in a unique perfect matching. The minimum anti-forcing number of G is the smallest cardinality of an edge subset of G whose deletion results in a graph with exactly one perfect matching. In this paper, we proved that for any convex hexagonal system $H(a_1, a_2, a_3)$ with a perfect matching, its minimum forcing and anti-forcing numbers are both equal to $\min\{a_1, a_2, a_3\}$ by applying perfect path systems.

1 Introduction

A *hexagonal system*, also called *benzenoid system*, is a 2-connected plane bipartite graph so that every interior face is a regular hexagon. A *perfect matching* of a graph is a set of disjoint edges covering all vertices of it. This concept coincides with that of a Kekulé structure in organic chemistry. The carbon-skeleton of a benzenoid hydrocarbon may be represented by a hexagonal system with a perfect matching. Kekulé structures of hexagonal systems have been extensively investigated; for example, see [5, 7].

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For a perfect matching M in a graph G, an edge subset $S \subseteq M$ is called a *forcing set* of M in G if $G - V(S)$ contains exactly one perfect matching. The smallest cardinality over all forcing sets of M is the *forcing number* of M, denoted by $f(G, M)$. The minimum and maximum values of forcing numbers of all perfect matchings of G are called the minimum and maximum forcing number of G, respectively, denoted by $f(G)$ and $F(G)$. The concept of "forcing number " in perfect matchings was first introduced by Randić and Klein [9] under name "*innate degree of freedom*", and then renamed by Harary et al. [8].

Forcing number of a Kekulé structure of a benzenoid system is related closely to resonance theory. According to Clar's aromatic sextet theory [4], for any two isometric benzenoid hydrocarbons, the one with larger Clar number is more stable. Xu et al. [19] showed that the maximum forcing number of a hexagonal system H is equal to its Clar number (or resonant number). Further Zhou and Zhang [27] showed that for each perfect matching M of H with the maximum forcing number, the maximum set of disjoint M-alternating hexagons has the size equal to the Clar number. For polyomino graphs and (4,6)-fullerenes, the former assertion also holds (cf. [16, 28]). Zhang and Li [21] characterized a hexagonal system with a forcing edge. Wang et al. [18] gave a linear algorithm to compute the minimum forcing number of a toroidal polyhex. Recently, Diwan [6] proved that for a hypercube Q_n, $f(Q_n) = 2^{n-2}$, which was ever conjectured by Pachter and Kim [14]. Afshani et al. [2] proved that determining the minimum forcing number is NP-complete for bipartite graphs with maximum degree 4.

As early as 1997, Li [12] characterized hexagonal systems with a forcing single edge (i.e. anti-forcing edge). In 2007, Vukičević and Trinajstić [17] proposed the anti-forcing number of a graph. Lei et al. [11] and Klein and Rosenfeld [10] independently generalized the idea of "anti-forcing" to every perfect matching. For a perfect matching M in a graph G, a set S of edges of G not in M is called an *anti-forcing set* of M if $G - S$ has a unique perfect matching M. The cardinality of a smallest anti-forcing set of M is called the anti-forcing number of M, denoted by $af(G, M)$. The minimum (resp. maximum) anti-forcing number of G is denoted by $af(G)$ (resp. $Af(G)$). Lei et al. [11] and Shi et al. [16] respectively proved that the maximum anti-forcing numbers of hexagonal systems and (4,6)-fullerenes are equal to their Fries numbers. The previous paper also characterized the hexagonal systems H with $af(H) = 2$.

The *inner dual graph* $T(H)$ of a hexagonal system H is the plane graph whose vertices consist of the centers of all hexagons of H, and two centers are joined by a segment as an edge of $T(H)$ if and only if the corresponding two hexagons have a common edge in H. Obviously, $T(H)$ is a triangulation graph.

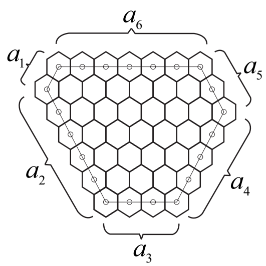
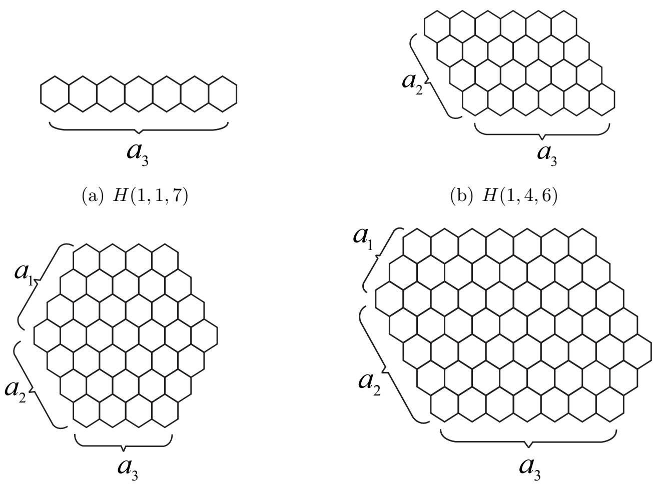


Figure 1. A general CHS $H(a_1, a_2, a_3, a_4, a_5, a_6)$.

A hexagonal systems is called *convex* if the boundary of its inner dual graph bounds a convex point set in the plane (see Fig. 1). Next a convex hexagonal systems will be abbreviated as CHS. Cyvin [5] showed that a CHS has a perfect matching if and only if it has equal opposite sides, that is, $a_1 = a_4$, $a_2 = a_5$ and $a_3 = a_6$. Such a CHS can be represented by $H(a_1, a_2, a_3)$. For example, see Fig. 2; some special cases are linear hexagonal chain $H(1, 1, a_3)$ and parallelogram HS $H(1, a_2, a_3)$ (see Fig. 2(a) and 2(b)).



(a) $H(1, 1, 7)$ (b) $H(1, 4, 6)$

(c) $H(3, 3, 3)$ (d) $H(3, 5, 7)$

Figure 2. Various examples for CHS $H(a_1, a_2, a_3)$.

In the following, we will discuss those CHS with at least one perfect matching. For $H(a_1, a_2, a_3)$, Cyvin [5] and Bodroža et al. [3] gave and proved a formula for the number of Kekulé structures. Zhang [22] got an expression of the Clar number, thus the maximum forcing number. For benzenoid parallelogram $H(1, a_2, a_3)$, Zhang and Li [21] and Li [12] showed that its minimum forcing numer and anti-forcing number are both equal to 1 respectively, and Zhao and Zhang [25, 26] derived explicit expressions of its forcing polynomial and anti-forcing polynomials by generating functions. For the definition of the forcing polynomial of a graph, see [24]. Zhu [29] showed that $f(H(2, 2, n)) = 2$ for all $n \geq 2$, and $f(H(3, 3, n)) = 3$ for all $n \geq 3$.

In this paper, we obtain the minimum forcing and anti-forcing numbers of $H(a_1, a_2, a_3)$ by applying the perfect path systems.

Theorem 1.1. Let $H(a_1, a_2, a_3)$ be a CHS. Then $f(H(a_1, a_2, a_3)) = af(H(a_1, a_2, a_3)) = \min\{a_1, a_2, a_3\}$.

2 Preliminary

In this section, we will introduce some notations and definitions. Let H be a hexagonal system embedded in the plane with some edges vertical. A *peak* (*valley*) of H is a vertex, all neighbors of which are below (above) it. Surely, all peaks and valleys have degree 2. Since H is a bipartite graph, its vertices can be colored white and black so that each pair of adjacent vertices receives distinct colors. We make a convention that all peaks (resp. valleys) are black (resp. white).

A *monotone path system* of H is a set of disjoint down paths of H, in which each path issues from a peak and ends at a valley. A *perfect path system* of H is a monotone path system covering all peaks and valleys of H.

Let M be a perfect matching of a graph G. We call a cycle (or path) of G is M-*alternating*, if its edges appear alternately in M or not. Sachs [15] gave a one-to-one correspondence between the perfect matchings and the perfect path systems of a hexagonal system.

Theorem 2.1. [15] Let H be a hexagonal system. Then H has a perfect matching if and only if it has a perfect path system. Further their one-to-one correspondence is given as follows (see Fig. 3).

(i) For a perfect path system $\mathcal{P}$, all non-vertical edges in and vertical edges not in the paths of $\mathcal{P}$ form a perfect matching of H.

(ii) If a perfect matching M is given, then we can delete all oblique edges not in M and all vertical edges in M together with their end vertices to obtain a perfect path system, where every path is an M-alternating path.

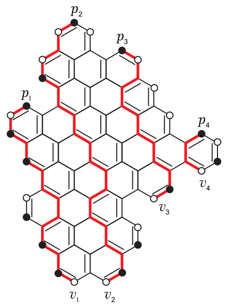


Figure 3. A perfect path system of H corresponding to a perfect matching and consisting of monotone paths from p_i to v_i, $1 \leq i \leq 4$.

Let M be a perfect matching of an HS H. Let $D(H,M)$ be a digraph obtained from H by directing every edge of M from black to white end-vertices, and directing each edge in $E(H)\backslash M$ from white to black end-vertices. Then there is a natural one-to-one corresponding between the directed cycles (resp. paths) and M-alternating cycles (resp. paths). Obviously, all arcs (directed edges) in $D(H,M)$ can be divided into six directions as shown in Fig. 4.

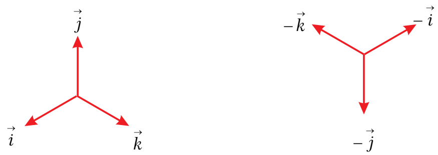


Figure 4. Six edge directions of a hexagonal system H.

An HS H has three plane drawings H_1 (the same as H), H_2 and H_3 such that they always have vertical edges and all peaks and valleys are black and white respectively. More precisely, rotating H 120 degrees counterclockwise and clockwise, we get H_2 and H_3 respectively. By Theorem 2.1, H_i has a perfect path system $\mathcal{P}_i(M)$ corresponding to M

for each $i \in \{1,2,3\}$. When H_2 and H_3 are returned to H, perfect path systems $\mathcal{P}_i(M)$ for $i = 2$ and 3 are imposed into H. In this point of view, H has three perfect path systems $\mathcal{P}_i(M)$ for $i = 1, 2$ and 3. For each path Q_i in $\mathcal{P}_i(M)$, its orientaion in $D(H, M)$ is a directed path. For convenience, we also use Q_i to represent its orientation; for an edge $e = xy$ in H, we also use $e = xy$ to represent an arc (i.e. directed edge) in $D(H, M)$ such that x and y are tail and head respectively.

In reference to the same H, we have the following three simple observations about each (directed or M-alternating) path in $\mathcal{P}_i(M)$ for $i = 1, 2$ and 3.

Observation 2.2. For each directed path $Q_1 \in \mathcal{P}_1(M)$, all arcs of Q_1 have directions $\vec{i}$, $\vec{k}$ and $-\vec{j}$, and Q_1 is a down path.

Observation 2.3. For each directed path $Q_2 \in \mathcal{P}_2(M)$, all arcs of Q_2 have directions $\vec{i}$, $\vec{j}$ and $-\vec{k}$. So all vertices of Q_2 are from right to left and the black (resp. white) vertices are from bottom to top along Q_2.

Observation 2.4. For each directed path $Q_3 \in \mathcal{P}_3(M)$, all arcs of Q_3 have directions $\vec{j}$, $\vec{k}$ and $-\vec{i}$. So all vertices of Q_3 are from left to right and the black (resp. white) vertices are from bottom to top along Q_3.

To prove our Theorem 1.1 we present some basic results on general graphs and topology. The following well-known Jordan curve theorem in the plane will be used repeatedly.

Theorem 2.5. [13] (Jordan curve theorem) Any simple closed curve D divides the points of the plane not on D into two distinct domains (with no points in common) of which D is the common boundary.

Equivalent definitions for a forcing set and an anti-forcing set of a perfect matching of a graph are described as follows.

Lemma 2.6. [1] Let M be a perfect matching of a graph G. Then an edge subset of M is a forcing set of M if and only if each M-alternating cycle intersects S.

Lemma 2.7. [11] Let G be a graph with a perfect matching M. Then $S \subseteq E(G)\backslash M$ is an anti-forcing set of M if and only if every M-alternating cycle intersects S.

The following gives relations between forcing and anti-forcing numbers of a graph.

Lemma 2.8. [11] Let G be a graph with a perfect matching M. Then $f(G, M) \leq af(G, M) \leq (\Delta - 1)f(G, M)$, and thus $f(G) \leq af(G)$.

3 Proof of Theorem 1.1

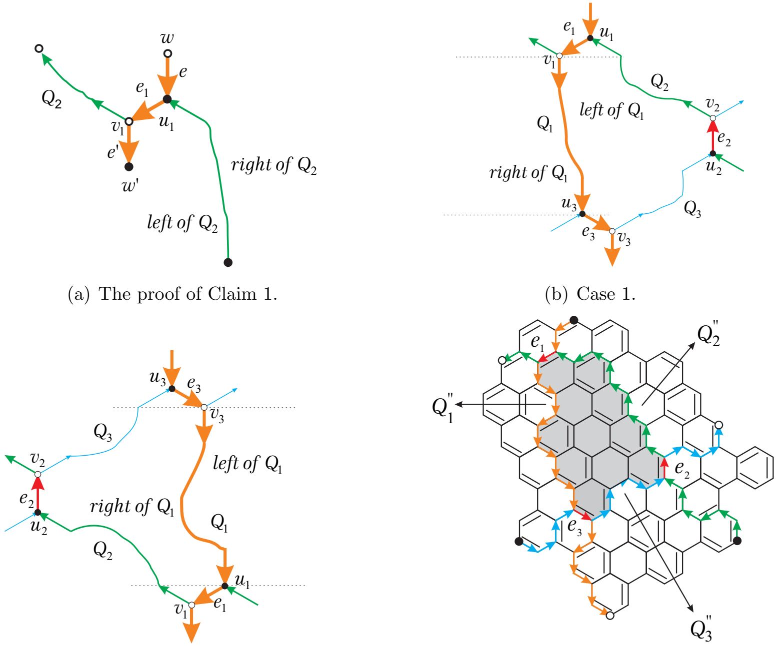
Our proof to Theorem 1.1 will be divided into three steps in this section. First we apply the three perfect path systems of $H(a_1, a_2, a_3)$ to get that the minimum forcing number of $H(a_1, a_2, a_3)$ has at least $\min\{a_1, a_2, a_3\}$. Then, by constructing a 3-coordinate system of $H(a_1, a_2, a_3)$, we can find a special perfect matching M of it such that $af(H(a_1, a_2, a_3), M) \leq \min\{a_1, a_2, a_3\}$. That implies that $H(a_1, a_2, a_3)$ has the minimum anti-forcing number at most $\min\{a_1, a_2, a_3\}$. Finally, by combining a known result [11] stating that the minimum forcing number of a graph is equal to or less than its minimum anti-forcing number (see also Lemma 2.8) with the previous facts, we can directly get that the minimum forcing and anti-forcing numbers of $H(a_1, a_2, a_3)$ are both equal to $\min\{a_1, a_2, a_3\}$.

Lemma 3.1. Let M be a perfect matching of a hexagonal system H. If three paths $Q_i \in \mathcal{P}_i(M)$, $i \in \{1, 2, 3\}$, pairwise intersect, then there is an M-alternating cycle of H formed by three subpaths on the three paths Q_i.

Proof. Since Q_i and Q_j are both M-alternating paths, $1 \leq i < j \leq 3$, they have at least one common edge belonging to M. Let $e_1 = u_1v_1$ be a common edge of Q_1 and Q_2 so that $e_1 \in M$. By Observations 2.2 and 2.3, e_1 is of direction $\vec{i}$.

Claim 1. Any pair of Q_1, Q_2 and Q_3 contains a unique common edge.

Proof. We only consider Q_1 and Q_2. The other cases are similar. Let $e = wu_1$ and $e' = v_1w'$ be two edges of Q_1 adjacent to e_1, if they exist. Then e and e' are both with direction $-\vec{j}$ and do not belong to Q_2 by Observation 2.2, which implies that w and w' lie on the right and on the left sides along the direction of Q_2, respectively. We can deduce that Q_1 goes through Q_2 always from the right to the left of Q_2 as shown in Fig. 5(a). That implies that the subpath of Q_1 from the peak to u_1 lies entirely on the right side of Q_2 and the subpath of Q_1 from the v_1 to the valley lies entirely on the left side of Q_2. Otherwise, we only need to consider the case that the latter does not holds. That is, the directed subpath Q_1' of Q_1 from w' to the end enters in the right side of Q_2. By the Jordan curve theorem, Q_1' intersects Q_2 at least one point, and Q_1' goes through Q_2 from the left to the right of Q_2, a contradiction. So Q_1 and Q_2 have exactly one common edge. ∎



(a) The proof of Claim 1.

(b) Case 1.

(c) Case 2.

(d) An M-alternating cycle bounded by Q_1, Q_2 and Q_3.

Figure 5. Illustration for the proof of Lemma 3.1.

By Claim 1, e_1 is the common edge of Q_1 and Q_2, and let $e_2 = u_2v_2$ (resp. $e_3 = u_3v_3$) be the common edge of Q_2 and Q_3 (resp. Q_1 and Q_3). By Observations 2.2 to 2.4, e_2 is of direction $\vec{j}$, and e_3 is of direction $\vec{k}$. So e_1, e_2 and e_3 are pairwise different edges in M. So we know that the u_i and v_i receive black and white, $1 \leq i \leq 3$, respectively.

Since e_i and e_{i-1} are both in Q_i, we can get a directed sub-path Q''_i of Q_i, connecting but not containing e_i and e_{i-1}, where $i = 1, 2, 3$, and $e_0 = e_3$. Then each Q''_i is an M-alternating path whose both end edges are not in M. So the first and final vertices of Q''_i respectively belong to $\{v_1, v_2, v_3\}$ and $\{u_1, u_2, u_3\}$. By Claim 1, any pair of Q''_1, Q''_2 and Q''_3 has no common edges. Further we have the following claim.

Claim 2. Any pair of Q''_1, Q''_2 and Q''_3 has no common vertices.

Proof. For two vertices x and y in Q_i such that x appears before y along Q_i, let $Q_i[x, y]$ denote the (directed) subpath of Q_i from x to y. There are two cases to distinguish.

Case 1. e_1 comes before e_3 along the path Q_1 (see Fig. 5(b)).

Then v_1 lies above u_3 and $Q_1'' = Q_1[v_1, u_3]$. It suffices to prove that e_i is before e_{i-1} along the path Q_i for $i = 2, 3$, that is, $Q_2'' = Q_1[v_2, u_1]$ and $Q_3'' = Q_3[v_3, u_2]$. Since $e_1 = u_1v_1$ is of direction $\vec{i}$, u_1 is above v_1. The entire subpath of Q_2 from v_1 lies on the right of Q_1 by Claim 1 and above v_1 by Observation 2.3. Since $e_3 = u_3v_3$ is of direction $\vec{k}$, u_3 is above v_3. By Claim 1 and Observation 2.4, the entire subpath of Q_3 to u_3 lies on the right of Q_1 and below u_3. So the subpath of Q_2 from v_1 and the subpath of Q_3 to u_3 are disjoint. Further, since Q_2 and Q_3 intersect at edge e_2, e_2 is the common edge of the subpath of Q_2 from the initial vertex to u_1 and the subpath of Q_3 from v_3 to the final vertex. That implies that e_3 appears before e_2 along the path Q_3 and Q_2 first passes through e_2 before e_1.

Case 2. e_3 comes before e_1 along the path Q_1 (see Fig. 5(c)).

Then v_3 is above u_1 and $Q_1'' = Q_1[v_3, u_1]$. Similar to Case 1, we just need to show that $Q_2'' = Q_2[v_1, u_2]$ and $Q_3'' = Q_3[v_2, u_3]$. Since u_1 is above v_1. By Claim 1 and Observation 2.3, the entire subpath of Q_2 to u_1 lies on the left of Q_1 and below u_1. Since u_3 is above v_3. The entire subpath of Q_3 from v_3 lies on the left of Q_1 and above v_3 by Claim 1 and Observation 2.4. Thus, the subpath of Q_2 to u_1 and the subpath of Q_3 from v_3 are disjoint. That is, e_2 is the common edge of the subpath of Q_2 from v_1 to the final vertex and the subpath of Q_3 from the initial vertex to u_3. That implies that $Q_2'' = Q_2[v_1, u_2]$ and $Q_3'' = Q_3[v_2, u_3]$. ■

From Claim 2, we know that the end vertices of Q_1'', Q_2'' and Q_3'' are different. So we can find a directed cycle $e_1 \cup Q_1'' \cup e_3 \cup Q_3'' \cup e_2 \cup Q_2''$, also an M-alternating cycle. ■

Let $H(a_1, a_2, a_3)$ be a CHS with a perfect matching M. Without loss of generality, we can assume that the number of peaks and valleys of H_i are both a_i for $i = 1, 2, 3$. By Theorem 2.1 the number of paths in a perfect path system of H_i is a_i, that is $|\mathcal{P}_i(M)| = a_i$.

Lemma 3.2. Let $H(a_1, a_2, a_3)$ be a CHS with a perfect matching and $a_1 \le a_2 \le a_3$. Then $f(H(a_1, a_2, a_3)) \ge a_1$.

Proof. Assume to the contrary that $f(H(a_1, a_2, a_3)) < a_1$. Let M be a perfect matching of $H(a_1, a_2, a_3)$ with the minimum forcing number. Then M has a forcing set S with cardinality smaller than a_1. By Theorem 2.1 (ii), for each $i \in \{1, 2, 3\}$, $\mathcal{P}_i(M)$ consists of a_i disjoint directed paths of $D(H, M)$. So there are three directed paths $Q_1 \in \mathcal{P}_1(M)$, $Q_2 \in \mathcal{P}_2(M)$ and $Q_3 \in \mathcal{P}_3(M)$ which each contains no edges of S.

For each pair $\{i, j\} \subseteq \{1, 2, 3\}$, since both Q_i and Q_j are inside the boundary of H (a closed polygon), and their end vertices cross along the boundary, by Jordan curve theorem, Q_i and Q_j intersect at least one point. By Lemma 3.1, Q_1, Q_2 and Q_3 form an M-alternating cycle containing no edges of S, contradicting that S is a forcing set of M by Lemma 2.6. Thus, we have $f(H(a_1, a_2, a_3)) \geq a_1$. ■

For any edge e of a graph G, we call it a 2-2 edge, if both end vertices of e have degree 2 in G. Obviously, $H(a_1, a_2, a_3)$ has exactly six 2-2 edges, and they are all on the border of $H(a_1, a_2, a_3)$. We label the six 2-2 edges by e_1, e_2, e_3, e_4, e_5, e_6 in clockwise order along the border of $H(a_1, a_2, a_3)$. Moreover, e_i and e_{i+3} are parallel, where $i = 1, 2, 3$.

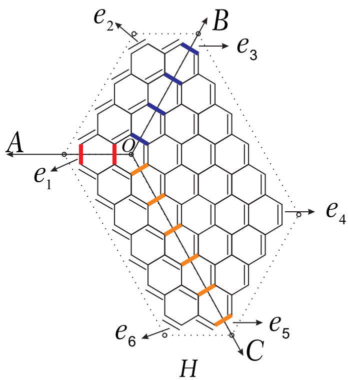


Figure 6. Illustration for the proof of Lemma 3.4: three anti-forcing sets of a perfect matching of $H(a_1, a_2, a_3)$, where $a_1 = 2$, $a_2 = 4$ and $a_3 = 6$.

Lemma 3.3. [20, 23] Let H be a hexagonal system with a perfect matching M. Then for any M-alternating cycle C of H, there is an M-alternating hexagon in C with its interior.

Lemma 3.4. Let $H(a_1, a_2, a_3)$ be a CHS with a perfect matching and $a_1 \leq a_2 \leq a_3$. Then $af(H(a_1, a_2, a_3)) \leq a_1$.

Proof. Take rays OA, OB and OC that are perpendicular bisectors of 2-2 edges e_1, e_3 and e_5 respectively so that they intersect at the center O of some hexagon h (see Fig. 6). Then $O - ABC$ can be seen as a 3-coordinate system of H, which divides the plane into three areas AOB, BOC and COA. Let L_A (resp. L_B and L_C) be the set of edges of H intersecting OA (resp. OB and OC). Then the cardinalities of L_A, L_B and L_C respectively are a_1, a_2 and a_3.

Let M be a perfect matching of H such that M does not contain an edge of L_A, L_B and L_C, and all edges of M in anyone of the three areas are parallel to each other, see Fig. 6. Then H contains exactly one M-alternating hexagon h whose center is O. For any M-alternating cycle C of H, by Lemma 3.3, h lies in the C with its interior, so O is a point in the interior of C. So each one of L_A, L_B and L_C intersects C. In addition, L_A, L_B and L_C are subsets of $E(H)\backslash M$. By Lemma 2.7, L_A, L_B and L_C are all anti-forcing sets of M. Hence we have that $af(H) \leq af(H, M) \leq a_1$. ■

Proof of Theorem 1.1. Without loss of generality, suppose that $a_1 = \min\{a_1, a_2, a_3\}$. Combining Lemmas 3.2, 3.4 and 2.8, we have the following inequalities.

$$a_1 \leq f(H(a_1, a_2, a_3)) \leq af(H(a_1, a_2, a_3)) \leq a_1,$$

which implies that all the above equalities hold. ■

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