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Anti-forcing numbers of perfect matchings of graphs

Hongchuan Lei [a,b], Yeong-Nan Yeh [b,*], Heping Zhang [c]

[a] College of Science, Zhejiang Sci-Tech University, Hangzhou, Zhejiang 310018, China
[b] Institute of Mathematics, Academia Sinica, Taipei 10617, Taiwan
[c] School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, China

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ABSTRACT

We define the anti-forcing number of a perfect matching M of a graph G as the minimal number of edges of G whose deletion results in a subgraph with a unique perfect matching M, denoted by $af(G, M)$. The anti-forcing number of a graph proposed by Vukičević and Trinajstić in Kekulé structures of molecular graphs is in fact the minimum anti-forcing number of perfect matchings. For plane bipartite graph G with a perfect matching M, we obtain a minimax result: $af(G, M)$ equals the maximal number of M-alternating cycles of G where any two either are disjoint or intersect only at edges in M. For a hexagonal system H, we show that the maximum anti-forcing number of H equals the Fries number of H. As a consequence, we have that the Fries number of H is between the Clar number of H and twice. Further, some extremal graphs are discussed.

1. Introduction

We only consider finite and simple graphs. Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A perfect matching or 1-factor M of a graph G is a set of edges of G such that each vertex of G is incident with exactly one edge in M.

A Kekulé structure of some molecular graph (for example, benzenoid and fullerene) coincides with a perfect matching of a graph. Randić and Klein [20,14] proposed the *innate degree of freedom* of a Kekulé structure, i.e. the least number of double bonds can determine this entire Kekulé structure, nowadays it is called the forcing number by Harary et al. [13].

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. $F(G)$). In general to compute the minimum forcing number of a graph with the maximum degree 3 is an NP-complete problem [3].

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 $E(G) \setminus M$.

Lemma 1.1 ([2,22]). *A subset $S \subseteq M$ is a forcing set of M if and only if each M-alternating cycle of G contains at least one edge of S.*

For planar bipartite graphs, Pachter and Kim obtained the following minimax theorem by using Lucchesi and Younger's result in digraphs [18].

* Corresponding author.
E-mail addresses: mayeh@math.sinica.edu.tw (Y.-N. Yeh), zhanghp@lzu.edu.cn (H. Zhang).

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Theorem 1.2 (*[19]*). *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.*

A hexagonal system (or benzenoid) is a 2-connected finite plane graph such that every interior face is a regular hexagon of side length one. It can also be formed by a cycle with its interior in the infinite hexagonal lattice on the plane (graphene). A hexagonal system with a perfect matching is viewed as the carbon-skeleton of a benzenoid hydrocarbon.

Let H be a hexagonal system with a perfect matching M. A set of *disjoint* M-alternating hexagons of H is called an *M-resonant set*. A set of M-alternating hexagons of H (the intersection is allowed) is called an *M-alternating set*. A maximum resonant set of H over all perfect matchings is a *Clar structure* or *Clar set*, and its size is the *Clar number* of H, denoted by $cl(H)$ (cf. [11]). A Fries set of H is a maximum alternating set of H over all perfect matchings and the Fries number of H, denoted by $Fries(H)$, is the size of a Fries set of H. Both Clar number and Fries number can measure the stability of polycyclic benzenoid hydrocarbons [6,1].

Theorem 1.3 (*[28]*). *Let H be a hexagonal system. Then $F(H) = cl(H)$.*

In this paper we consider the anti-forcing number of a graph, which was previously defined by Vukičević and Trinajstić [26,27] as the smallest number of edges whose removal results in a subgraph with a single perfect matching (see Refs. [5,8,9,15,29,30] for some researches on this topic). By an analogous manner as the forcing number we define the anti-forcing number, denoted by $af(G, M)$, of a perfect matching M of a graph G as the minimal number of edges not in M whose removal to fix a single perfect matching M of G. We can see that the anti-forcing number of a graph G is the minimum anti-forcing number of all perfect matchings of G. We also show that the anti-forcing number has a close relation with the forcing number: For any perfect matching M of G, $f(G, M) \leq af(G, M) \leq (\Delta - 1)f(G, M)$, where Δ denotes the maximum degree of G. For a plane bipartite graph G, we obtain a minimax result: For any perfect matching M of G, the anti-forcing number of M equals the maximal number of M-alternating cycles of G any two members of which either are disjoint or intersect only at edges in M. For a hexagonal system H, we show that the maximum anti-forcing number of H equals the Fries number of H. As a consequence, we have that the Fries number of H is between the Clar number of H and twice. Discussions for some extremal graphs about the anti-forcing numbers show the anti-forcing number of a graph G with the maximum degree three can achieve the minimum forcing number or twice.

2. Anti-forcing number of perfect matchings

An anti-forcing set S of a graph G is a set of edges of G such that $G - S$ has a unique perfect matching. The smallest cardinality of anti-forcing sets of G is called the *anti-forcing number* of G and denoted by $af(G)$.

Given a perfect matching M of a graph G. If C is an M-alternating cycle of G, then the symmetric difference $M \oplus C$ is another perfect matching of G. Here C may be viewed as its edge-set, and for two sets A and B, $A \oplus B := (A \cup B) \setminus (A \cap B)$. A subset $S \subseteq E(G) \setminus M$ is called an anti-forcing set of M if $G - S$ has a unique perfect matching, that is, M.

Lemma 2.1. *A set S of edges of G not in M is an anti-forcing set of M if and only if S contains at least one edge of every M-alternating cycle of G.*

Proof. If S is an anti-forcing set of M, then $G - S$ has a unique perfect matching, i.e. M. So $G - S$ has no M-alternating cycles. Otherwise, if $G - S$ has an M-alternating cycle C, then the symmetric difference $M \oplus C$ is another perfect matching of $G - S$ different from M, a contradiction. Hence each M-alternating cycle of G contains at least one edge of S. Conversely, suppose that S contains at least one edge of every M-alternating cycle of G. That is, $G - S$ has no M-alternating cycles, so $G - S$ has a unique perfect matching. □

The smallest cardinality of anti-forcing sets of M is called the anti-forcing number of M and denoted by $af(G, M)$. So we have the following relations between the forcing number and anti-forcing number.

Theorem 2.2. *Let G be a graph with the maximum degree Δ. For any perfect matching M of G, we have*

$$f(G, M) \leq af(G, M) \leq (\Delta - 1)f(G, M).$$

Proof. Given any anti-forcing set S of M. For each edge e in S, let e_1 and e_2 be the edges in M adjacent to e. All such edges e in S are replaced with one of e_1 and e_2 to get another set S' of edges in M. It is obvious that $|S'| \leq |S|$. Further we claim that S' is a forcing set of M. For any M-alternating cycle C of G, by Lemma 2.1 C must contain an edge e in S. Then C must pass through both e_1 and e_2. By the definition for S', C contains at least one edge of S'. So Lemma 1.1 implies that S' is a forcing set of M. Hence the claim holds. So $f(G, M) \leq |S'| \leq |S|$, and the first inequality is proved.

Now we consider the second inequality. Let F be a minimum forcing set of M. Then $f(G, M) = |F|$. For each edge e in F, we choose all the edges not in M incident with one end of e. All such edges form a set F' of size no larger than $(\Delta - 1)|F|$, which is disjoint with M. We claim that F' is an anti-forcing set of M. Otherwise, Lemma 2.1 implies that $G - F'$ contains an M-alternating cycle C. Since each edge in F is a pendant edge of $G - F'$, C does not pass through an edge of F. This contradicts that F is a forcing set of M by Lemma 1.1. Hence $af(G, M) \leq |F'| \leq (\Delta - 1)|F|$. □

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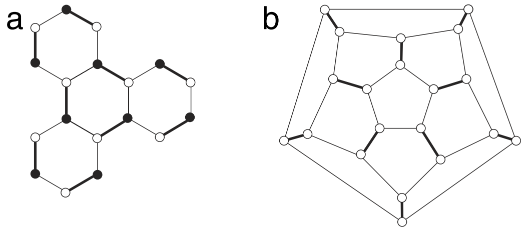

Fig. 1. (a) Triphenylene. (b) Dodecahedron.

Lemma 2.3. *$af(G) = \min\{af(G, M) : M$ is a perfect matching of $G\}$.*

By the definitions the above result is immediate. Hence we may say, $af(G)$ is the *minimum anti-forcing number* of G. Whereas,

$$Af(G) := \max\{af(G, M) : M \text{ is a perfect matching of } G\}$$

is the *maximum anti-forcing number* of G.

The following is an immediate consequence of Theorem 2.2.

Corollary 2.4. *Let G be a graph with a perfect matching and the maximum degree Δ. Then*

$$f(G) \le af(G) \le (\Delta - 1)f(G), F(G) \le Af(G) \le (\Delta - 1)F(G).$$

Further, $\mathrm{Spec}_f(G) := \{f(G, M) : M$ is a perfect matching of $G\}$ and $\mathrm{Spec}_{af}(G) := \{af(G, M) : M$ is a perfect matching of $G\}$ are called the *forcing spectrum* [3] and the *anti-forcing spectrum* of G respectively. For example, $\mathrm{Spec}_{af}(\text{Triphenylene}) = \{2, 3, 4\}$ and $\mathrm{Spec}_f(\text{Triphenylene}) = \{1, 3\}$ (see Fig. 1(a)), $\mathrm{Spec}_f(\text{Dodecahedron}) = \{3\}$ [32] (see Fig. 1(b)). Randić and Vukičević [25,21] computed the distributions of forcing numbers of Kekulé structures of C_{60} and C_{70} respectively; see also the forcing polynomial of a graph [34].

For any given graph G with a perfect matching M, we now consider the anti-forcing number $af(G, M)$. If G has two M-alternating cycles that either are disjoint or intersect only at edges in M, then by Lemma 2.1 any anti-forcing set of M contains an edge of each one of such M-alternating cycles. Thus it naturally motivates us to propose a novel concept: a collection A of M-alternating cycles of G is called a *compatible M-alternating set* if any two members of A either are disjoint or intersect only at edges in M. Let $c'(M)$ denote the maximum cardinality of compatible M-alternating sets of G. By the above discussion we have the following immediate result.

Lemma 2.5. *For any perfect matching M of a graph G, we have $af(G, M) \ge c'(M)$.*

For plane bipartite graphs G we can show that the equality in the above lemma always holds. The vertices of G are colored with white and black such that any pair of adjacent vertices receive different colors. Such two color classes form a bipartition of G.

Theorem 2.6. *Let G be a planar bipartite graph with a perfect matching M. Then*

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

To obtain such a minimax result we need a classical result of Lucchesi and Younger [18] about directed graphs; Its shorter proof was ever given by Lovász [16]. Let D be a finite directed graph. A *feedback set* of D is a set of arcs that contains at least one arc of each directed cycle of D.

Theorem 2.7 (*Lucchesi and Younger [18]*). *For a finite planar digraph, a minimum feedback set has cardinality equal to that of a maximum collection of arc-disjoint directed cycles.*

Proof of Theorem 2.6. First assign a specific orientation of G concerning M to obtain a digraph $\vec{G}(M)$: any edge in M is directed from white end to black end, and the edges not in M are directed from black ends to white ends. Obviously the M-alternating cycles of G correspond naturally to directed cycles of its orientation. Then contract each edge of M in $\vec{G}(M)$ to a vertex (i.e. delete the edge and identify its ends) to get a new digraph, denoted by $\vec{G} \cdot M$. We can see that there is a one-to-one correspondence between the M-alternating cycles of G and directed cycles of $\vec{G} \cdot M$. That is, an M-alternating cycle of G becomes a directed cycle $\vec{G} \cdot M$, and a directed cycle of $\vec{G} \cdot M$ can produce an M-alternating cycle of G when each vertex is restored to an edge of M. So by Lemma 2.1 a subset $S \subseteq E(G) \setminus M$ is an anti-forcing set of M if and only if S is a feedback set of $\vec{G} \cdot M$. Hence $af(G, M)$ equals the smallest cardinality of feedback sets of $\vec{G} \cdot M$. On the other hand, a compatible M-alternating set of G corresponds to a set of arc-disjoint directed cycles of $\vec{G} \cdot M$. That implies that $c'(M)$ equals the maximum number of arc-disjoint directed cycles of $\vec{G} \cdot M$. Note that $\vec{G} \cdot M$ is a planar digraph. So Theorem 2.7 implies $af(G, M) = c'(M)$. □

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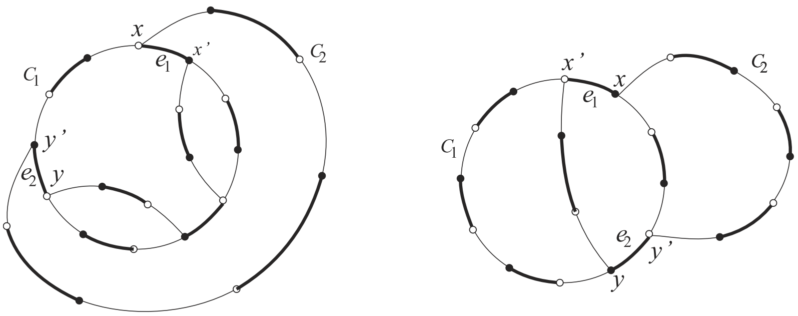

Fig. 2. Two ways of crossing M-alternating cycles C_1 and C_2 (bold lines are edges in M), where e_1 and e_2 are their crossings.

However, the equality in Lemma 2.5 does not necessarily hold in general. That is, Theorem 2.6 does not hold for general graphs. A counterexample is dodecahedron (see Fig. 1(b)); For this specific perfect matching M marked by bold lines, we can check that its anti-forcing number equals five. But there are at most four M-compatible alternating cycles. In fact, it has only M-alternating cycles of length 16 and 8. Any two M-alternating cycles of length 16 are not compatible. Further, each M-alternating cycles of length 8 always bounds two pentagons, so it is compatible with at most two other M-alternating cycles of length 8. Hence the dodecahedron has at most three compatible M-alternating cycles of length 8. For short, the maximum number of compatible M-alternating cycles of dodecahedron equals 4.

3. Maximum anti-forcing number

In this section we restrict our consideration to a hexagonal system H with a perfect matching M. Without loss of generality, H is placed in the plane such that an edge-direction is vertical and the peaks (i.e. those vertices of H that just have two low neighbors, but no high neighbors) are black. An M-alternating cycle C of H is said to be *proper* (resp. *improper*) if each edge of C in M goes from white end to black end (resp. from black end to white end) along the clockwise direction of C. The boundary of H means the boundary of the outer face. An edge on the boundary is a boundary edge.

The following main result shows that the maximum anti-forcing number equals the Fries number in a hexagonal system.

Theorem 3.1. *Let H be a hexagonal system with a perfect matching. Then $Af(H) = Fries(H)$.*

Proof. Since any Fries set of H is a compatible M-alternating set A for some perfect matching M of H, we have that $Af(H) \geq Fries(H)$ from Theorem 2.6. So we now prove that $Af(H) \leq Fries(H)$. It suffices to prove that for a compatible alternating set A of H with $|A| = Af(H)$, we can find a Fries set F of H such that $|A| \leq |F|$.

Given any compatible M-alternating set A of H with a perfect matching M. Two cycles C_1 and C_2 in A are *crossing* if they share an edge e in M and the four edges adjacent to e alternate in C_1 and C_2 (i.e. C_1 enters into C_2 from one side and leaves from the other side via e). Such an edge e is said to be a crossing. For example, see Fig. 2. We say A is *non-crossing* if any two cycles in A are not crossing.

Claim 1. For any compatible M-alternating set A of H, we can find the corresponding non-crossing compatible M-alternating set A' of H such that $|A'| = |A|$.

Proof. Suppose A has a pair of crossing members C_1 and C_2. In fact C_1 and C_2 have even number of crossings. Let e_1 and e_2 be two consecutive crossings, which are edges in M. So we may suppose along the counterclockwise direction of C_2 from edge $e_1 = xx'$ enters into the interior of C_1, then reaches the crossing $e_2 = yy'$. Note that x is the first vertex of C_2 entering in C_1 and y' the first vertex of C_2 leaving from C_1 after x. For convenience, if a cycle C in H has two vertices s and t, we always denote by $C(s, t)$ the path from s to t along C clockwise. If C_1 is a proper M-alternating cycle and C_2 is an improper M-alternating cycle, let $C_1' := C_1(y, x') + C_2(y, x')$ and $C_2' := C_1(x', y) + C_2(x', y)$ (see Fig. 2 (left)). If C_1 and C_2 both are proper (resp. improper) M-alternating cycles, let $C_1' := C_1(y', x) + C_2(x, y')$ and $C_2' := C_1(x, y') + C_2(y', x)$ (see Fig. 2 (right)). In all such cases C_1 and C_2 in A can be replaced with C_1' and C_2' to get a new compatible M-alternating set of H and such a pair of crossings e_1 and e_2 disappeared. Since such a change cannot produce any new crossings, by repeating the above process we finally get a compatible M-alternating set A' of H that is non-crossing. It is obvious that $|A'| = |A|$. □

For a cycle C of H, let $h(C)$ denote the number of hexagons in the interior of C. By Claim 1 we can choose a perfect matching M of H and a maximum compatible M-alternating set A satisfying that (i) $|A| = Af(H)$ and (ii) A is non-crossing, and $h(A) := \sum_{C\in A} h(C)$ is as minimal as possible subject to (i) and (ii). We call $h(A)$ the *area* of A.

By the above choice we know that for any two cycles in A their interiors either are disjoint or one contains the other one. Hence the cycles in 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. [33]), we immediately obtain the following claim.

Claim 2. Every minimal member of A is a hexagon.

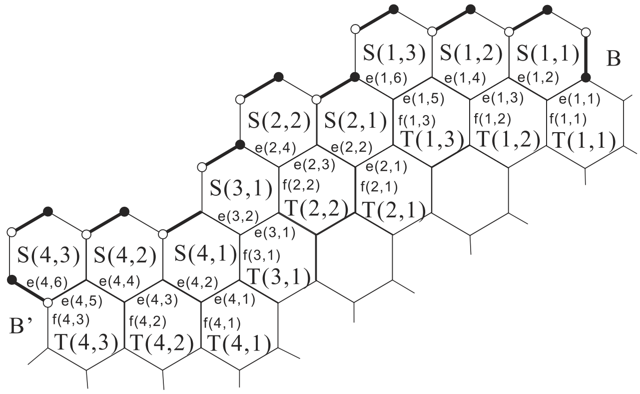

Fig. 3. Illustration for the proof of Claim 3 (bold lines are edges in M, $m = 4$, $n(1) = 3$, $n(2) = 2$, $n(3) = 1$, $n(4) = 3$).

It suffices to prove that all members of A are hexagons. Suppose to the contrary that A has at least one non-hexagon member. Let C be a minimal non-hexagon member in A. Then C is an M-alternating cycle. We consider a new hexagonal system H' formed by C and its interior as a subgraph of H. Without loss of generality, suppose that C is a proper M-alternating cycle (otherwise, analogous arguments are implemented on right-top corner of H'). So we can find a substructure of H' in its left-top corner as follows.

We follow the notations of Zheng and Chen [35]. Let $S(i, j)$, $1 \le i \le m$ and $1 \le j \le n(i)$, be a series of hexagons on the boundary of H' as Fig. 3 that form a hexagonal chain and satisfy that neither B nor B' is contained in H'. We denote edges, if any, by $e(i, k)$, $1 \le i \le m$ and $1 \le k \le 2n(i)$, and by $f(i, j)$, $1 \le i \le m$ and $1 \le j \le n(i)$; and denote the hexagons (not necessarily contained in H') with both edges $f(i, j)$ and $e(i, 2j - 1)$, by $T(i, j)$, $1 \le i \le m$ and $1 \le j \le n(i)$ (see Fig. 3).

Claim 3. (a) $n(1) = 1$, and $m \ge 2$,

(b) $n(i) = 1$ or 2 for all $1 \le i \le m$,

(c) for all $1 \le i \le m$, $f(i, n(i)) \in M$, and

(d) if $n(i) = 2$, $2 \le i \le m$, then $S(i, 1) \in A$.

Proof. We now prove the claim by induction on i. We first consider $i = 1$. If $e(1, 2) \in M$, then $S(1, 1)$ is a proper M-alternating hexagon. So C in A can be replaced with $S(1, 1)$ to produce a new compatible M-alternating set A'. That is, $A' := (A \cup S(1, 1)) - \{C\}$, but $|h(A')| < |h(A)|$, a contradiction. So $e(1, 2) \notin M$, which implies that $f(1, 1) \in M$ and all edges $e(1, 3), e(1, 5), \ldots, e(1, 2n(1) - 1)$ belong to M. Hence $S(2, 1)$ is a hexagon of H' and $m \ge 2$. If $n(1) \ge 2$, since the boundary C of H' is a proper M-alternating cycle, none of the edges $e(1, 2), e(1, 3), \ldots, e(1, 2n(1))$ is a boundary edge of H'. In this case the cycle C can be replaced with $C \oplus S(1, n(1))$ to get another compatible M-alternating set with the area less than A, also a contradiction. Hence $n(1) = 1$. So the claim holds for $i = 1$.

Suppose $1 \le i < m$ and Claim 3 holds for any integer $1 \le i' \le i$. We want to show that it holds for $i + 1$. There are two cases to be considered.

Case 1. $n(i) = 1$. Suppose that $n(i+1) \ge 3$. If $e(i+1, 2) \notin M$, then $e(i+1, 3), e(i+1, 5), \ldots, e(i+1, 2n(i)-1)$ all belong to M. By an analogous argument as above, we have that $T(i + 1, 2), \ldots, T(i + 1, n(i + 1)), S(i + 2, 1)$ are hexagons of H', and C can be replaced with $C \oplus S(i + 1, n(i + 1))$ to get another M-compatible alternating set with the area less than A, also a contradiction. Hence $e(i + 1, 2) \in M$. By the induction hypothesis we have $f(i, 1) \in M$, and $S(i + 1, 1)$ is an M-alternating hexagon. If $e(i + 1, 4) \notin M$, the similar contradiction occurs. So $e(i + 1, 4) \in M$. We can see that none of members of A but C intersect $S(i + 1, 1)$. Then $(A \cup \{S(i, 1), S(i + 1, 1), S(i + 1, 2)\}) - \{C\}$ is a compatible $M \oplus S(i + 1, 1)$-alternating set, which is larger than A, contradicting the choice of A. Hence $n(i + 1) \le 2$. If $n(i + 1) = 1$, then $f(i + 1, 1) \in M$. Otherwise, C in A would be replaced with $S(i + 1, 1)$ to obtain a similar contradiction. If $n(i + 1) = 2$, by the similar arguments we have that $e(i + 1, 2) \in M$ and $f(i + 1, 2) \in M$. So $S(i + 1, 1) \in A$.

Case 2. $n(i) = 2$. Choose an integer i_0 with $1 \le i_0 < i$ such that $n(i_0) = 1$, and $n(i_0 + 1) = n(i_0 + 2) = \cdots = n(i) = 2$. By the induction hypothesis, we have that the right vertical edge of hexagon $S(i_0, 1)$ belongs to M, the hexagons $S(i_0 + 1, 1), S(i_0 + 2, 1), \ldots, S(i, 1)$ are all proper M-alternating hexagons, which all belong to A, and $f(i, 2) \in M$. If $e(i + 1, 2) \notin M$, then $f(i + 1, 1) \in M$. We have that $n(i + 1) = 1$; otherwise, $n(i + 1) \ge 2$ and C would be replaced with $C \oplus S(i + 1, n(i + 1))$ to get another M-compatible alternating set with the area less than A, also a contradiction. So suppose that $e(i + 1, 2) \in M$. Then $S(i + 1, 1)$ is a proper M-alternating hexagon. We claim that $n(i + 1) = 2$ and $f(i + 1, n(i + 1)) \in M$. If $n(i + 1) = 1$, then $e(i + 1, 2)$ belongs to C. So C can be replaced with $S(i + 1, 1)$ also to get a contradiction. Hence $n(i + 1) \ge 2$. Suppose $e(i + 1, 4) \in M$. Let $M' = M \oplus S(i + 1, 1) \oplus S(i, 1) \oplus \cdots \oplus S(i_0 + 1, 1)$. Then M' is a perfect matching of H so that $S(i + 1, 2), S(i + 1, 1), S(i, 2), S(i, 1), \ldots, S(i_0 + 1, 2), S(i_0 + 1, 1), S(i_0, 1)$ are M-alternating hexagons. Let $A' := (A \cup \{S(i + 1, 2), S(i, 2), \ldots, S(i_0 + 1, 2), S(i_0, 1)\}) - \{C, T(i, 2), \ldots, T(i_0 + 1, 2)\}$. Then A' is a compatible M'-alternating set of H with $|A| < |A'|$, contradicting the choice for A. Hence $e(i + 1, 4) \notin M$ and $f(i + 1, 2) \in M$. If $n(i + 1) \ge 3$, then $e(i + 1, 5), e(i + 1, 7), \ldots, e(i + 1, 2n(i + 1) - 1)$ all belong to M, so C can be replaced with $C \oplus S(i+1, n(i+1))$ to get a similar contradiction. Hence $n(i+1) = 2$ and the claim holds. Further we have that $S(i+1, 1) \in A$

Now we have completed the proof of Claim 3. □

By Claim 3 we have that $f(m, n(m)) \in M$. That implies that $e(m, 2n(m)) \notin M$. So $S(m+1, 1)$ exists in H', a contradiction. Hence each member of A is a hexagon. □

Combining Theorems 1.3 and 3.1 with Corollary 2.4, we immediately obtain the following relations between the Clar number and Fries number.

Corollary 3.2. *Let H be a hexagonal system. Then $cl(H) \leq Fries(H) \leq 2cl(H)$.*

4. Some extremal classes

4.1. All-kink catahexes

Let H be a hexagonal system. The inner dual H^* of H is a plane graph: the center of each hexagon h of H is placed a vertex h^* of H^*, and if two hexagons of H share an edge, then the corresponding vertices are joined by an edge. H is called catacondensed if its inner dual is a tree. Further H is called *all-kink catahex* [13] if it is catacondensed and there is no hexagon such that its intersections with two other hexagons are two parallel edges. The following result due to Harary et al. gives a characterization for a hexagonal system to have the Fries number (or the maximum anti-forcing number) achieving the number of hexagons.

Theorem 4.1 (*[13]*). *For a hexagonal system H with n hexagons, $Fries(H) \leq n$, and equality holds if and only if H is an all-kink catahex.*

An independent (or stable) set of a graph G is a set of vertices no two of which are adjacent. The independence number of G, denoted by $\alpha(G)$, is the largest cardinality of independent sets of G. A matching of G is a set of edges of G no two of which are adjacent. The matching number of G, denoted by $\nu(G)$, is the maximum size of matchings of G.

Theorem 4.2. *For an all-kink catahex H, $Af(H) = 2F(H)$ if and only if the inner dual H^* has a perfect matching.*

Proof. By Theorem 4.1, $Af(H)$ equals the number n of vertices of H^*. Note that any set of disjoint hexagons of H is a resonant set. By Theorem 1.3, $F(H) = cl(H) = \alpha(H^*)$. Since H^* is a bipartite graph, $\nu(H^*) + \alpha(H^*) = n$. So this equality implies the result. □

For a hexagonal system H with a perfect matching M, let $fries(M)$ be the number of M-alternating hexagons of H. Then $Fries(H)$ is the maximal value of $fries(M)$ over all perfect matchings. The minimal value of $fries(M)$ over all perfect matchings M is called the *minimum fries number*, denoted by $fries(H)$. For an all-kink catahex, each hexagon has two choices for three disjoint edges, and just one's edges can be glued with other hexagons, so these three edges are called *fusing edges*. If a fusing edge is on the boundary, then an additive hexagon is glued along it to get a larger all-kink catahex.

A *dominating set* of a graph G is a set S of vertices of G such that every vertex not in S has a neighbor in S. An independent dominating set of G is a set of vertices of G that is both dominating and independent in G [10]. The independent domination number of G, denoted by $i(G)$, is the minimum size of independent dominating sets of G. (For a survey on independent domination, see [10].)

Theorem 4.3. *For an all-kink catahex H, $f(H) = i(H^*) = fries(H)$.*

Proof. For any perfect matching M of H, by Theorem 1.2 we have that $f(H, M) = c(M)$. Note that H has no interior vertices. Since each M-alternating cycle of H contains an M-alternating hexagon in its interior, $c(M)$ equals the maximum number of disjoint M-alternating hexagons of H. It is obvious that for a hexagon of H a non-fusing edge belongs to M if and only if the three non-fusing edges belong to M.

Choose a perfect matching M of H such that $f(H) = f(H, M)$. Let S be a maximum set of disjoint M-alternating hexagons of H and $S^* := \{h^* : h \in S\}$. Then $f(H) = |S^*|$. We claim that S^* is an independent dominating set of H^*. Let h be any hexagon of H not in S. If some hexagon h' of H adjacent to h has the three non-fusing edges in M, then $h' \in S$. Otherwise, h is an M-alternating hexagon. Since $h \notin S$ and S is maximum, some hexagon of H adjacent to h must belong to S. So the claim holds, and $f(H) \geq i(H^*)$. Conversely, given a minimum independent dominating set S^* of H^*. Construct a perfect matching M_0 of H as follows. The three non-fusing edges of each hexagon in S are chosen as edges of M_0. For any hexagon of H not in S, a fusing edge that is a boundary edge or shared by the other hexagon not in S is also an edge of M_0. So we can see that M_0 is a perfect matching of H and any hexagon of H not in S is not M_0-alternating. Hence S is the maximum set of M_0-alternating hexagons of H. So $i(H^*) = f(H, M_0) \geq f(H)$. Hence $i(H^*) = f(H)$.

According to the above construction, S is the set of all M_0-alternating hexagons of H. Hence $f(H) = h(M_0) \geq fries(H)$. On the other hand, for any perfect matching M of H, $c(M) \leq fries(M)$, and thus $f(H) \leq fries(H)$. Both inequalities imply the second equality. □

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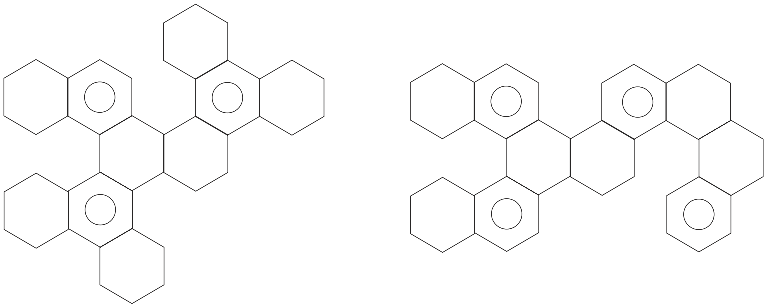

Fig. 4. All-kink catahexes with the minimum forcing numbers 3 and 4.

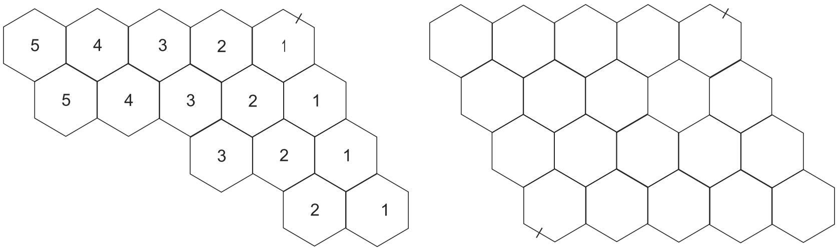

Fig. 5. Truncated parallelograms $H(5, 5, 3, 2)$ and $H(5, 5, 5, 5)$.

Beyer et al. [4] observed an algorithm of linear time to compute the independent domination number of a tree. So the minimum forcing number of all-kink catahexes can be computed in linear time. For example, Fig. 4 gives the minimum forcing numbers of two all-kink catahexes. But the anti-forcing number of an all-kink catahex may be larger than its minimum forcing number; for example, the triphenylene has the minimum forcing number 1 and the anti-forcing number 2 (see Fig. 1(a)).

4.2. $af(H) = 1, 2$

Li [15] gave the structure of hexagonal systems with an anti-forcing edge (i.e. an edge that itself forms an anti-forcing set). For integers $n_1 \geq n_2 \geq \cdots \geq n_k \geq 1$, $k \geq 1$, let $H(n_1, n_2, \ldots, n_k)$ be a hexagonal system with k horizontal rows of $n_1 \geq n_2 \geq \cdots \geq n_k$ hexagons and last hexagon of each row being immediately below and to the right of the last one in the previous row, and we call it *truncated parallelogram* [7]; For example, see Fig. 5. In particular, $H(r, r, \ldots, r)$ with $k \geq 2$ and $r \geq 2$ and $H(r)$ with $r \geq 2$ are parallelogram and linear chain respectively. Note that a truncated parallelogram can be placed and represented in other ways.

Theorem 4.4 ([15]). *Let H be a hexagonal system. Then $af(H) = 1$ if and only if H is a truncated parallelogram.*

Precisely, a single hexagon has six anti-forcing edges, a linear chain has four anti-forcing edges, and a parallelogram has two anti-forcing edges. A true truncated parallelogram has just one anti-forcing edge (see Fig. 5). In the following we will give a construction for hexagonal systems with the anti-forcing number 2.

Some necessary preliminary is needed. Let G be a connected bipartite graph with a perfect matching. An edge of G is said to be *fixed single* (resp. *double*) if it belongs to no (resp. all) perfect matchings of G. An edge of G is *fixed* if it is either fixed double edge or fixed single edge. G is *normal* or *elementary* if G has no fixed edges. The non-fixed edges of G form a subgraph whose components are normal and thus 2-connected graphs, which are called *normal components* of G. Further, if G is plane, then a normal component of G is called a *normal block* if it is formed by a cycle of G with its interior. A pendant vertex of a graph is a vertex of degree one, and its incident edge is a pendant edge.

Lemma 4.5. *Let G be a bipartite graph with the normal components $G_1, G_2, \ldots, G_m$, $m \geq 1$. Then $af(G) = \sum_{i=1}^{m} af(G_i)$.*

Proof. For $S \subseteq E(G)$ that contains no fixed double edges of G, let $S_i := S \cap E(G_i)$, $i = 1, 2, \ldots, m$. It suffices to prove that S is an anti-forcing set of G if and only if every S_i is an anti-forcing set of G_i, $i = 1, 2, \ldots, m$. From the definition any perfect matching of G consists of a perfect matching of each G_i, $i = 1, 2, \ldots, m$, and the fixed double edges of G. So, if S is an anti-forcing set of G, then $G - S$ has a unique perfect matching. Further each S_i is an anti-forcing set of G_i, $i = 1, 2, \ldots, m$; otherwise, there would be i such that $G_i - S_i$ has at least two perfect matchings, so $G - S$ also has at least two perfect matchings, a contradiction. Conversely, suppose that every S_i is an anti-forcing set of G_i, $i = 1, 2, \ldots, m$. Then $G - S$ has a perfect matching M. If $G - S$ has an M-alternating cycle C, then C does not pass through fixed edges, so C lies entirely in

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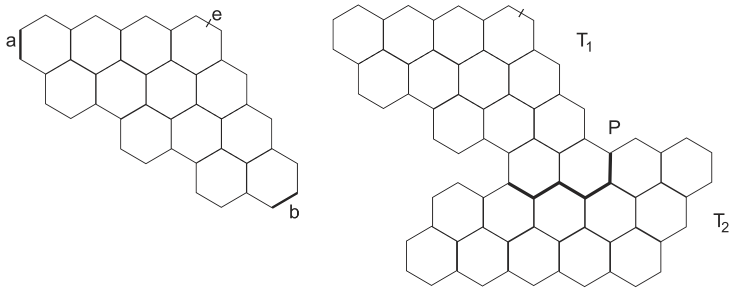

Fig. 6. (a) A truncated parallelogram with specific edges a and b. (b) Gluing two truncated parallelograms.

some normal component G_i. This implies that $G_i - S_i$ has at least two perfect matchings, a contradiction. Hence $G - S$ has a unique perfect matching and S is an anti-forcing set of G. □

The following known results are useful in the subsequent discussions.

Lemma 4.6 ([17]). *If a bipartite graph has a unique perfect matching, then it has a pair of pendant vertices with different colors.*

Lemma 4.7 ([24]). *Let H be a connected plane bipartite graph with a perfect matching. If all pendant vertices of G are of the same color and lie on the boundary, then G has at least one normal block. If G has a fixed single edge and $\delta(G) \geq 2$, then G has at least two normal blocks.*

Lemma 4.8 ([23]). *Let H be a hexagonal system with a perfect matching. Let $E = \{e_1, e_2, \ldots, e_r\}$ be a set of parallel edges of H such that e_i and e_{i+1} belong to the same hexagon and the e_1 and e_r are boundary edges. Then E is an edge-cut of H and $|E \cap M|$ is invariant for all perfect matchings M of H.*

Theorem 4.9. *Let H be a hexagonal system with a fixed single edge. Then $af(H) = 2$ if and only if H has exactly two normal components, which are both truncated parallelograms.*

Proof. By Lemma 4.7 H has at least two normal components. Such normal components have the anti-forcing number at least one since they are normal hexagonal systems and have at least two perfect matchings. By Lemma 4.5 we have that the anti-forcing number of H equals the sum of the anti-forcing numbers of such normal components. Hence $af(H) = 2$ if and only if H has exactly two normal components, which are truncated parallelograms by Theorem 4.4. □

Theorem 4.10. *Let H be a normal hexagonal system. Then $af(H) = 2$ if and only if H is not truncated parallelogram and H can be obtained by gluing two truncated parallelograms T_1 and T_2 along their boundary parts as a fused path P of odd length such that*

(i) *an anti-forcing edge of T_1 remains on the boundary,*

(ii) *the hexagons of each T_i with an edge of P form a linear chain or a chain with one kink (i.e. the inner dual is a path with exactly one turning vertex), and*

(iii) *when the fused path P passes through edge b or a of T_1, the hexagons of T_1 (resp. T_2) with an edge of P form a linear chain (resp. a chain with one kink) (see Fig. 6).*

Proof. Suppose that $af(H) = 2$. Then H has distinct edges e and e' such that $H' := H - e - e'$ has a unique perfect matching M. So by Lemma 4.6 H' has two pendant vertices with different colors. Then one of e and e', say e, must be a boundary edge of H; otherwise H' has at most one pendant vertex, a contradiction.

Claim 1. e has at least one end with degree two in H.

Otherwise, suppose that e has both ends with degree three. Then $H - e$ has the minimum degree two. If $H - e$ is 2-connected, it must be a hexagonal system other than truncated parallelogram, contradicting that $H - e$ has an anti-forcing edge e'. If $H - e$ has a cut edge, by Lemma 4.7 $H - e$ has at least two normal components. So $af(H - e) \geq 2$, also a contradiction, and Claim 1 holds.

So $H - e$ has a pendant vertex x. The edge e_0 between x and its neighbor belongs to all perfect matchings of $H - e$, and is thus anti-forced by e. Deleting the ends of this edge and their incident edges, any pendant edges of the resulting graph also belong to all perfect matchings of $H - e$, such pendant edges are anti-forced by e. Repeating the above process, until to get a graph without pendant vertices, denoted by $H \ominus e$.

Claim 2. $H \ominus e$ is a truncated parallelogram with an anti-forcing edge e'.

If $H \ominus e$ is empty, then e is an anti-forcing edge of H, a contradiction. Otherwise, $H \ominus e$ has a perfect matching and the minimum degree two. Note that the interior faces of $H \ominus e$ are hexagons. By the similar arguments as the proof of Claim 1, we have that $H \ominus e$ is a hexagonal system with an anti-forcing edge e'. Hence Claim 2 holds.

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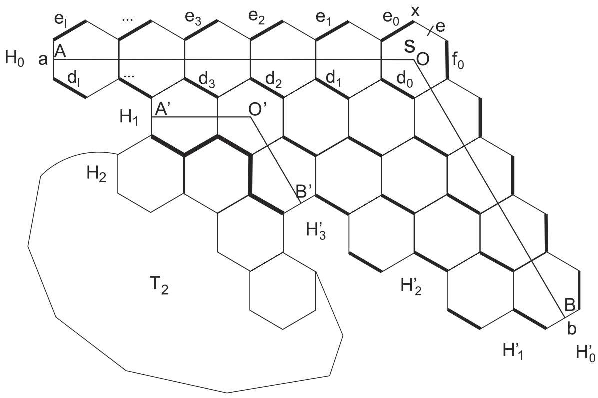

Fig. 7. Illustration for the proof of Theorem 4.10 ($m = 1$, $m' = 3$).

Without loss of generality, suppose that edge e is from the left-up end x to the right-low end so that e_0 is a slant edge. Let s be the hexagon with edge e, f_0 the vertical edge of s adjacent to e, d_0 the other edge of s parallel to e. From the center O of s draw a ray perpendicular to and away from f_0 (resp. e_0) intersecting a boundary edge a at A (resp. edge b at B) such that OA (resp. OB) only passes through hexagons of H. Let H_0 and H_0' be the linear chains of H consisting of hexagons intersecting OA and OB; See Fig. 7. By the similar reasons as Claim 1, we have the following claim.

Claim 3. It is impossible that H has not only hexagons adjacent above to H_0 but also hexagons adjacent right to H_0'.

By Claim 3 we may suppose that H has no hexagons adjacent above to H_0. Let $e_1, e_2, \ldots, e_l$ denote a series of edges in H_0 parallel to e_0 and above OA, $d_1, d_2, \ldots, d_l$ denote a series of edges in H_0 parallel to d_0 and below OA (see Fig. 7), where $l \geq 0$ and e_l is adjacent to a. Hence $e_0, e_1, \ldots, e_l$ are anti-forced by e in turn and thus belong to M.

Let H_1 be the graph consisting of the hexagons adjacent to H_0 and below it. If d_l is a boundary edge of H, then $d_l, \ldots, d_1, d_0$ are further anti-forced by e and thus belong to M. So H_1 is a linear chain with an end hexagon in H_0', and thus H_1 has at most many hexagons as H_0. Otherwise, by Lemma 4.8 we have that some vertical edges in H_1 are fixed single edges, contradicting that H is normal. In general, for $i \geq 0$ we define H_{i+1} recursively as the graph consisting of the hexagons adjacent to H_i and below it. Suppose that for each $0 \leq i \leq m$, H_{i+1} has no hexagon adjacent left to the left end hexagon of H_i. By the same reasons as above we can show recursively that H_{i+1} is a linear chain with an end hexagon in H_0' and the bottom edges in H_i parallel to d_0 are anti-forced by e and thus belong to M. There are two cases to be considered.

Case 1. H has no hexagons adjacent right to H_0'.

In this case there must be a non-negative integer m such that for each $1 \leq i \leq m$, H_i is a linear chain with an end hexagon in H_0' and H_i has at most many hexagons as H_{i-1}, but H_{m+1} has a hexagon adjacent left to the left end hexagon of H_m. Otherwise H is a truncated parallelogram, a contradiction. Along chain H_0', similarly as rows H_i we can define H_j' in turn and have the similar fact: there must be a non-negative integer m' such that for each $1 \leq j \leq m'$, H_j' is a linear chain with an end hexagon in H_0 and H_j' has at most many hexagons as H_{j-1}', but $H_{m'+1}$ has a hexagon adjacent below to the lowest hexagon of $H_{m'}'$ (see Fig. 7). Note that $m = 0$ or $m' = 0$ is allowed. Then H_m and $H_{m'}'$ have exactly one hexagon s' in common. Let O' be the center of s', A' the center of the most-left vertical edge of H_m and B' the center of the lowest right edge of $H_{m'}'$. By Claim 2 $T_2 := H \ominus e$ is a truncated parallelogram just lying in left-low side of the broken line $A'O'B'$. Let T_1 be the graph consisting of $H_0, \ldots, H_m$ and $H_0', \ldots, H_{m'}'$. It is obvious that T_1 is a truncated parallelogram, T_1 and T_2 intersect at a path of odd length, and statements (i) and (ii) hold.

Case 2. H has a hexagon adjacent right to H_0'.

Let H_0'' be the graph consisting of hexagons of H adjacent right to H_0'. Let m be the least non-negative integer such that H_m has the right end hexagon adjacent to a hexagon of H_0''. Let $f_0, f_1, \ldots, f_m$ be a series of vertical edges of H_0' on its right side (see Fig. 8). Then the edges $f_0, f_1, \ldots, f_{m-1}$ are anti-forced by e and thus belong to M. If every H_i is a linear chain and H_i has no hexagons adjacent left to the left-end hexagon of H_{i-1}, then H_0'' is a linear chain. This implies that H_0'' intersect H_0' at a path of odd length, so $T_2 = H \ominus e$ must be a truncated parallelogram consisting of H_0'' and its right side. Otherwise, by analogous arguments we have that for each $1 \leq i \leq m$, H_i is a linear chain with an end hexagon in H_0' and H_i has at most many hexagons as H_{i-1}, but H_{m+1} has a hexagon adjacent left to the left end hexagon of H_m. Let s' be the right end hexagon of H_m, O' the center of s', A' the center of the most-left vertical edge of H_m and B' the center of the edge of s' adjacent above to f_m. Then $T_2 := H \ominus e$ just lies in the low and right side of the broken line $A'O'B'$, and T_1 consists of $H_0, H_1, \ldots, H_m$ (see Fig. 8). So the necessity is proved.

Conversely, suppose that H is obtained from the construction that the theorem states. We can see that the anti-forcing edge e of T_1 can anti-force all double and single edges of T_1 except for the path P. That is, $H \ominus e = T_2$. Hence $af(H) \leq 2$. Since H is not truncated parallelogram, $af(H) = 2$. □

Finally we give some examples of applying the construction of Theorem 4.10 as shown in Fig. 9. The last graph has the minimum forcing number one. In fact, Zhang and Li [31], and Hansen and Zheng [12] determined hexagonal systems with a

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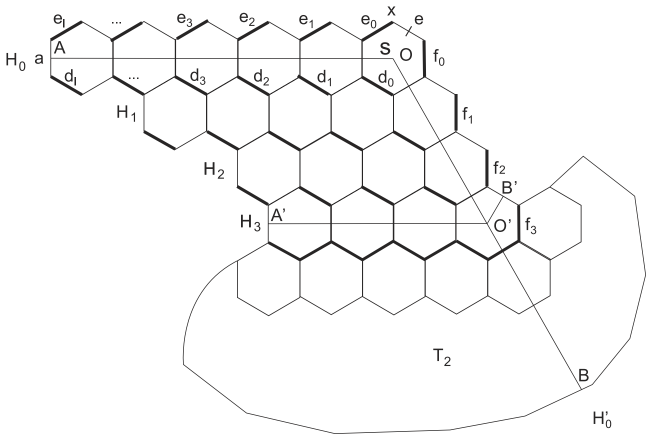

Fig. 8. Illustration for the proof of Theorem 4.10 ($m = 3$).

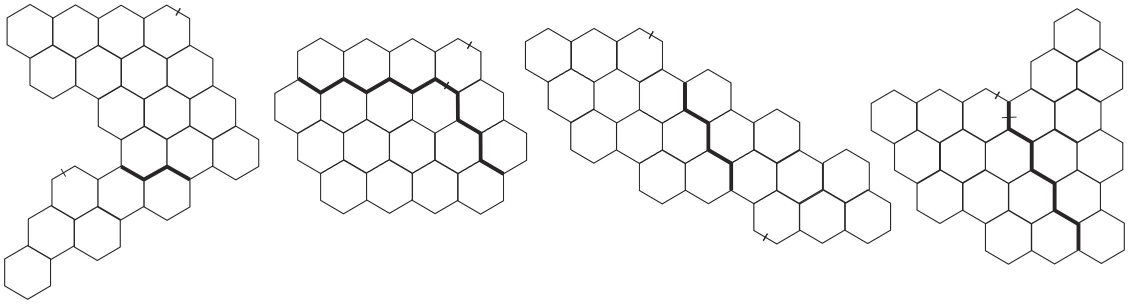

Fig. 9. Four examples for gluing two truncated parallelograms along a path of odd length (marked by bold line) to get hexagonal systems with the anti-forcing number 2.

forcing edge. In hexagonal systems H with $af(H) \leq 2$, we can see that in addition to the kind of last graphs, we always have that $af(H) = f(H)$.

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