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Minimum Maximal Matchings in Phenylene Chains

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Abstract

A matching M in a graph G is a set of pairwise non-adjacent edges. M is maximal if it is not contained in any other matching of G. A minimum maximal matching is a maximal matching of minimum size, and its cardinality is the saturation number of G. Maximal matchings serve as an effective model for characterizing certain real-world problems, while the saturation number captures information about their worst-case scenarios in a certain sense. In this paper, we prove that the saturation number of any phenylene chain with n benzenoids is $2n$. We also derive a formula to enumerate minimum maximal matchings via the transfer matrix method. Furthermore, we determine the extremal phenylene chains with n benzenoids achieving the largest and smallest number of minimum maximal matchings, respectively.

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1 Introduction

Let $V(G)$ and $E(G)$ denote the vertex set and edge set of a graph G, respectively. Let $M \subseteq E(G)$. If no two edges in M are adjacent, then M is called a *matching* or *independent edge set* of G. A matching M is *maximum* if there is no matching in G with more edges than M. The cardinality of a maximum matching in G is called the *matching number* of G and is denoted by $\nu(G)$. A matching M is *maximal* if no other matching in G contains it as a proper subset. Maximum matchings must be maximal, but the opposite is generally not true. The maximal matching with the fewest edges is called the *minimum maximal matching*. The cardinality of a minimum maximal matching is called the *saturation number* of the graph G and is denoted by $s(G)$. The saturation number of G satisfies $\frac{1}{2}\nu(G) \leq s(G) \leq \nu(G)$ [4]. Although the computation of the matching number is in polynomial time, the computation of the saturation number is NP-complete. In fact, $M \subseteq E(G)$ is a maximal matching if and only if it is an *independent edge-dominating set* [22] (i.e., a matching such that every edge of G is adjacent to an edge in it). Therefore, the saturation number equals both the independent edge-dominating number and the edge-dominating number. It was proved that computing the edge-dominating number is NP-complete even for planar graphs or bipartite graphs of maximum degree 3 [22]. Furthermore, stronger intractability and inapproximability results have also been confirmed [6, 7, 14].

Maximal matchings are an effective model for characterizing problems such as communication network routing [22], block allocation of sequential resources [8], and dimer adsorption on molecular surfaces [9]. The saturation number quantifies worst-case scenario characteristics of these systems. Matsumoto et al. [15] proposed a 2-approximation algorithm based on the edge-coloring number of graphs to compute the saturation number. Taşkın et al. [19] studied the saturation numbers of general graphs with integer programming formulation. Saturation numbers for some special graphs have been determined, yielding either exact values or tight upper and lower bounds. Examples include hypercube graphs [12, 13], trees [22], chordal graphs [14], series-parallel graphs [16], complete multipartite graphs [18], lexicographic product graphs [20], and graphs with bounded maximum degree [2,3,5], etc. Within chemistry, saturation numbers have been determined for several classes of molecular graphs, including lattice animals [10], benzenoid graphs [11], fullerene graphs [1, 9], as well as nanocones and nanotubes [17, 21].

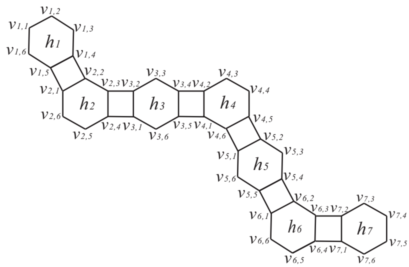


Figure 1. A phenylene chain with seven hexagons.

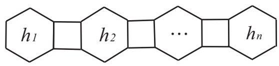


Figure 2. The linear phenylene chain with n hexagons.

In this paper, we focus on phenylene chains. A phenylene chain consists of alternating benzenoids and cyclobutadiene units, and its molecular graph is formed by connecting hexagons and squares in a linear alternating sequence. In this structure, hexagons are only adjacent to squares, and each square is adjacent to exactly two hexagons. For a phenylene chain with n (≥ 2) hexagons, we label the n hexagons as $h_1, h_2, \cdots, h_n$ in sequence, and denote the chain by $H(h_1, h_2, \cdots, h_n)$. To simplify notation, $H(h_1, h_2, \cdots, h_n)$ will be written as H_n when unambiguous, i.e., $H_n = H(h_1, h_2, \cdots, h_n)$. In a phenylene chain, if an internal hexagon has two adjacent vertices of degree 2, it is said to be *angular-fused*. Otherwise, it is *linear-fused*. The terminal hexagons h_1 and h_n are regard as linear-fused. As shown in Fig. 1, H_7 denotes a phenylene chain with seven hexagons, where h_2, h_4, and h_6 are angular-fused. A phenylene chain is called a *linear chain* if all its hexagons are linear-fused (see Fig. 2). In Section 2, Theorem 3 establishes that the saturation number is exactly

$2n$ for every chain consisting of n hexagons. In Section 3, using transfer matrix methods, we derive a formula for the number of minimum maximal matchings. In Section 4, we identify the extremal phenylene chains that attain the largest and smallest numbers of minimum maximal matchings. Specifically, Theorem 3, together with Example 1, shows that among all n-hexagon chains, the largest number of minimum maximal matchings is asymptotically 3^{n-2}, achieved by the linear chain depicted in Fig. 2. Theorem 3, together with Example 2, further shows that the smallest number of such matchings is asymptotically $(1+\sqrt{2})^{n-2}$, attained by the helical chain depicted in Fig. 8.

2 Saturation numbers of phenylene chains

Let M be a matching in a graph G. A vertex of G is called *M-covered* if it is incident to an edge in M; otherwise, it is *M-uncovered*. The graph $G - V(M)$ is obtained by deleting all vertices covered by M and all their incident edges. A set $S \subseteq V(G)$ is an *independent set* if no two vertices in S are adjacent. The *independence number* of G is the maximum size of an independent set in G.

Proposition 1. *[18] Let M be a matching of graph G. M is maximal if and only if $G - V(M)$ is an independent set of graph G.*

Proposition 2. *Let M be a maximal matching in the phenylene chain H_n. Then each hexagon h_i ($1 \le i \le n$) contains at most two M-uncovered vertices within it.*

Proof. Since the independence number of any hexagon h_i in H_n is at most three, Proposition 1 implies that h_i contains at most three M-uncovered vertices. Suppose there exists a hexagon h_k ($1 \le k \le n$) that contains three M-uncovered vertices. Label its vertices consecutively as $v_1, v_2, \cdots, v_6$ in clockwise order. Consequently, the three M-uncovered vertices must form an independent set, leaving v_1, v_3, v_5 and v_2, v_4, v_6 as the only possibilities. If they are v_1, v_3, v_5, then at least one vertex from v_2, v_4, v_6 must also be M-uncovered, a contradiction. Symmetrically, the case v_2, v_4, v_6 leads to the same contradiction. Therefore, h_k contains at most two M-uncovered vertices. ■

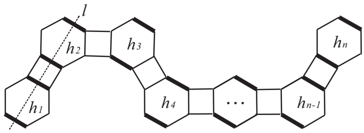


Figure 3. Illustration of the proof of Theorem 3.

Theorem 3. *For a phenylene chain H_n, $s(H_n) = 2n$.*

Proof. Let M be a minimum maximal matching of H_n. By Proposition 2, there are at most $2n$ M-uncovered vertices in H_n. So $|V(H_n) - V(M))| = 6n - |V(M)| \leq 2n$, i.e., $|M| \geq 2n$. We have $s(H_n) = |M| \geq 2n$.

On the other hand, let l be the straight line passing through the centers of hexagons h_1 and h_2. The set of all edges perpendicular to l in H_n forms a maximal matching M', as shown in Fig. 3, where thick edges represent M'. Since each hexagon has exactly two edges perpendicular to l, we have $|M'| = 2n$. Therefore, we conclude that $s(H_n) \leq 2n$. ■

Theorem 3 demonstrates that the saturation number of any phenylene chain depends solely on its number of hexagons, regardless of the fusion pattern of the hexagons. Consequently, the following conclusion holds.

Corollary. *Let M be a maximal matching of H_n. Then M is minimum if and only if each hexagon contains exactly two M-uncovered vertices.*

Proof. Let M be a minimum maximal matching. Suppose there exists a hexagon with fewer than two M-uncovered vertices. According to Proposition 2, $|V(H_n) - V(M)| = 6n - |V(M)| < 2n$, i.e., $|M| > 2n$, which contradicts Theorem 3. Therefore, each hexagon contains exactly two M-uncovered vertices.

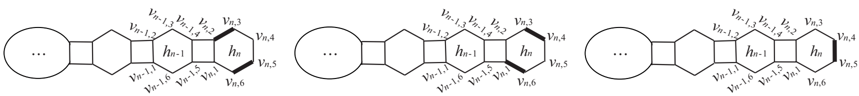
Conversely, if each hexagon contains exactly two M-uncovered vertices, then $|V(M)| = 6n - 2n = 4n$, i.e., $|M| = 2n$. By Theorem 3, M is a minimum maximal matching. ■

3 Counting minimum maximal matchings

Let l_i $(1 \le i \le n-2)$ be the straight line passing through the centers of hexagons h_i and h_{i+1} in H_n $(n \ge 3)$. Then, h_{i+2} is called *straight-linear type* if it intersects l_i, and is denoted S-type. Furthermore, h_{i+2} is called l*eft-turning type* (resp. *right-turning type*) if it is on the left (resp. right) side of l_i along the direction from h_i to h_{i+1}, and is denoted L-type (resp. R-type) (see Fig. 4).

Let the vertices of the i-th hexagon h_i $(1 \le i \le n)$ in H_n be labeled as $v_{i,1}$, $v_{i,2}$, $v_{i,3}$, $v_{i,4}$, $v_{i,5}$, $v_{i,6}$ in clockwise order. For $i = 1$, let $v_{1,4}v_{1,5}$ be the shared edge of h_1 and its right-adjacent square. For $2 \le i \le n$, let $v_{i,1}v_{i,2}$ be the shared edge of h_i and its left-adjacent square (see Fig. 1). Let M be any minimum maximal matching of H_n. By Proposition 1 and Corollary 1, there are exactly two M-uncovered vertices in the n-th hexagon h_n, and they can only be $\{v_{n,1}, v_{n,4}\}$, $\{v_{n,2}, v_{n,5}\}$, or $\{v_{n,3}, v_{n,6}\}$. Let $m(H_n)$ denote the number of minimum maximal matchings in H_n, and let $m_k(H_n)$ $(k = 1, 2, 3)$ denote the number of minimum maximal matchings with $v_{n,k}$, $v_{n,k+3}$ uncovered. Then

$$m(H_n) = m_1(H_n) + m_2(H_n) + m_3(H_n). \tag{1}$$



(a) $v_{n,1}$ and $v_{n,4}$ are M-uncovered. **(b)** $v_{n,2}$ and $v_{n,5}$ are M-uncovered. **(c)** $v_{n,3}$ and $v_{n,6}$ are M-uncovered.

Figure 4. Illustrations of the proof of Lemma 1.

Lemma 1. *If the end hexagon h_n of H_n is S-type, then*

$$m(H_n) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_S \cdot \mathbf{1},$$

where $\mathbf{1} = [1,1,1]^\top$, $\quad A_S = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 2 \end{bmatrix}$.

Proof. Let M be a minimum maximal matching of H_n. According to the positions of the two M-uncovered vertices in h_n, there are three cases to be discussed.

Case 1. If $v_{n,1}$ and $v_{n,4}$ are M-uncovered, then M must contain the edge set $\{v_{n,2}v_{n,3}, v_{n,5}v_{n,6}\}$ (see Fig. 5(a)), and the number of such minimum maximal matchings is $m_1(H_n)$. By maximality of M, $v_{n-1,5}$ must be M-covered. If $v_{n-1,4}v_{n-1,5} \in M$, then $v_{n-1,3}$ and $v_{n-1,6}$ in h_{n-1} have to be M-uncovered. The number of such minimum maximal matchings is $m_3(H_{n-1})$. If $v_{n-1,5}v_{n-1,6} \in M$, then $v_{n-1,1}$ and $v_{n-1,4}$ must be M-uncovered. The number of such minimum maximal matchings is $m_1(H_{n-1})$. Therefore

$$m_1(H_n) = 1 \cdot m_1(H_{n-1}) + 0 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{2}$$

Case 2. If $v_{n,2}$ and $v_{n,5}$ are M-uncovered, then $\{v_{n,3}v_{n,4}, v_{n,1}v_{n,6}\} \subseteq M$ (see Fig. 5(b)), and the number of such minimum maximal matchings is $m_2(H_n)$. By maximality of M, $v_{n-1,4}$ must be M-covered. If $v_{n-1,3}v_{n-1,4} \in M$, then $v_{n-1,2}$ and $v_{n-1,5}$ must be M-uncovered. The number of such minimum maximal matchings is $m_2(H_{n-1})$. If $v_{n-1,4}v_{n-1,5} \in M$, then $v_{n-1,3}$ and $v_{n-1,6}$ have to be $M-$uncovered. The number of such minimum maximal matchings is $m_3(H_{n-1})$. Hence

$$m_2(H_n) = 0 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{3}$$

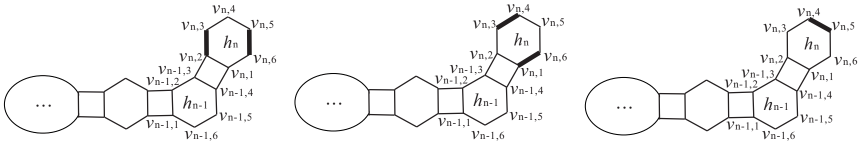
Case 3. If $v_{n,3}$ and $v_{n,6}$ are M-uncovered, then $v_{n,4}v_{n,5} \subseteq M$ (see Fig. 5(c)). The number of such minimum maximal matchings is $m_3(H_n)$. By maximality of M, $v_{n,1}$ and $v_{n,2}$ both are M-covered. If $v_{n,1}v_{n,2} \in M$, then $M \setminus \{v_{n,1}v_{n,2}, v_{n,4}v_{n,5}\}$ is a minimum maximal matching of H_{n-1}. By the formula (1), the number of such minimum maximal matchings is $m_1(H_{n-1}) + m_2(H_{n-1}) + m_3(H_{n-1})$. If $\{v_{n,1}v_{n-1,5}, v_{n,2}v_{n-1,4}\} \subseteq M$, then $v_{n-1,3}$ and $v_{n-1,6}$ are M-uncovered. The number of such minimum maximal matchings is $m_3(H_{n-1})$. Thus

$$m_3(H_n) = 1 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 2 \cdot m_3(H_{n-1}). \tag{4}$$

By Formulas (2), (3) and (4), we have

$$(m_1(H_n), m_2(H_n), m_3(H_n)) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_S.$$

According to the Formula (1), the conclusion holds. ■



(a) $v_{n,1}$ and $v_{n,4}$ are M-uncovered. **(b)** $v_{n,2}$ and $v_{n,5}$ are M-uncovered. **(c)** $v_{n,3}$ and $v_{n,6}$ are M-uncovered.

Figure 5. Illustrations of the proof of Lemma 2.

Lemma 2. *If the end hexagon h_n of H_n is L-type, then*

$$m(H_n) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_L \cdot \mathbf{1},$$

where $A_L = \begin{bmatrix} 0 & 1 & 1 \\ 1 & 1 & 2 \\ 1 & 0 & 1 \end{bmatrix}.$

Proof. Let M be a minimum maximal matching of H_n. According to the positions of the two M-uncovered vertices in h_n, there are three cases to be discussed.

Case 1. If $v_{n,1}$ and $v_{n,4}$ are M-uncovered in h_n, then $\{v_{n,2}v_{n,3}, v_{n,5}v_{n,6}\} \subseteq M$ (see Fig. 6(a)). By maximality of M, $v_{n-1,4}$ must be M-covered. If $v_{n-1,3}v_{n-1,4} \in M$, then $v_{n-1,2}$ and $v_{n-1,5}$ have to be M-uncovered in h_{n-1}. The number of such minimum maximal matchings is $m_2(H_{n-1})$. If $v_{n-1,4}v_{n-1,5} \in M$, then $v_{n-1,3}$ and $v_{n-1,6}$ must be M-uncovered. The number of such minimum maximal matchings is $m_3(H_{n-1})$. Therefore

$$m_1(H_n) = 0 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{5}$$

Case 2. If $v_{n,2}$ and $v_{n,5}$ are M-uncovered, then $\{v_{n,3}v_{n,4}, v_{n,1}v_{n,6}\} \subseteq M$ (see Fig. 6(b)). By maximality of M, $v_{n-1,3}$ must be M-covered. If $v_{n-1,2}v_{n-1,3} \in M$, then $v_{n-1,1}$ and $v_{n-1,4}$ must be M-uncovered in h_{n-1}. The number of such minimum maximal matchings is $m_1(H_{n-1})$. If $v_{n-1,3}v_{n-1,4} \in M$, then $v_{n-1,2}$ and $v_{n-1,5}$ have to be M-uncovered. The number of such minimum maximal matchings is $m_2(H_{n-1})$. So

$$m_2(H_n) = 1 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 0 \cdot m_3(H_{n-1}). \tag{6}$$

Case 3. If $v_{n,3}$ and $v_{n,6}$ are M-uncovered, then the edge $v_{n,4}v_{n,5} \subseteq M$

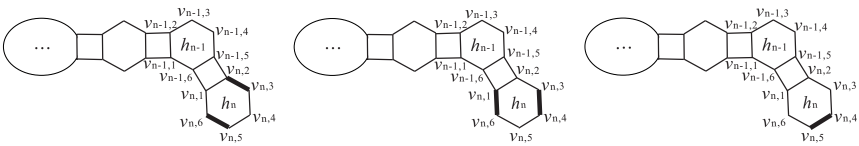
(see Fig. 6(c)). By maximality of M, $v_{n,1}$ and $v_{n,2}$ both are M-covered. If $v_{n,1}v_{n,2} \in M$, then $M \setminus \{v_{n,1}v_{n,2}, v_{n,4}v_{n,5}\}$ is a minimum maximal matching of H_{n-1}. By Formula (1), the number of such minimum maximal matchings is $m_1(H_{n-1})+m_2(H_{n-1})+m_3(H_{n-1})$. If $\{v_{n,1}v_{n-1,4}, v_{n,2}v_{n-1,3}\} \subseteq M$, then $v_{n-1,2}$ and $v_{n-1,5}$ are M-uncovered. The number of such minimum maximal matchings is $m_2(H_{n-1})$. Hence

$$m_3(H_n) = 1 \cdot m_1(H_{n-1}) + 2 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{7}$$

By Formulas (5), (6) and (7), we have

$$(m_1(H_n), m_2(H_n), m_3(H_n)) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_L.$$

According to Formula (1), the conclusion holds. ■



(a) $v_{n,1}$ and $v_{n,4}$ are M-uncovered. **(b)** $v_{n,2}$ and $v_{n,5}$ are M-uncovered. **(c)** $v_{n,3}$ and $v_{n,6}$ are M-uncovered.

Figure 6. Illustrations of the proof of Lemma 3.

Lemma 3. *If the end hexagon h_n of H_n is R-type, then*

$$m(H_n) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_R \cdot \mathbf{1},$$

where $A_R = \begin{bmatrix} 1 & 1 & 2 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}$.

Proof. Let M be a minimum maximal matching of H_n. According to the positions of the two M-uncovered vertices in h_n, there are three cases to be discussed.

Case 1. If $v_{n,1}$ and $v_{n,4}$ are M-uncovered, then $\{v_{n,2}v_{n,3}, v_{n,5}v_{n,6}\} \subseteq M$ (see Fig. 7(a)). By maximality of M, $v_{n-1,6}$ must be M-covered. If $v_{n-1,5}v_{n-1,6} \in M$, then $v_{n-1,1}$ and $v_{n-1,4}$ have to be M-uncovered in h_{n-1}. The number of such minimum maximal matchings is $m_1(H_{n-1})$.

If $v_{n-1,1}v_{n-1,6} \in M$, then $v_{n-1,2}$ and $v_{n-1,5}$ must be M-uncovered. The number of such minimum maximal matchings is $m_2(H_{n-1})$. So

$$m_1(H_n) = 1 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 0 \cdot m_3(H_{n-1}). \tag{8}$$

Case 2. If $v_{n,2}$ and $v_{n,5}$ are M-uncovered, then $\{v_{n,3}v_{n,4}, v_{n,1}v_{n,6}\} \subseteq M$ (see Fig. 7(b)). By maximality of M, $v_{n-1,5}$ must be M-covered. If $v_{n-1,5}v_{n-1,6} \in M$, then $v_{n-1,1}$ and $v_{n-1,4}$ have to be M-uncovered. The number of such minimum maximal matchings is $m_1(H_{n-1})$. If $v_{n-1,4}v_{n-1,5} \in M$, then $v_{n-1,3}$ and $v_{n-1,6}$ must be M-uncovered. The number of such minimum maximal matchings is $m_3(H_{n-1})$. Therefore

$$m_2(H_n) = 1 \cdot m_1(H_{n-1}) + 0 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{9}$$

Case 3. If $v_{n,3}$ and $v_{n,6}$ are M-uncovered, then $v_{n,4}v_{n,5} \subseteq M$ (see Fig. 7(c)). By maximality of M, $v_{n,1}$ and $v_{n,2}$ both are M-covered. If $v_{n,1}v_{n,2} \in M$, then $M \setminus \{v_{n,1}v_{n,2}, v_{n,4}v_{n,5}\}$ is a minimum maximal matching of H_{n-1}. By the Formula (1), the number of such minimum maximal matchings is $m_1(H_{n-1})+m_2(H_{n-1})+m_3(H_{n-1})$. If $\{v_{n,1}v_{n-1,6}, v_{n,2}v_{n-1,5}\} \subseteq M$, then $v_{n-1,1}$ and $v_{n-1,4}$ have to be M-uncovered. The number of such minimum maximal matchings is $m_1(H_{n-1})$. Hence

$$m_3(H_n) = 2 \cdot m_1(H_{n-1}) + 1 \cdot m_2(H_{n-1}) + 1 \cdot m_3(H_{n-1}). \tag{10}$$

By Formulas (8), (9) and (10), we have

$$(m_1(H_n), m_2(H_n), m_3(H_n)) = (m_1(H_{n-1}), m_2(H_{n-1}), m_3(H_{n-1})) \cdot A_R.$$

According to the Formula (1), the conclusion holds. ■

By Lemmas 1, 2, and 3, we obtain the counting formula for the minimum maximal matching of any phenylene chain as follows:

Theorem 4. *For a phenylene chain H_n with n hexagons,*

$$m(H_n) = \mathbf{1}^\top \cdot A_2 \cdot A_3 \cdot \cdots \cdot A_{n-1} \cdot A_n \cdot \mathbf{1},$$

where for each $i = 2, 3, \ldots, n$,

$$A_i = \begin{cases} A_S, & \text{if } h_i \text{ is } S\text{-type}, \\ A_L, & \text{if } h_i \text{ is } L\text{-type}, \\ A_R, & \text{if } h_i \text{ is } R\text{-type}. \end{cases}$$

Proof. According to Lemmas 1, 2, and 3, we can derive that

$$(m_1(H_n), m_2(H_n), m_3(H_n)) = (m_1(H_2), m_2(H_2), m_3(H_2)) \cdot A_3 \cdot \cdots \cdot A_{n-1} \cdot A_n.$$

For $3 \leq i \leq n$, $A_i = A_S$ if h_i is S-type, $A_i = A_L$ if h_i is L-type, and $A_i = A_R$ if h_i is R-type.

Note that

$$(m_1(H_2), m_2(H_2), m_3(H_2)) = (2, 2, 4) = \mathbf{1}^\top \cdot A_S = \mathbf{1}^\top \cdot A_L = \mathbf{1}^\top \cdot A_R.$$

Therefore, h_2 can be regarded as any of the S-, L-, or R-types. Combined with the Formula (1), this allows us to derive the conclusion. ■

In fact, the first two hexagons h_1 and h_2 in H_n can be considered as S-type; thus H_n can be represented by a sequence of hexagon types. For instance, Fig. 1 illustrates a phenylene chain encoded as $H_7(S, S, L, S, R, S, L)$.

Example 1. For the linear chain $H_n(S, S, \cdots, S)$, see Fig. 2. By Theorem 4,

$$m(H_n(S, S, \cdots, S)) = \mathbf{1}^\top \cdot A_S^{n-1} \cdot \mathbf{1}.$$

Note that A_S can be diagonalized as

$$T^{-1} A_S T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{bmatrix},$$

where $T = \begin{bmatrix} -1 & -1 & 1 \\ -1 & 1 & 1 \\ 1 & 0 & 2 \end{bmatrix}$.

Therefore

$$A_S^{n-1} = \begin{bmatrix} \frac{1+3^{n-2}}{2} & \frac{3^{n-2}-1}{2} & 3^{n-2} \\ \frac{3^{n-2}-1}{2} & \frac{1+3^{n-2}}{2} & 3^{n-2} \\ 3^{n-2} & 3^{n-2} & 2\cdot 3^{n-2} \end{bmatrix}.$$

We have

$$m(H_n(S,S,\cdots,S)) = \mathbf{1}^\top \cdot A_S^{n-1} \cdot \mathbf{1} = 8\cdot 3^{n-2} \quad (n \geq 2).$$

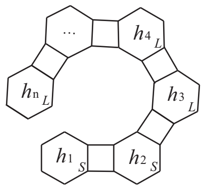


Figure 7. The helical phenylene chain.

Example 2. H_n is called a *helical chain* if hexagons $h_3, h_4, \cdots, h_n$ all are R-types or L-types. For the helical chain $H_n(S,S,L,\cdots,L)$, see Fig. 7. By Theorem 4,

$$m(H_n(S,S,L,\cdots,L)) = \mathbf{1}^\top \cdot A_S \cdot A_L^{n-2} \cdot \mathbf{1}.$$

The eigenvalues of the matrix A_L are $\lambda_1 = 0$, $\lambda_2 = 1+\sqrt{2}$, and $\lambda_3 = 1-\sqrt{2}$. The matrix can be diagonalized as

$$T^{-1}A_LT = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 1+\sqrt{2} & 0 \\ 0 & 0 & 1-\sqrt{2} \end{bmatrix},$$

where $T = \begin{bmatrix} -1 & \sqrt{2} & -\sqrt{2} \\ -1 & 1+\sqrt{2} & 1-\sqrt{2} \\ 1 & 1 & 1 \end{bmatrix}$.

So

$$A_L{}^{n-2} = \begin{bmatrix} \frac{(2-\sqrt{2})\lambda_2^{n-2}+(2+\sqrt{2})\lambda_3^{n-2}}{2} & \frac{(\sqrt{2}-1)\lambda_2^{n-2}-(\sqrt{2}+1)\lambda_3^{n-2}}{2} & \frac{\lambda_2^{n-2}+\lambda_3^{n-2}}{2} \\ \frac{\lambda_2^{n-2}+\lambda_3^{n-2}}{2} & \frac{\lambda_2^{n-2}-\lambda_3^{n-2}}{2\sqrt{2}} & \frac{(2+\sqrt{2})\lambda_2^{n-2}+(2-\sqrt{2})\lambda_3^{n-2}}{4} \\ \frac{(\sqrt{2}-1)\lambda_2^{n-2}-(\sqrt{2}+1)\lambda_3^{n-2}}{2} & \frac{(\sqrt{2}-1)\lambda_2^{n-2}+(\sqrt{2}+1)\lambda_3^{n-2}}{2\sqrt{2}} & \frac{\lambda_2^{n-2}-\lambda_3^{n-2}}{2\sqrt{2}} \end{bmatrix}.$$

We can derive that

$$m(H_n(S,S,L,\cdots,L)) = (4+3\sqrt{2})(1+\sqrt{2})^{n-2} + (4-3\sqrt{2})(1-\sqrt{2})^{n-2} \quad (n \geq 2).$$

Note that $H_n(S,S,L,\cdots,L)$ is isomorphic to $H_n(S,S,R,\cdots,R)$. So $m(H_n(S,S,R,\cdots,R)) = m(\ H_n(S,\ S,\ L,\ \cdots\ ,L))$.

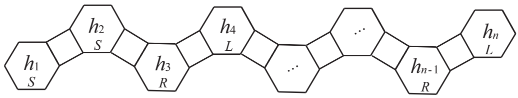


Figure 8. The zigzag phenylene chain.

Example 3. H_n is called a *zigzag chain* if hexagons $h_3, h_4, \cdots, h_n$ are alternately connected in R-type and L-type, see Fig. 8.

For $n \equiv 0 \pmod 2$, by Theorem 4,

$$m(H_n(S,S,R,L,\cdots,R,L)) = \mathbf{1}^\top \cdot A_S \cdot (A_R \cdot A_L)^{\frac{n-2}{2}} \cdot \mathbf{1}.$$

The matrix $A_R \cdot A_L$ has three distinct eigenvalues $\lambda_1 = 0$, $\lambda_2 = \frac{7+3\sqrt{5}}{2}$, and $\lambda_3 = \frac{7-3\sqrt{5}}{2}$. It can be diagonalized as

$$T^{-1}(A_R \cdot A_L)T = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{7+3\sqrt{5}}{2} & 0 \\ 0 & 0 & \frac{7-3\sqrt{5}}{2} \end{bmatrix},$$

where $T = \begin{bmatrix} -1 & 5\lambda_2 - 1 & 5\lambda_3 - 1 \\ -1 & 2\lambda_2 - 1 & 2\lambda_3 - 1 \\ 1 & 3\lambda_2 & 3\lambda_3 \end{bmatrix}.$

Therefore

$$(A_R \cdot A_L)^{\frac{n-2}{2}} = \begin{bmatrix} \frac{\sqrt{5}(\lambda_2^{\frac{n-2}{2}} - \lambda_3^{\frac{n-2}{2}})}{5} & \frac{(5-\sqrt{5})\lambda_2^{\frac{n-2}{2}} + (5+\sqrt{5})\lambda_3^{\frac{n-2}{2}}}{10} & \frac{(5+\sqrt{5})\lambda_2^{\frac{n-2}{2}} + (5-\sqrt{5})\lambda_3^{\frac{n-2}{2}}}{10} \\ \frac{(3\sqrt{5}-5)\lambda_2^{\frac{n-2}{2}} + (-3\sqrt{5}-5)\lambda_3^{\frac{n-2}{2}}}{10} & \frac{(5-2\sqrt{5})\lambda_2^{\frac{n-2}{2}} + (5+2\sqrt{5})\lambda_3^{\frac{n-2}{2}}}{5} & \frac{(5-\sqrt{5})\lambda_2^{\frac{n-2}{2}} + (5+\sqrt{5})\lambda_3^{\frac{n-2}{2}}}{10} \\ \frac{(5-\sqrt{5})\lambda_2^{\frac{n-2}{2}} + (5+\sqrt{5})\lambda_3^{\frac{n-2}{2}}}{10} & \frac{(3\sqrt{5}-5)\lambda_2^{\frac{n-2}{2}} + (-3\sqrt{5}-5)\lambda_3^{\frac{n-2}{2}}}{10} & \frac{\sqrt{5}(\lambda_2^{\frac{n-2}{2}} - \lambda_3^{\frac{n-2}{2}})}{5} \end{bmatrix}$$

We have

$$m(H_n(S,S,R,L,\cdots,R,L))$$
$$=\frac{20+8\sqrt{5}}{5}\left(\frac{7+3\sqrt{5}}{2}\right)^{\frac{n-2}{2}}+\frac{20-8\sqrt{5}}{5}\left(\frac{7+3\sqrt{5}}{2}\right)^{\frac{n-2}{2}} \quad (n\geq 2).$$

For $n \equiv 1 \pmod 2$, we can similarly derive

$$m(H_n(S,S,R,L,\cdots,R,L,R)) = \mathbf{1}^\top \cdot A_S \cdot (A_R \cdot A_L)^{\frac{n-3}{2}} \cdot A_R \cdot \mathbf{1}$$
$$=\frac{50+22\sqrt{5}}{5}\left(\frac{7+3\sqrt{5}}{2}\right)^{\frac{n-3}{2}}+\frac{50-22\sqrt{5}}{5}\left(\frac{7+3\sqrt{5}}{2}\right)^{\frac{n-3}{2}} \quad (n\geq 3).$$

4 The extremal phenylene chains

In this section, we determine the extremal phenylene chains with n hexagons that attain, respectively, the largest and smallest numbers of minimum maximal matchings. Let $\mathcal{M} = \{[\boldsymbol{m}_1,\ \boldsymbol{m}_2,\ \boldsymbol{m}_3] \in \mathbb{R}^{3\times 3} \mid \boldsymbol{m}_3 = \boldsymbol{m}_1 + \boldsymbol{m}_2, \boldsymbol{m}_i \in \mathbb{R}^{3\times 1}, i = 1,2,3\}$. The following lemma is crucial for characterizing these extremal chains.

Lemma 4. *If $A, B \in \mathcal{M}$, then $A \cdot B \in \mathcal{M}$.*

Proof. Let $A, B = [\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3] \in \mathcal{M}$, and $C = A \cdot B = [\boldsymbol{c}_1, \boldsymbol{c}_2, \boldsymbol{c}_3]$. Then $\boldsymbol{c}_1 = A \cdot \boldsymbol{b}_1$, $\boldsymbol{c}_2 = A \cdot \boldsymbol{b}_2$ and $\boldsymbol{c}_3 = A \cdot \boldsymbol{b}_3$. Since $\boldsymbol{b}_3 = \boldsymbol{b}_1 + \boldsymbol{b}_2$, $\boldsymbol{c}_3 = A \cdot \boldsymbol{b}_3 = A \cdot \boldsymbol{b}_1 + A \cdot \boldsymbol{b}_2 = \boldsymbol{c}_1 + \boldsymbol{c}_2$. Thus $A \cdot B \in \mathcal{M}$. ■

Clearly, $A_S, A_L, A_R \in \mathcal{M}$, and thus any finite product of these matrices remains in $\mathcal{M}$. Based on this conclusion, we can derive the following theorem.

Theorem 5. $m(H_n(S,S,L,\cdots,L)) \leq m(H_n) \leq m(H_n(S,S,S,\cdots,S))$. *Furthermore, the upper bound (resp. lower bound) is attained if and only if H_n corresponds to the linear chain (resp. helical chain).*

Proof. According to Theorem 4,

$$m(H_n) = \mathbf{1}^\top \cdot A_2 \cdot A_3 \cdot \cdots \cdot A_{n-1} \cdot A_n \cdot \mathbf{1},$$

where $A_i \in \{A_S, A_L, A_R\}$, $i = 2, 3, \ldots, n$.

Let $A = A_2 \cdot A_3 \cdot \cdots \cdot A_{n-1}$. By Lemma 4, $A \in \mathcal{M}$. Consequently, $\mathbf{1}^\top \cdot A$ must be of the form $(a, b, a+b)$ for some positive integers a and b, proving that

$$m(H_{n-1}) = (a, b, a+b) \cdot \mathbf{1} = 2(a+b).$$

We argue by induction. To establish the upper bound, we first examine the base case $n = 3$, for which the bound holds by direct computation. Suppose the upper bound holds for $n-1$, i.e., $m(H_{n-1}) \leq \mathbf{1}^\top \cdot A_S^{n-2} \cdot \mathbf{1}$.

Let $\mathbf{1}^\top \cdot A_S^{n-2} = (x, y, x+y)$, where x and y both are positive integers. Then

$$m(H_{n-1}(S, S, S, \cdots, S)) = \mathbf{1}^\top \cdot A_S^{n-2} \cdot \mathbf{1} = 2(x+y),$$

$$m(H_n(S, S, S, \cdots, S)) = \mathbf{1}^\top \cdot A_S^{n-1} \cdot \mathbf{1} = 6(x+y).$$

By the inductive hypothesis,

$$a + b \leq x + y.$$

For H_n, there are three cases to be considered.

If $A_n = A_S$, then $m(H_n) = (a, b, a+b) \cdot A_S \cdot \mathbf{1} = (a, b, a+b) \cdot (2, 2, 4)^\top = 6(a+b) \leq 6(x+y)$.

If $A_n = A_L$, then $m(H_n) = (a, b, a+b) \cdot A_L \cdot \mathbf{1} = (a, b, a+b) \cdot (2, 4, 2)^\top = 4a + 6b < 6(a+b) \leq 6(x+y)$.

If $A_n = A_R$, then $m(H_n) = (a, b, a+b) \cdot A_R \cdot \mathbf{1} = (a, b, a+b) \cdot (4, 2, 2)^\top = 6a + 4b < 6(a+b) \leq 6(x+y)$.

Therefore, the upper bound holds for n, completing the induction. Moreover, in the above statement, equality occurs if and only if $A_n = A_S$, meaning the bound is attained precisely when H_n is a linear chain.

We proceed to prove the lower bound. The base case $n = 3$ is confirmed by direct computation, showing the lower bound holds. Assume the lower bound holds for all integers k with $3 \leq k < n$.

Let $\mathbf{1}^\top \cdot A_2 \cdot A_3 \cdot \cdots \cdot A_{n-2} = (a', b', a'+b')$, $\mathbf{1}^\top \cdot A_S \cdot A_L^{n-4} = (p', q', p'+q')$ and $\mathbf{1}^\top \cdot A_S \cdot A_L^{n-3} = (p, q, p+q)$. Then

$$m(H_{n-2}) = \mathbf{1}^\top \cdot A_2 \cdot A_3 \cdot \cdots \cdot A_{n-2} \cdot \mathbf{1} = 2(a' + b'),$$

$$m(H_{n-2}(S,S,L,\cdots,L)) = \mathbf{1}^\top \cdot A_S \cdot A_L^{n-4} \cdot \mathbf{1} = 2(p'+q'),$$

$$m(H_{n-1}(S,S,L,\cdots,L)) = \mathbf{1}^\top \cdot A_S \cdot A_L^{n-3} \cdot \mathbf{1} = 2(p+q).$$

By the inductive hypothesis,

$$p'+q' \leq a'+b', p+q \leq a+b.$$

Since $(p',q',p'+q') \cdot A_L = (p,q,p+q)$, $p = p'+2q'$ and $q = p'+q'$. Thus

$$m(H_n(S,S,L,\cdots,L)) = (p,q,p+q) \cdot A_L \cdot \mathbf{1} = 4p+6q = 10p'+14q'.$$

For H_n, we discuss the following three cases.

Case 1. If $A_{n-1} = A_S$, then $(a',b',a'+b') \cdot A_S = (a,b,a+b)$. Thus $a = 2a'+b'$ and $b = a'+2b'$. We now analyze three distinct subcases based on the possible choices of A_n.

If $A_n = A_S$, then $m(H_n) = 6(a+b) \geq 6(p+q) > 4p+6q$.

If $A_n = A_L$, then $m(H_n) = 4a+6b = 14a'+16b' > 14(a'+b') \geq 14(p'+q') > 10p'+14q'$.

If $A_n = A_R$, then $m(H_n) = 6a+4b = 16a'+14b' > 14(a'+b') \geq 14(p'+q') > 10p'+14q'$.

Case 2. If $A_{n-1} = A_L$, then $(a',b',a'+b') \cdot A_L = (a,b,a+b)$. So

$$a = a'+2b' > a'+b' = b \geq p'+q' = q.$$

In parallel to the previous analysis, we now consider three subcases arising from the choice of A_n. The case $A_n = A_S$ is identical to Case 1.

For $A_n = A_L$, $m(H_n) = 4a+6b = 4(a+b)+2b \geq 4(p+q)+2q = 4p+6q$.

For $A_n = A_R$, $m(H_n) = 6a+4b = 4(a+b)+2a > 4(p+q)+2q = 4p+6q$.

Case 3. If $A_{n-1} = A_R$, then $(a',b',a'+b') \cdot A_R = (a,b,a+b)$. Therefore

$$b = 2a'+b' > a'+b' = a \geq p'+q' = q.$$

Similarly, only need to consider the following two subcases.

If $A_n = A_L$, then $m(H_n) = 4a+6b = 4(a+b)+2b > 4(p+q)+2q = 4p+6q$.

If $A_n = A_R$, then $m(H_n) = 6a + 4b = 4(a + b) + 2a \geq 4(p + q) + 2q = 4p + 6q$.

In conclusion, the lower bound holds for all n, completing the inductive proof. Furthermore, in the proof above, equality holds if and only if $A_{n-1} = A_n = A_L$ or $A_{n-1} = A_n = A_R$, which implies that the lower bound is attained exactly when H_n forms a helical chain. ■

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