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The anti-forcing number of double hexagonal chains[1]

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Abstract

The anti-forcing number of a graph is the smallest number of edges that have to be removed so that the remaining graph contains only one perfect matching. In this paper, the anti-forcing number of double hexagonal chains is determined and the extremal graphs are characterized.

1 Introduction

The anti-forcing number was recently introduced by Vukičević and Trinajstić [1]. The roots of these concepts can be traced to reports by Randić and Klein [2] and Harary et al. [3]. Randić and Klein introduced the term the innate degree of freedom or the forcing number of a Kekulé structure. Later Harary et al. discussed the concept of forcing number in more detail.

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The forcing number is equal to the smallest number of double bonds that completely determine the Kekulé structure of a given benzenoid. After the initial report [3], several papers appeared reporting the forcing number of hexagonal systems and square grids [4,5].

Later, Vukičevic, Sedlar and Došlić [14-15,6] introduced the global forcing number of a graph and gave several results concerning global forcing sets and numbers of grid and benzenoid graphs. In particular, Došlić proved that all catacondensed benzenoids and catafused coronoids with n hexagons have the global forcing number equal to n, and that for pericondensed benzenoids the global forcing number is always strictly smaller than the number of hexagons.

All graphs in this paper are simple, connected, and have a perfect matching, if not explicitly stated otherwise. For all terms and notation not defined here we refer the reader to [7].

A perfect matching in a graph G is a set M of edges of G such that every vertex of G is incident with exactly one edge from M.

Let $G = (V, E)$ be a graph G with a perfect matching. In [1], an anti-forcing set of G is a subset A of E such that $G - A$ has a unique Kekulé structure. An anti-forcing set of the smallest cardinality is called a minimal anti-forcing set, and its cardinality is the anti-forcing number of G. We denote it by $af(G)$. It is the smallest number of edges that have to be removed from a benzenoid to obtain a graph with a single Kekulé structure. The minimal anti-forcing set and the anti-forcing number of the benzenoid parallelogram ([8-10]) $B_{m,n}$ are determined in [1], where $B_{m,n}$ is consisting of $m \times n$ hexagons, arranged in m rows, each row consisting of n hexagons. It was proved there that $af(B_{m,n}) = 1$. In [11], the author gave an algorithm for computing the anti-forcing number of hexagonal chains and determine the bounds of the anti-forcing number of hexagonal chains.

The aim of this paper is to analyze the anti-forcing number of double hexagonal chains.

2 The anti-forcing number of double hexagonal chains

Let us now consider the main subject of the present paper, the double hexagonal chains. Hexagonal systems are of great importance for theoretical chemistry because they are the molecular graphs (or, more precisely, the graphs representing the carbon-atom skeleton) of benzenoid hydrocarbons. The mathematical theory of hexagonal systems is nowadays being greatly expanded.

Our standard reference for any terminology of hexagonal systems is [8,12-13].

A hexagonal system is a 2-connected plane graph whose every interior face is bounded by a regular hexagon of unit length 1. A vertex of a hexagonal system belongs to at most three hexagons. A vertex shared by three hexagons is called an internal vertex of the respective hexagonal system. A hexagonal system H is said to be catacondensed if it does not possess internal vertices, otherwise H is said to be pericondensed. A hexagonal chain is a catacondensed hexagonal system which has no hexagon adjacent to more than two hexagons. An n-tuple hexagonal chain consists of n condensed identical hexagonal chains. When $n = 2$, we call it a double hexagonal chain [9].

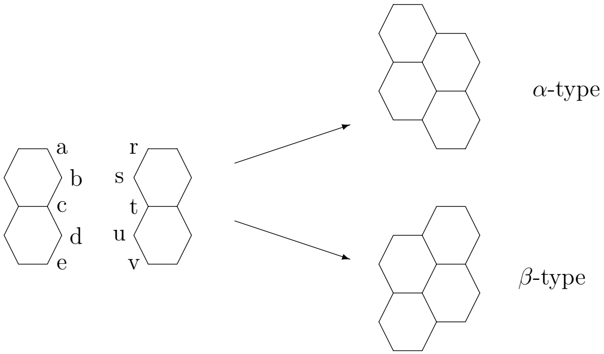


Figure 1. α-type fusing, β-type fusing.

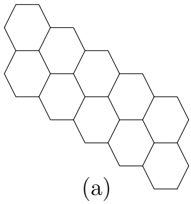
A double hexagonal chain can be constructed inductively. Let us orient the naphthalene so that its interior edges are horizontal. There are two types of fusion of two naphthalenes: (i) $b \equiv r$, $c \equiv s$, $d \equiv t$, $e \equiv u$; (ii) $a \equiv s$, $b \equiv t$, $c \equiv u$, $d \equiv v$ as shown in Figure 1. We call them α-type and β-type fusing, respectively. Any double hexagonal chain can be obtained from a naphthalene B by a stepwise fusion of new naphthalene, and at each step a type of fusion is selected from θ-type fusing, where $\theta \in \{\alpha, \beta\}$.

Let $B(\theta_1, \theta_2, \cdots, \theta_n)$ be the double hexagonal chain obtained from a naphthalene B by θ_1-type, θ_2-type, $\cdots$, θ_n-type, successively. Then, $B(\theta_1, \theta_2, \cdots, \theta_n)$ has $n+1$ naphthalenes or $2(n+1)$ hexagons. And $B(\alpha, \alpha, \cdots, \alpha)$ or $B(\beta, \beta, \cdots, \beta)$, i.e., $\theta_i = \theta_{i+1}$ for each i, is called the double linear hexagonal chain and denoted by DL_n; if $\theta_i \neq \theta_{i+1}$ for each i, then $B(\theta_1, \theta_2, \cdots, \theta_n)$ is called the double zig-zag hexagonal chain and denoted by DZ_n (see Figure 2(a)(b)).

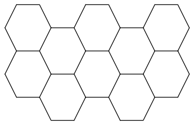
Let

$$\overline{\theta} = \begin{cases} \beta, & \text{if } \theta = \alpha; \\ \alpha, & \text{if } \theta = \beta. \end{cases}$$

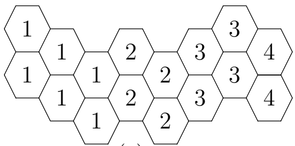
Then $B(\theta_1, \theta_2, \cdots, \theta_n)$ and $B(\overline{\theta_1}, \overline{\theta_2}, \cdots, \overline{\theta_n})$ are isomorphic, i.e., $B(\theta_1, \theta_2, \cdots, \theta_n) \cong B(\overline{\theta_1}, \overline{\theta_2}, \cdots, \overline{\theta_n})$. If $n \geq 1$, the double hexagonal chain $B(\theta_1, \theta_2, \cdots, \theta_n)$ is a pericondensed hexagonal system.



(a)



(b)



(c)

Figure 2. (a) The double linear hexagonal chain $DL_4 = B(\alpha, \alpha, \alpha, \alpha)$;
(b) The double zig-zag hexagonal chain $DZ_4 = B(\alpha, \beta, \alpha, \beta)$;
(c) The double hexagonal chain $B(\alpha, \alpha, \beta, \alpha, \beta, \beta, \alpha)$.

Now we define a segment in a double hexagonal chain. We scan a double hexagonal chain G from left to right. The first maximal sub-double-linear-chain S_1 in G is called the first segment of G; if $G \neq S_1$, let $G_1 = G - S_1$, where the last three fusing edges of S_1 are left, then the first segment S_2 of G_1 is called the second segment of G, and so on. The number of the naphthalenes in a segment S is called its length and is denoted by $l(S)$. The length of a segment is always at least 2, except, possible, for the last segment of G. For example, there are four segments in $B(\alpha, \alpha, \beta, \alpha, \beta, \beta, \alpha)$ with lengths $3, 2, 2, 1$, respectively (see Figure 2(c)). The double linear hexagonal chain DL_n has only one segment and the double zig-zag hexagonal chain DZ_n has $[\frac{n}{2}] + 1$ segments, where $[x]$ is the integer part of x.

Lemma 1. Let $G = (V, E)$ be a graph obtained from a double hexagonal chain G_0 by gluing to it a (single) linear hexagonal chain in the way shown in Fig.3. Then $af(G) \geq af(G_0)$.

Proof. Let A be an anti-forcing set of the smallest cardinality in G and M the unique perfect matching in $G - A$. Then either both the edges x and

y are in M, or no one of them is in M.

If $x, y \notin M$, then $A_0 = A \cap E(G)$ is an anti-forcing set of G_0. So, $af(G) = |A| \geq |A_0| \geq af(G_0)$.

If $x, y \in M$, then there is a conjugated circuit of M in part of the single linear hexagonal chain of G, and A contains at least one edge of the single linear hexagonal chain. Let $M_0 = (M \cap E(G_0)) \cup \{z\}$, $A_0 = (A \cap E(G_0)) \cup \{w\} - \{z\}$ if $z \in A$ and $A_0 = A \cap E(G_0)$ if $z \notin A$. Then M_0 is the unique perfect matching of $G_0 - A_0$ and A_0 is an anti-forcing set of G_0. So, $af(G) = |A| \geq |A_0| \geq af(G_0)$.

Therefore, the result holds.

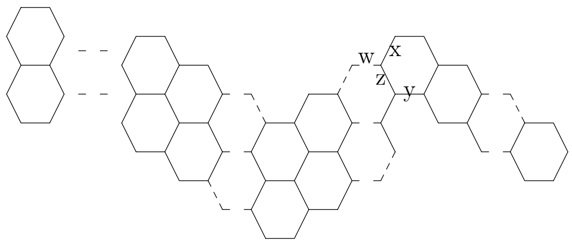


Figure 3. The graph G in Lemma 1.

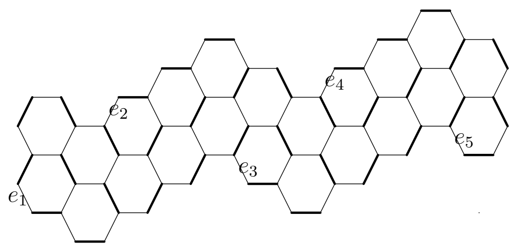


Figure 4. A double hexagonal chain with an anti-forcing set.

Lemma 2. Let $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ be a double hexagonal chain with $n+1$ naphthalenes and k segments. Then $af(G) \leq k$.

Proof. Without loss of generality, we may assume that $\theta_1 = \alpha$. S_i is the $i-$th segment of G, $1 \leq i \leq k$. We only need to find an anti-forcing set of G with k edges.

Let e_i be the oblique edge at the bottom or the oblique edge at the top on the first column of S_i depend on S_i down or up from left to right (see Figure 4). Then $A = \{e_1, e_2, \cdots, e_k\}$ is an anti-forcing set of G with k edges since each $S_i - e_i$ has a unique perfect matching for $1 \leq i \leq k$.

So, $af(G) \leq k$.

Theorem 3. Let $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ be a double hexagonal chain with $n+1$ naphthalenes and k segments. Then $af(G) = k$.

Proof. We prove the result by induction on n. When $n = 1$, G is the benzenoid parallelogram $B_{1,2}$ with $k = 1$, and $af(G) = 1$. When $n = 2$, G is the benzenoid parallelogram $B_{2,2}$ if $\theta_1 = \theta_2$, i.e., $k = 1$, and then $af(G) = 1$; If $\theta_1 \neq \theta_2$, i.e., $k = 2$, then $G = B(\alpha, \beta)$ or $G = B(\beta, \alpha)$. For any edge e of G, the graph $G - \{e\}$ has a perfect matching with a conjugated circuit, and hence $af(G) = 2$. The result holds for $n = 1, 2$. Now we assume inductively that the result holds for all double hexagonal chains with at most $n+1$ naphthalenes, $n \geq 2$. We need to prove that if $G = B(\theta_1, \theta_2, \cdots, \theta_{n+1})$ be the double hexagonal chain with $n+2$ naphthalenes, then $af(G) = k$, where k is the number of segments in G.

By Lemma 2, we only need to prove that $af(G) \geq k$.

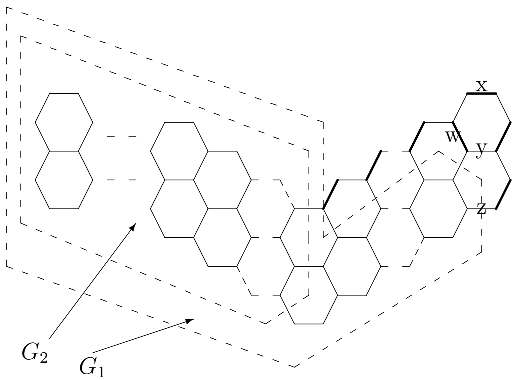


Figure 5. The graphs in Case I.

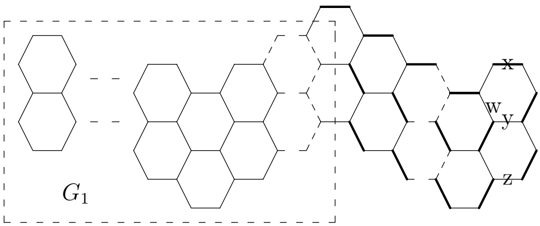
Without loss of generality, we may assume $\theta_{n+1} = \beta$. If $k = 1$, then G is a double linear hexagonal chain and it is a benzenoid parallelogram, its anti-forcing number is 1. The result holds. In the following, we assume $k \geq 2$. Let A be an anti-forcing set of the smallest cardinality in G and M the unique matching in $G - A$. If x, y, z are the three horizontal edges in the last naphthalene, then exactly one of x, y, z belongs to M.

Case I. $x \in M$. Then $y, z \notin M$.

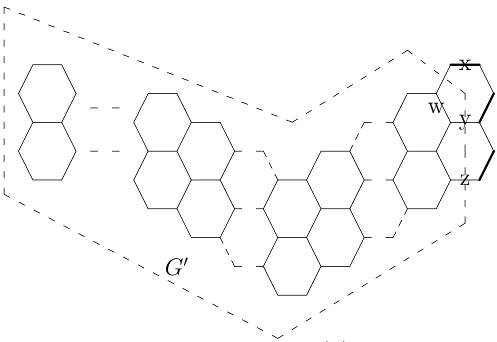
(i) If $w \in M$, see Figure 5, then $A_1 = A \cap E(G_1)$ is an anti-forcing set of G_1, and $|A| \geq |A_1| + 1$ since there is a conjugated circuit of M in $G - E(G_1)$. So, $af(G) = |A| \geq |A_1| + 1 \geq af(G_1) + 1$. Note that G_2 is a double hexagonal chain with at most n naphthalenes and at least $k-1$ segments. By Lemma 1 and the inductive hypothesis, we have

$$af(G_1) \geq af(G_2) \geq k - 1$$

and $af(G) \geq k$.



(a)



(b)

Figure 6.

(ii) If $w \notin M$, then G is shown in Figure 6(a) when the length of the last segment is 1. Let $A_1 = A \cap E(G_1)$, then A_1 is an anti-forcing set of G_1, and $|A| \geq |A_1| + 2$ since $G - E(G_1)$ has two conjugated circuits of M whose common edge is in M. So, $af(G) = |A| \geq |A_1| + 2 \geq af(G_1) + 2$. G_1 is a double hexagonal chain with at most $n-1$ naphthalenes and $k-2$ segments. By the inductive hypothesis, we have $af(G_1) = k - 2$, and $af(G) \geq k$.

When the length of the last segment in G is at least 2, G is shown in Figure 6(b). Then A is also an anti-forcing set of G', and G' is a double hexagonal chain with $n+1$ naphthalenes and k segments, $af(G') = k$ by the inductive hypothesis. We have $af(G) = |A| \geq af(G') = k$.

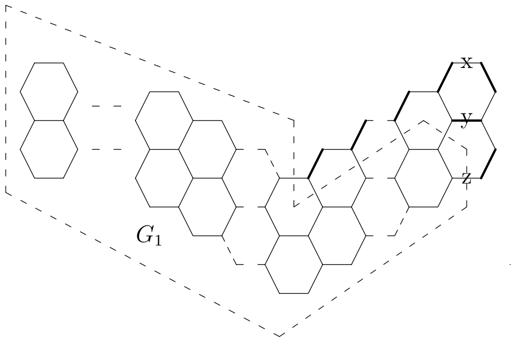


Figure 7. The graphs in Case II.

Case II. $y \in M$. Then $x, z \notin M$ and G is showed in Figure 7. As in Case I(i), we have $af(G) \geq k$.

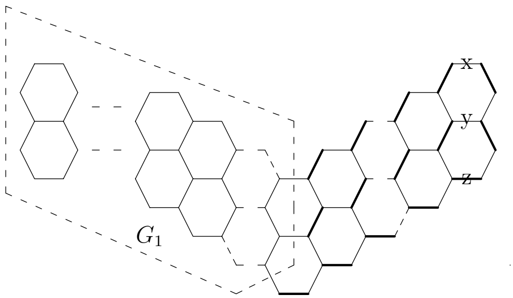


Figure 8. The graphs in Case III.

Case III. $z \in M$. Then $x, y \notin M$ and G is showed in Figure 8.

Let $A_1 = A \cap E(G_1)$. A_1 is an anti-forcing set of G_1, and $|A| \geq |A_1| + 1$ since $G - E(G_1)$ has a conjugated circuits of M. So, $af(G) = |A| \geq |A_1| + 1 \geq af(G_1) + 1$. Note that G_1 is a double hexagonal chain with at most n naphthalenes and $k-1$ segments. By the inductive hypothesis, we have

$af(G_1) = k - 1$, and $af(G) \geq k$.

So, $af(G) \geq k$, and hence $af(G) = k$ by Lemma 2.

The following results are immediate from Theorem 3.

Corollary 4. Let $G = DZ_n$ be a double zig-zag hexagonal chain with $n + 1$ segments. Then $af(G) = [\frac{n}{2}] + 1$, where $[x]$ is the integer part of x.

If a double hexagonal chain with $n+1$ segments $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ has only one segment, then $G \cong DL_n$. And if k is the the number of segments of $G = B(\theta_1, \theta_2, \cdots, \theta_n)$, then $n + 1 \geq 2k - 1$ since the lengths of segments except the last segment are at least 2. So, $k \leq \frac{n}{2} + 1$, and $k \leq [\frac{n}{2}] + 1$ since k is an integer. We can obtain the following result.

Corollary 5. Let $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ be any double hexagonal chain with $n + 1$ naphthalenes. Then

$$1 = af(DL_n) \leq af(G) \leq af(DZ_n) = [\frac{n}{2}] + 1$$

with the left equality if and only if $G \cong DL_n$ and the right equality if and only if

(i) the sequence of lengths of segments in G is $2, \cdots, 2, 1$ when n is even;

(ii) the sequence of lengths of segments in G is $2, 2, \cdots, 2$ or $3, 2, \cdots, 2, 1$ when n is odd, where the sequence of lengths of segments in G is the ordering of lengths of all segments in G from large to small.

3 Conclusion

How difficult it would be to generalize the results to the case of n-tuple hexagonal chains? From our proofs, it seems that only real difficulty is in the case I(i) and II of Theorem 3. In fact, we need a result analogous to Lemma 1: If G be a graph obtained from a n-tuple hexagonal chain G_1 by gluing to it a m-tuple linear hexagonal chain G_2, $1 \leq m \leq n - 1$, then $af(G) \geq af(G_1)$. But then it is complicated since any $2k$ $(0 \leq 2k \leq m + 1)$ edges of the $m + 1$ edges in $G - E(G_1)$ and neighbor to G_1 can belong to a perfect matching M.

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