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Došlić, Tomislav; Short, Taylor

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Maximal matchings in polyspiro and benzenoid chains

Tomislav Došlić*
Faculty of Civil Engineering
University of Zagreb
doslic@grad.hr

Taylor Short†
Department of Mathematics
University of South Carolina
shorttm2@mailbox.sc.edu

Abstract

A matching M of a graph G is maximal if it is not a proper subset of any other matching in G. Maximal matchings are much less known and researched than their maximum and perfect counterparts. In particular, almost nothing is known about their enumerative properties. In this paper we present the recurrences and generating functions for the sequences enumerating maximal matchings in two classes of chemically interesting linear polymers: polyspiro chains and benzenoid chains. We also analyze the asymptotic behavior of those sequences and determine the extremal cases.

Keywords: maximal matching; benzenoid chain; polyspiro chain

1 Introduction

A matching in a graph is a collection of its edges such that no two edges in this collection have a vertex in common. Matchings in graphs serve as successful models of many phenomena in engineering, natural and social sciences. A strong initial impetus to their study came from the chemistry of benzenoid compounds after it was observed that the stability of benzenoid compounds is related to the existence and the number of perfect matchings in the corresponding graphs. That observation gave rise to a number of enumerative results that were accumulated over the course of several decades;

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we refer the reader to monograph [3] for a survey. Further motivation came from the statistical mechanics *via* the Kasteleyn's solution of the dimer problem [13, 14] and its applications to evaluations of partition functions for a given value of temperature. In both cases, the matchings under consideration are perfect, i.e., their edges are collectively incident to all vertices of G. It is clear that perfect matchings are as large as possible and that no other matching in G can be "larger" than a perfect one. It turns out that in all other applications we are also interested mostly in large matchings.

Basically, there are two ways to quantify the largeness of a matching. One way, by using the number of edges, gives rise to the idea of *maximum matchings*. Maximum matchings are well researched and well understood; there is a well developed structural theory and enumerative results are abundant. The classical monograph by Lóvasz and Plummer [16] is an excellent reference for all aspects of the theory.

An alternative way is to say that a matching is large if no other matching contains it as a proper subset; this gives rise to the concept of *maximal matchings*. Every maximum matching is also maximal, but the opposite is usually not true. Unlike their maximum counterparts, maximal matchings can have different cardinalities (unless the graph is *equimatchable*; see [10]) and the recurrences used for their enumeration are essentially non-local. As a consequence, maximal matchings are much less understood then the maximum ones. There is nothing analogous to the structural theory of maximum matchings and the enumerative results are scarce and scattered through the literature [7, 15, 18].

In spite of their obscurity, maximal matchings are natural models for several problems connected with adsorption of dimers on a structured substrate and block-allocation of a sequential resource. One can find them also in the context of polymerization of organic molecules, as witnessed by an early paper of Flory [9]. A probabilistic approach to the same problem can be found in [11]. We refer the reader to papers [1, 4, 6, 7] for some structural and enumerative results on those models. In this paper our goal is to further the line of research of reference [7] by considering graphs with more complicated connectivity patterns and richer structure of basic units. We provide enumerative and extremal results on maximal matchings in two classes of linear polymers of chemical interest: the polyspiro chains and benzenoid chains. We extablish the recurrences and generating functions for the enumerating sequences of maximal matchings in three classes of uniform polyspiro chains and use the obtained results to determine the asymptotic behavior and to find the extremal chains. Further, we also enumerate maximal matchings in three classes of benzenoid chains and show that one of them is extremal with respect to the number of maximal matchings. Our results show that maximal matchings behave in a radically different way that the perfect matchings; chains rich in maximal matchings are poor in perfect matchings and vice versa. We end by comparing our results with enumerative results for other type of structures in similar polymers and by discussing some possible directions of future research.

2 Preliminaries

Our terminology and notations are mostly standard and taken from [16, 19]. All graphs G considered in this paper will be finite and simple, with vertex set $V(G)$ and edge set $E(G)$. For a subset of vertices S of $V(G)$, we make use of the notation $G-S$ (or $G-v$ if $S=\{v\}$) to denote the subgraph of G obtained by deleting the vertices of S and all edges incident to them. For a graph G and subset of edges X of G, we use the notation $G \setminus X$ (or $G \setminus e$ if $X=\{e\}$) to denote the subgraph of G obtained by deleting the endpoints of the edges in X as well as all incident edges to these endpoints.

A *matching* M in G is a set of edges of G such that no two edges from M have a vertex in common. The number of edges in M is called its *size*. A matching in G with the largest possible size is called a *maximum matching*. If a matching in G is not a subset of a larger matching of G, it is called a *maximal matching*. Let $\Psi(G)$ denote the number of maximal matchings of G.

In this paper we are mainly concerned with counting maximal matchings in two classes of linear polymers (or *facsiagraphs*, [12]) with simple connectivity patterns. The first class are 6-uniform cactus chains. Chain cacti are in chemical literature known as *polyspiro chains*.

A *cactus graph* is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same length m, the cactus is *m-uniform*.

A *hexagonal cactus* is a 6-uniform cactus, i.e., a cactus in which every block is a hexagon. A vertex shared by two or more hexagons is called a *cut-vertex*. If each hexagon of a hexagonal cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two hexagons, we say that G is a *chain hexagonal cactus*. The number of hexagons is called the *length* of the chain. An example of a chain hexagonal cactus is shown in Figure 1.

Furthermore, any chain hexagonal cactus of length greater than one has exactly two hexagons with only one cut-vertex; such hexagons are called

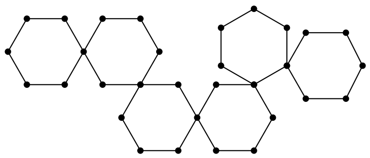

Figure 1: A chain hexagonal cactus of length 6.

terminal and all other hexagons with two cut-vertices are called *internal*.

Internal hexagons can be one of three types depending upon the distance between its cut-vertices: in an *ortho-hexagon* cut vertices are adjacent, in a *meta-hexagon* they are at distance two, and in a *para-hexagon* cut-vertices are at distance three. The terminology is borrowed from the theory of benzenoid hydrocarbons; see [5, 6, 7] for more details. These give rise to the following three types of hexagonal cactus chains of length n: the unique chain whose internal hexagons are all para-hexagons is P_n, the unique chain whose internal hexagons are all meta-hexagons is M_n, and the unique chain whose internal hexagons are all ortho-hexagons is O_n.

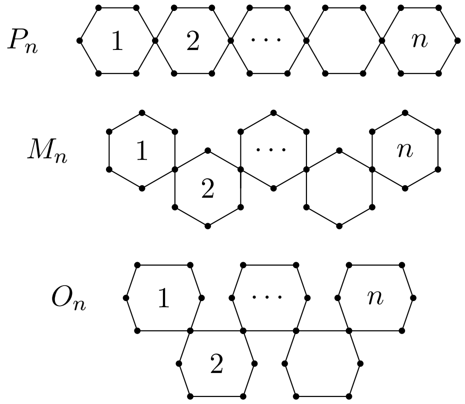

Figure 2: The hexagonal cactus chains P_n, M_n, and O_n.

The other class of unbranched polymers we consider are benzenoid chains. A *benzenoid system* is a is a connected, plane graph without cut-vertices in which all faces, except the unbounded one, are hexagons. Two hexagonal faces are either disjoint or they share exactly one common edge (adjacent hexagons). A vertex of a benzenoid system belongs to at most three hexagonal faces and the benzenoid system is called *catacondensed* if it does not posses such a vertex. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the benzenoid is a *chain* see Figure 3.

The number of hexagons in a benzenoid chain is called its *length*. In each benzenoid chain there are exactly two hexagons adjacent to one other hexagon; those two hexagons are called *terminal*, while any other hexagons are called *interior*. An interior hexagon has two vertices of degree 2. If these two vertices are not adjacent, then hexagon is called *straight*. If the two vertices are adjacent, then the hexagon is called *kinky*.

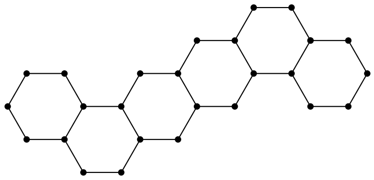

Figure 3: A benzenoid chain of length 6.

If all $n-2$ interior hexagons of a benzenoid chain with n hexagons are straight, we call the chain a *polyacene* and denote it by L_n. If all interior hexagons are kinky, the chain is called a *polyphenacene*. Since the number of perfect matchings in a polyphenacene of length n is equal to the $(n+2)$-nd Fibonacci number F_{n+2}, these chains are also known as *fibonacenes* [3]. We consider two specific families of polyphenacenes depicted in Figure 4: the *zig-zag polyphenacene*, Z_n, and *helicene*, H_n.

3 Chain hexagonal cacti

3.1 Generating functions

In this section, we obtain ordinary generating functions for the number of maximal matchings in the hexagonal chain cacti P_n, M_n, and O_n. To do this, we first find recursions for the number of maximal matchings using auxiliary graphs (initial conditions are obtained by direct counting). These recursions can be verified via casework. By introducing generating functions for the number of maximal matchings in each auxiliary graph, the recursions can be transformed into a solvable system of equations in terms of unknown generating functions. Finally, we solve this system of equations for the desired generating function. We omit the details of most of these computations.

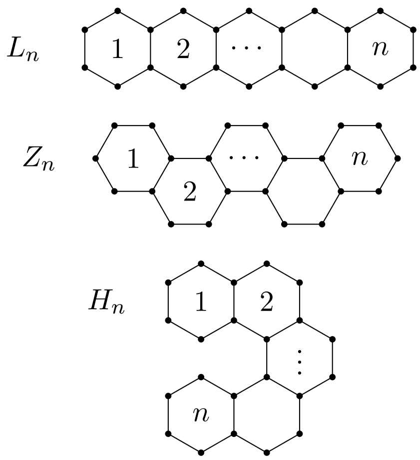

Figure 4: The polyacene, zig-zag polyphenacene, and helicene chains.

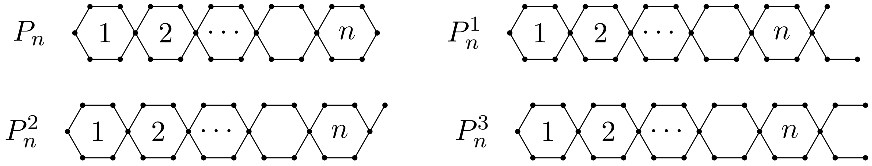

Figure 5: Auxiliary graphs for P_n.

Lemma 3.1. *Let p_n be the number of maximal matchings in P_n and p_n^i be the number of maximal matchings in the auxiliary graph P_n^i in Figure 5. Then*

(i) $p_n = 2p_{n-1}^1 + p_{n-1}$,

(ii) $p_n^1 = p_n^2 + p_{n-1}^3$,

(iii) $p_n^2 = p_{n-1}^3 + 2p_{n-1}^1$,

(iv) $p_n^3 = p_n + 2p_{n-1}^3$,

with the initial conditions $p_0 = 1$, $p_0^1 = 2$, $p_0^2 = 1$, *and* $p_0^3 = 3$.

Lemma 3.2. *Let m_n be the number of maximal matchings in M_n and m_n^i*

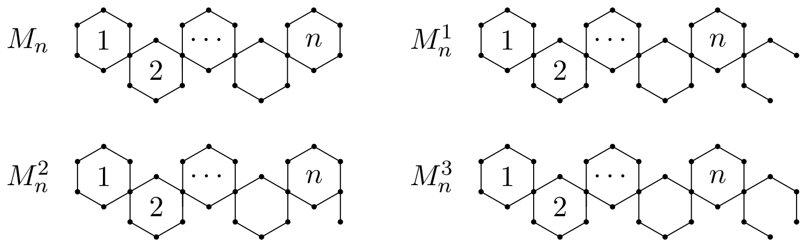

Figure 6: Auxiliary graphs for M_n.

be the number of maximal matchings in the auxiliary graph M_n^i in Figure 6. Then

(*i*) $m_n = 2m_{n-1}^1 + m_{n-1}$,

(*ii*) $m_n^1 = m_n^2 + m_{n-1}^3$,

(*iii*) $m_n^2 = m_{n-1}^3 + m_{n-1}^1 + m_{n-1}^2 + m_{n-1}$,

(*iv*) $m_n^3 = 2m_{n-1}^3 + m_{n-1}^1 + m_{n-1}^2 + m_{n-1} + m_n^2$,

with the initial conditions $m_0 = 1$, $m_0^1 = 2$, $m_0^2 = 1$, *and* $m_0^3 = 3$.

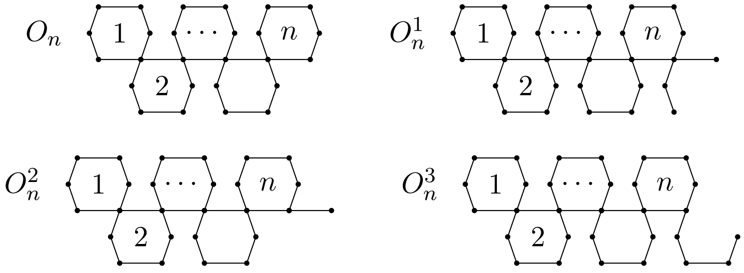

Figure 7: Auxiliary graphs for O_n.

Lemma 3.3. *Let o_n be the number of maximal matchings in O_n and o_n^i be the number of maximal matchings in the auxiliary graph O_n^i in Figure 7. Then* *(i)* $o_n = 2o^1_{n-1} + o_{n-1}$,

(ii) $o^1_n = o^2_n + o^3_{n-1}$,

(iii) $o^2_n = o^3_{n-1} + o^2_{n-1} + o_{n-1} + 2o^3_{n-2}$,

(iv) $o^3_n = o_n + o^3_{n-1} + o^2_n$,

with the initial conditions $o_0 = 1$, $o^1_0 = 2$, $o^2_0 = 1$, $o^2_1 = 7$, *and* $o^3_0 = 3$.

Theorem 3.4. *Let* $P(x)$, $M(x)$, *and* $O(x)$ *be the ordinary generating functions for the sequences* p_n, m_n, *and* o_n, *respectively. Then*

(i)

$$P(x) = \frac{1 + 4x^2}{1 - 5x + 4x^2 - 4x^3},$$

(ii)

$$M(x) = \frac{1 - x - 2x^2}{1 - 6x + 3x^2 - 2x^3},$$

(iii)

$$O(x) = \frac{1 + x + x^2}{1 - 4x - 4x^2 - x^3}.$$

Since $P(x)$, $M(x)$, and $O(x)$ are rational functions, we can conclude that the numbers p_n, m_n, and o_n each satisfy a third order linear recurrence with constant coefficients. The initial conditions can be verified by direct computations.

Corollary 3.5.

(i) $p_n = 5p_{n-1} - 4p_{n-2} + 4p_{n-3}$

with initial conditions $p_0 = 1$, $p_1 = 5$, $p_2 = 25$,

(ii) $m_n = 6m_{n-1} - 3m_{n-2} + 2m_{n-3}$

with initial conditions $m_0 = 1$, $m_1 = 5$, $m_2 = 25$,

(iii) $o_n = 4o_{n-1} + 4o_{n-2} + o_{n-3}$

with initial conditions $o_0 = 1$, $o_1 = 5$, $o_2 = 25$.

None of the obtained sequences appear in *The On-Line Encyclopedia of Integer Sequences* [17].

Now we can apply a version of Darboux's theorem to deduce the asymptotic behavior of the sequences p_n, m_n, and o_n. We refer the reader to any of standard books on generating functions, such as [2, 20] for more information on these techniques.

Theorem 3.6 (Darboux)**.** *Let* $f(x) = \sum_{n=0}^{\infty} a_n x^n$ *denote the ordinary generating function of a sequence* a_n*. If* $f(x)$ *can be written as*

$$f(x) = \left(1 - \frac{x}{w}\right)^{\alpha} g(x),$$

where w *is the smallest modulus singularity of* f *and* g *is analytic at* w*, then*

$$a_n \sim \frac{g(w)}{\Gamma(-\alpha)} w^{-n} n^{-\alpha-1}.$$

Here $\Gamma(x)$ *denotes the gamma function.*

Corollary 3.7.

(i) $p_n \sim 1.37804 \cdot 4.28428^n$*,*

(ii) $m_n \sim 0.81408 \cdot 5.52233^n$*,*

(iii) $o_n \sim 1.05177 \cdot 4.86454^n$*.*

The characteristic equations of the three recurrences can be solved exactly, but the resulting formulas tend to be too cumbersome to be of any use. The equation for meta-chains, however, allows a compact formula for the smallest (and the only) positive root: it is equal to $\frac{1}{2}(1 + \sqrt[3]{3} - \sqrt[3]{9})$.

The obtained asymptotics suggest that meta-chains could be the richest and para-chains the poorest in maximal matchings among all polyspiro chains of the same length. In the next subsection we prove that this is, indeed, the case.

3.2 Extremal structures

Theorem 3.8. *Let* G_n *be a hexagonal cactus of length* n*. Then*

$$\Psi(P_n) \leq \Psi(G_n) \leq \Psi(M_n).$$

Let G_m be an arbitrary hexagonal cactus of length m. Observe that we can always draw G_m as in Figure 8, where h_m is a terminal hexagon and the hexagon adjacent to the left of h_{m-1} may attach at any of the vertices b, a, k, j, or i. Let us assume the hexagons of G_m are labeled $h_1, \ldots, h_m$ according to their ordering in Figure 8 where (h_1 is the other terminal hexagon).

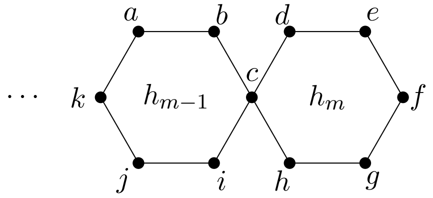

Figure 8: A terminal hexagon, h_m, and its adjacent hexagon, h_{m-1}, in the hexagonal chain cactus G_m.

In what follows, for $1 \leq \ell, p \leq m$ let H_ℓ be the subgraph of G_m induced by the vertices of the hexagons $h_1, \ldots, h_\ell$ and let $H_{\ell,p}$ denote the subgraph of G_m induced by the vertices of the two hexagons h_ℓ and h_p. We will need the following lemmas. The proof of the first lemma is immediate.

Lemma 3.9. *If H is a subgraph of the graph G, then $\Psi(H) \leq \Psi(G)$.*

Lemma 3.10. *Any maximal matching in G_m must contain exactly one of the edges cb, cd, ch, or ci, or the maximal matching must contain all the edges ab, de, ji, and hg.*

Proof. Take a maximal matching M in G_m. For sake of contradiction, suppose that M does not contain any of the edges cb, cd, ch, or ci and that M does not contain all of the edges ab, de, ji, and hg. Then at least one of the edges ab, de, ji, and hg is missing, say ab. Since ab is not in M, then we can add the edge bc to M, which is a contradiction to the fact that M is a maximal matching. The lemma follows. □

Lemma 3.11. *For the subgraph H_{m-1} of G_m, at least one of the following holds:*

(i) $2 \cdot \Psi(H_{m-1} - \{b, c\}) \geq \Psi(H_{m-1} - c)$
(ii) $2 \cdot \Psi(H_{m-1} - \{c, i\}) \geq \Psi(H_{m-1} - c)$

Proof. The proof depends on where the hexagon h_{m-2} attaches to h_{m-1}. By symmetry, suppose that h_{m-2} attaches at either i, j, or k (the case a, b, k

is similar). Consider a maximal matching of $H_{m-1} - c$. If such a matching contains the edge ab, then the remaining edges give a maximal matching of $H_{m-1} - \{a, b, c\}$. If a maximal matching does not contain the edge ab, then the matching must also be maximal in the graph $H_{m-1} - \{b, c\}$. Thus by Lemma 3.9 we have

$$\begin{aligned}\Psi(H_{m-1} - \{c\}) &= \Psi(H_{m-1} - \{a, b, c\}) + \Psi(H_{m-1} - \{b, c\}) \\ &\leq 2 \cdot \Psi(H_{m-1} - \{b, c\}).\end{aligned}$$

□

Proof (of Theorem 3.8). Take a hexagonal cactus C of length $n - 1$. Let us set $m = n - 1$ and suppose that C is drawn as in Figure 8 with vertices labeled as such, so that we may refer to this picture to aid this proof. We consider three cases of extending C by an nth hexagon h_n.

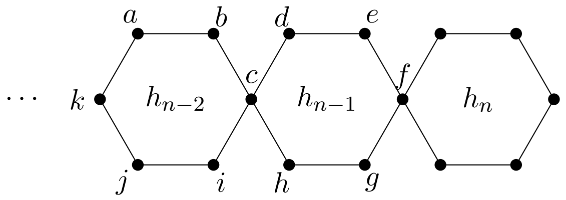

Figure 9: The hexagonal cactus CP.

Case 1. The hexagon h_n attaches in the para position to the vertex f and let us denote the resulting graph by CP, see Figure 9. To compute $\Psi(CP)$ we make use of Lemma 3.10. Consider maximal matchings in CP containing the edge bc. The remaining edges of the matching must be a maximal matching of $H_{n-2} - \{b, c\}$ and a maximal matching of $H_{n-1,n} - c$. By direct counting, we find that $\Psi(H_{n-1,n} - c) = 11$ and hence, the number of maximal matchings containing the edge bc is $11 \cdot \Psi(H_{n-2} - \{b, c\})$. We count the maximal matchings containing the edges ci, cd, or ch as well as the maximal matchings containing all the edges ab, de, ji, and hg similarly, to obtain

$$\begin{aligned}\Psi(CP) =& 11(\Psi(H_{n-2} - \{b, c\}) + \Psi(H_{n-2} - \{c, i\})) + 20 \cdot \Psi(H_{n-2} - c) \\ &+ 5 \cdot \Psi(H_{n-2} - \{a, b, c, i, j\}).\end{aligned}$$

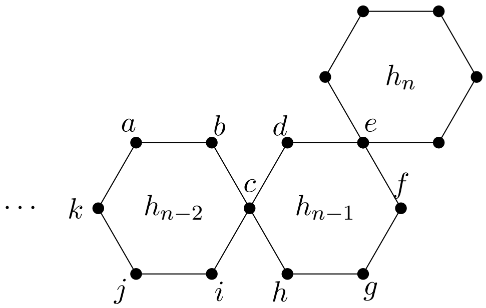

Figure 10: The hexagonal cactus CM.

Case 2. The hexagon h_n attaches in the meta position to the vertex e and let us denote the resulting graph by CM, see Figure 10. Counting similarly to Case 1 above we obtain

$$\begin{aligned}\Psi(CM) =&17(\Psi(H_{n-2} - \{b,c\}) + \Psi(H_{n-2} - \{c,i\})) + 22 \cdot \Psi(H_{n-2} - c)\\ &+ 3 \cdot \Psi(H_{n-2} - \{a,b,c,i,j\}).\end{aligned}$$

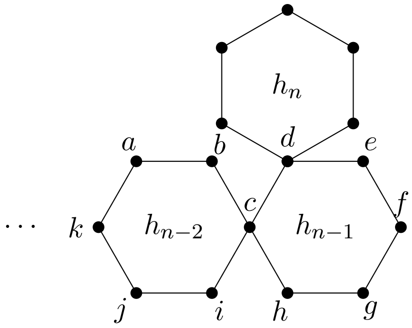

Figure 11: The hexagonal cactus CO.

Case 3. The hexagon h_n attaches in the ortho position to the vertex d and let us denote the resulting graph by CO, see Figure 11. Counting as in Cases 1 and 2,

$$\begin{aligned}\Psi(CO) =&15(\Psi(H_{n-2} - \{b,c\}) + \Psi(H_{n-2} - \{c,i\})) + 18 \cdot \Psi(H_{n-2} - c)\\ &+ 3 \cdot \Psi(H_{n-2} - \{a,b,c,i,j\}).\end{aligned}$$

Now $\Psi(CM) \geq \Psi(CO)$ follows immediately by comparing terms. By Lemma 3.9, we have $\Psi(H_{n-2}-c) \geq \Psi(H_{n-2}-\{a,b,c,i,j\})$ and by comparing the remaining terms we see that $\Psi(CM) \geq \Psi(CP)$. The preceding shows that attaching a hexagon in the meta position yields the most maximal matchings, implying

$$\Psi(G_n) \leq \Psi(M_n)$$

as desired.

To get the remaining inequality of our theorem, we need only show that $\Psi(CO) \geq \Psi(CP)$. Now we must have either (i) or (ii) of Lemma 3.11, say (i) holds. Then $4 \cdot \Psi(H_{n-2} - \{b, c\}) \geq 2 \cdot \Psi(H_{n-2} - c)$ and by Lemma 3.9 we have $\Psi(H_{n-2} - \{c, i\}) \geq \Psi(H_{n-2} - \{a, b, c, i, j\})$, showing that

$$\begin{aligned} \Psi(CO) \geq\ & 11\Psi(H_{n-2} - \{b, c\}) + 13\Psi(H_{n-2} - \{c, i\}) + 20 \cdot \Psi(H_{n-2} - c) \\ & + 5 \cdot \Psi(H_{n-2} - \{a, b, c, i, j\}). \end{aligned} \tag{1}$$

Now by comparing the terms of $\Psi(CP)$ with the inequality (1), it follows that $\Psi(CO) \geq \Psi(CP)$, which completes the proof. □

It is instructive to compare the above results with the corresponding results for all matchings and for independent sets from reference [5] (Theorems 3.23 and 4.14, respectively). It can be seen that with respect to the richest chains, the number of maximal matchings behaves more like the number of independent sets than the number of all matchings. A possible explanation might be the fact that maximal matchings in any graph G are in a bijective correspondence with *nice* independent sets in G. (A set of vertices S is *nice* if $G - S$ has a perfect matching.)

4 Benzenoid chains

4.1 Generating functions

Now we turn our attention to benzenoid chains. Here the connectivity increases to two, and one can expect that this will result in longer recurrences, as indicated in [7]. This is, indeed, the case.

Using the same techniques outlined in subsection 3.1, we obtain ordinary generating functions for the number of maximal matchings in the benzenoid chains L_n, Z_n, and H_n.

Lemma 4.1. *Let* ℓ_n *be the number of maximal matchings in* L_n *and* ℓ_n^i *be the number of maximal matchings in the auxiliary graph* L_n^i *in Figure 12. Then*

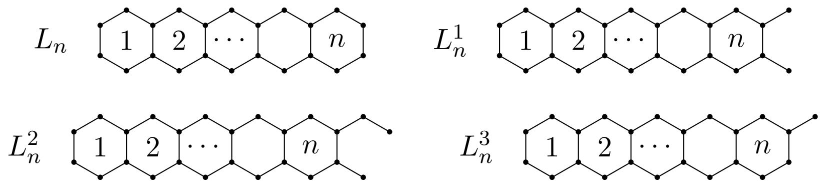

Figure 12: Auxiliary graphs for L_n.

(i) $\ell_n = \ell^1_{n-1} + \ell_{n-1} + 2\ell^2_{n-2}$,

(ii) $\ell^1_n = 2\ell^1_{n-1} + \ell_{n-1} + 2\ell^3_{n-1}$,

(iii) $\ell^2_n = \ell^3_n + \ell^1_{n-1} + \ell^3_{n-1}$,

(iv) $\ell^3_n = \ell^1_{n-1} + \ell_{n-1} + \ell^3_{n-1} + \ell^2_{n-2} + \ell^1_{n-2} + \ell^3_{n-2}$,

with the initial conditions $\ell_0 = 1$, $\ell_1 = 5$, $\ell^1_0 = 2$, $\ell^2_0 = 3$, $\ell^3_0 = 2$, *and* $\ell^3_1 = 7$.

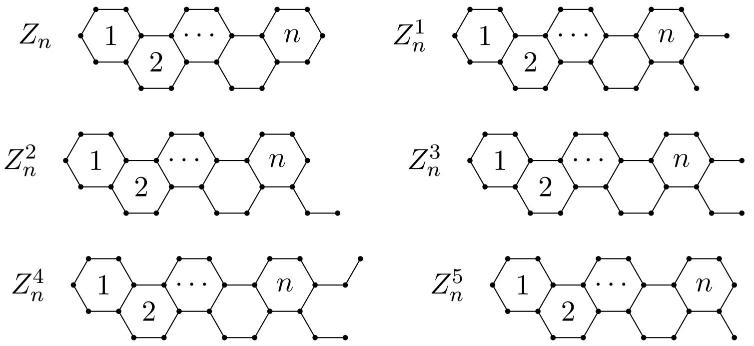

Figure 13: Auxiliary graphs for Z_n.

Lemma 4.2. *Let* z_n *be the number of maximal matchings in* Z_n *and* z^i_n *be the number of maximal matchings in the auxiliary graph* Z^i_n *in Figure 13. Then*

(i) $z_n = z^1_{n-1} + z^2_{n-1} + z^3_{n-2}$,

(*ii*) $z_n^1 = 2z_{n-1}^2 + z_{n-2}^4 + z_{n-1}^5 + z_{n-2}^3 + z_{n-2}^2$,

(*iii*) $z_n^2 = z_n + z_{n-1}^5 + z_{n-1}$,

(*iv*) $z_n^3 = 2z_{n-1}^2 + z_{n-1}^3 + z_{n-1}^1 + z_{n-1}^5$,

(*v*) $z_n^4 = z_n + z_{n-1}^5 + z_{n-1} + z_{n-1}^2 + z_{n-1}^3$,

(*vi*) $z_n^5 = z_{n-1}^5 + z_{n-2}^4 + z_{n-1}^2 + z_{n-2}^3 + z_{n-1}$,

with the initial conditions $z_0 = 1$, $z_1 = 5$, $z_0^1 = 2$, $z_1^1 = 9$, $z_0^2 = 2$, $z_0^3 = 3$, $z_0^4 = 4$, $z_0^5 = 2$, *and* $z_1^5 = 7$.

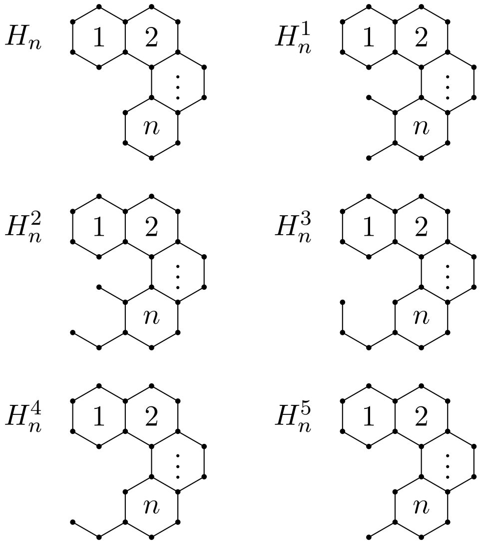

Figure 14: Auxiliary graphs for H_n.

Lemma 4.3. *Let* z_n *be the number of maximal matchings in* Z_n *and* z_n^i *be the number of maximal matchings in the auxiliary graph* Z_n^i *in Figure 13. Then*

(*i*) $h_n = h_{n-1} + h_{n-1}^1 + h_{n-2}^2 + h_{n-2}^3$,

(*ii*) $h_n^1 = 2h_{n-1}^4 + h_{n-1}^5 + h_{n-2}^3 + 2h_{n-2}^4 + h_{n-2}^5$, *(iii)* $h_n^2 = h_{n-1}^3 + 2h_{n-1}^4 + 2h_{n-2}^4 + 2h_{n-2}^3 + h_{n-2}^5$,

(iv) $h_n^3 = h_n^5 + h_n$,

(v) $h_n^4 = h_n + h_{n-1}^2$,

(vi) $h_n^5 = h_{n-1}^2 + h_{n-1}^4 + h_{n-1}^1$,

with the initial conditions $h_0 = 1$, $h_1 = 5$, $h_0^1 = 2$, $h_1^1 = 9$, $h_0^2 = 3$, $h_1^2 = 11$, $h_0^3 = 3$, $h_0^4 = 2$, *and* $h_0^5 = 2$.

Theorem 4.4. *Let* $L(x)$, $Z(x)$, *and* $H(x)$ *be the ordinary generating functions for the sequences* ℓ_n, z_n, *and* h_n, *respectively. Then*

(i)

$$L(x) = \frac{1 + x - x^3}{1 - 4x - x^4 - x^5},$$

(ii)

$$Z(x) = \frac{1 + 2x + 4x^2 + 4x^3 + 6x^4 + 4x^5 + x^6}{1 - 3x - x^2 - 6x^3 - 7x^4 - 7x^5 - 5x^6 - x^7},$$

(iii)

$$H(x) = \frac{1 + 4x + 8x^2 + 8x^3 + 7x^4 + 4x^5 + 2x^6}{1 - x - 7x^2 - 12x^3 - 6x^4 - 7x^5 - 4x^6 - 2x^7}.$$

Since $L(x)$, $Z(x)$, and $H(x)$ are rational functions, we can examine their denominators to obtain linear recurrences for the sequences ℓ_n, z_n, and h_n. The initial conditions can be verified by direct computations.

Corollary 4.5.

(i) $\ell_n = 4\ell_{n-1} + \ell_{n-4} + \ell_{n-5}$

with initial conditions $\ell_0 = 1$, $\ell_1 = 5$, $\ell_2 = 20$, $\ell_3 = 79$, *and* $\ell_4 = 317$,

(ii) $z_n = 3z_{n-1} + z_{n-2} + 6z_{n-3} + 7z_{n-4} + 7z_{n-5} + 5z_{n-6} + z_{n-7}$

with initial conditions $z_0 = 1$, $z_1 = 5$, $z_2 = 20$, $z_3 = 75$, $z_4 = 288$, $z_5 = 1105$, *and* $z_6 = 4234$,

(iii) $h_n = h_{n-1} + 7h_{n-2} + 12h_{n-3} + 6h_{n-4} + 7h_{n-5} + 4h_{n-6} + 2h_{n-7}$

with initial conditions $h_0 = 1$, $h_1 = 5$, $h_2 = 20$, $h_3 = 75$, $h_4 = 288$, $h_5 = 1094$, *and* $h_6 = 4171$.

Again we can use Darboux's Theorem to deduce the asymptotics of the sequences ℓ_n, z_n, and h_n. The smallest modulus singularity of $L(x)$ is approximately $x = 0.248804$. Hence, the asymptotic behavior of ℓ_n is given by $\ell_n \sim 4.01923^{n+1}$ for large n. Similarly, we deduce that $z_n \sim 3.83256^{n+1}$ and $h_n \sim 3.81063^{n+1}$ for large n.

4.2 Extremal structure

In this subsection, we prove the linear polyacene has most maximal matchings among all benzenoid chains of the same length.

Theorem 4.6. *Let* G_n *be a benzenoid chain of length* n. *Then*

$$\Psi(G_n) \leq \Psi(L_n).$$

Let G_m be an arbitrary benzenoid chain of length m. Observe that we can always draw G_m as in Figure 15, where h_m is a terminal hexagon and the hexagon adjacent to the left of h_{m-1} may attach at any of the edges f, g, or h. Let us assume the hexagons of G_m are labeled $h_1, \ldots, h_m$ according to their ordering in Figure 15 where (h_1 is the other terminal hexagon).

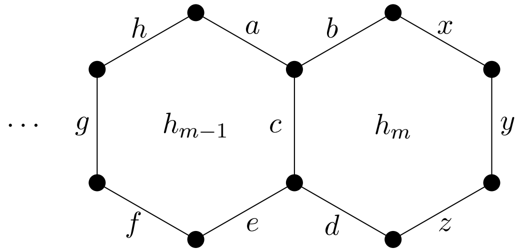

Figure 15: A terminal hexagon, h_m, and its adjacent hexagon, h_{m-1}, in the benzenoid chain G_m.

In what follows, let us adopt all of the same notation introduced in section 3.2. We also make use of Lemma 3.9 introduced previously, since this holds for arbitrary graphs.

Lemma 4.7. *Any maximal matching of* G_m *must contain at least one of the edges* a, b, c, d *or* e. *Moreover, any maximal matching of* G_m *contains exactly one of these edges, or contains exactly one of the following pairs of edges:* a *and* e, a *and* d, b *and* e, *or* b *and* d.

Proof. Take a maximal matching M. For sake of contradiction, suppose M contains none of the edges a, b, c, d or e. Then we could add the edge c to M, which is a contradiction to M being a maximal matching. Hence at least one of the edges a, b, c, d or e. The remaining part of the lemma follows by considering which pairs of edges can belong to the same matching. ☐

Proof. (of theorem 4.6). Take a benzenoid chain B of length $n-1$. Let us set $m = n-1$ and suppose that B is drawn as in Figure 15 with edges labeled as such, so that we may refer to this picture to aid this proof. We consider two cases of extending B by an nth hexagon h_n.

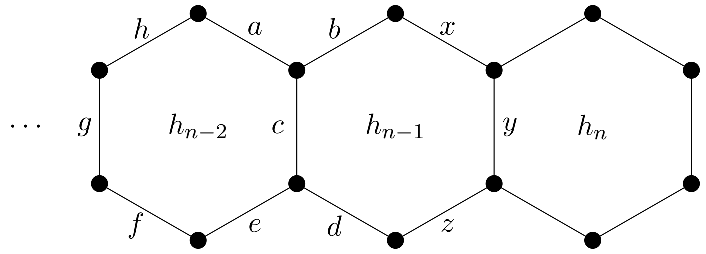

Figure 16: The benzenoid chain BL.

Case 1. The hexagon h_n attaches in the linear position to the edge y and let us denote the resulting graph by BL, see Figure 16. To compute $\Psi(BL)$ we make use of Lemma 4.7 and count matchings based on which of the edges a, b, c, d, e are saturated. Of the possibilities in Lemma 4.7, consider the maximal matchings of BL containing only the edge a. Such a matching must also contain the edges f and z, else this matching would contain one of the other edges d or e. The remaining edges of the matching must be a maximal matching of $H_{n-2} \setminus \{a, f\}$ and a maximal matching of $H_{n-1,n} \setminus z$. By directly counting, we find that $\Psi(H_{n-1,n} \setminus z) = 4$ and hence, the number of maximal matchings containing only the edge a is $4 \cdot \Psi(H_{n-2} \setminus \{a, f\})$. We count the remaining cases from Lemma 4.7 similarly. We note that a $H_{n-1} \setminus c$ is used to count maximal matchings containing the edges b or d, since these edges do not belong to the subgraph H_{n-2}. For example, the number of maximal matchings containing only the edge b is $3 \cdot \Psi(H_{n-2} \setminus \{c, f\})$. Thus

$$\begin{aligned}\Psi(BL) = {} & 4 \cdot \Psi(H_{n-2} \setminus \{a, f\}) + 3 \cdot \Psi(H_{n-2} \setminus \{c, f\}) + 14 \cdot \Psi(H_{n-2} \setminus c) \\ & + 4 \cdot \Psi(H_{n-2} \setminus \{e, h\}) + 3 \cdot \Psi(H_{n-2} \setminus \{c, h\}) + 9 \cdot \Psi(H_{n-2} \setminus \{a, e\}) \\ & + 7 \cdot \Psi(H_{n-2} \setminus \{a, c\}) + 7 \cdot \Psi(H_{n-2} \setminus \{c, e\}).\end{aligned}$$

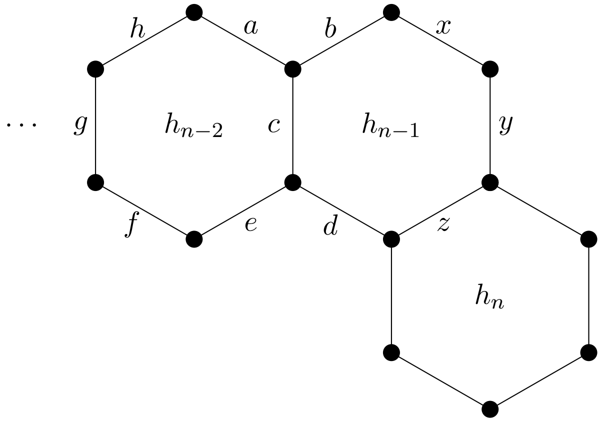

Figure 17: The benzenoid chain BK.

Case 2. The hexagon h_n attaches in the kinky position to the edge z and let us denote the resulting graph by BK, see Figure 17. Counting as in Case 1 above we obtain

$$\begin{aligned}\Psi(BK) = {} & 6 \cdot \Psi(H_{n-2} \setminus \{a, f\}) + 5 \cdot \Psi(H_{n-2} \setminus \{c, f\}) + 12 \cdot \Psi(H_{n-2} \setminus c) \\ & + 5 \cdot \Psi(H_{n-2} \setminus \{e, h\}) + 3 \cdot \Psi(H_{n-2} \setminus \{c, h\}) + 8 \cdot \Psi(H_{n-2} \setminus \{a, e\}) \\ & + 5 \cdot \Psi(H_{n-2} \setminus \{a, c\}) + 7 \cdot \Psi(H_{n-2} \setminus \{c, e\}).\end{aligned}$$

Now considering the terms in $\Psi(BL)$, by Lemma 3.9 we have

$$\begin{aligned}\Psi(H_{n-2} \setminus \{a, c\}) &\geq \Psi(H_{n-2} \setminus \{a, f\}), \\ \Psi(H_{n-2} \setminus \{c\}) &\geq \Psi(H_{n-2} \setminus \{c, f\}), and \\ \Psi(H_{n-2} \setminus \{a, e\}) &\geq \Psi(H_{n-2} \setminus \{e, h\}),\end{aligned}$$

implying that

$$\begin{aligned}\Psi(BL) \geq {} & 6 \cdot \Psi(H_{n-2} \setminus \{a, f\}) + 5 \cdot \Psi(H_{n-2} \setminus \{c, f\}) + 12 \cdot \Psi(H_{n-2} \setminus c) \\ & + 5 \cdot \Psi(H_{n-2} \setminus \{e, h\}) + 3 \cdot \Psi(H_{n-2} \setminus \{c, h\}) + 8 \cdot \Psi(H_{n-2} \setminus \{a, e\}) \\ & + 5 \cdot \Psi(H_{n-2} \setminus \{a, c\}) + 7 \cdot \Psi(H_{n-2} \setminus \{c, e\}) \\ & \geq \Psi(BK).\end{aligned}$$

The above proves that attaching a hexagon linearly gives more maximal matchings than attaching a hexagon in the kinky position. The inequality stated in the theorem follows. □

Again, we can see that the number of maximal matchings follows the same pattern as the number of independent sets, contrary to the number of all and of perfect matchings. While the last two increase with the number of kinky hexagons, the number of maximal matchings decreases. Further, unlike the number of perfect matchings which does not discriminate between left and right kinks, the number of maximal matchings seems to be sensitive to the direction of successive turns. It seems that the helicenes have the smallest number of maximal matchings among all benzenoid chains of the same length.

5 Further developments

In this last section we list some unresolved problems and indicate some possible directions of future research. We start by stating a conjecture about the extremal benzenoid chains.

Conjecture 5.1. *Let B_n be a benzenoid chain of length n. Then $\Psi(H_n) \leq \Psi(B_n)$.*

Now we turn to some structural properties. The cardinality of any smallest maximal matching in G is called the *saturation number* of G. The saturation number is of interest in the context of random sequential adsorption, since it gives the information on the worst possible case of clogging the substrate; see [7] for a discussion and [1, 6, 4] for some specific cases. However, it is not enough to know the size of the worst possible case; it is also imprtant to know how (un)likely is it to happen. This brings us back to enumerative problems, since the answer to this question depends on the ability to count maximal matchings of a given size. A neat way to handle information about maximal matchings of different sizes is to use the *maximal matching polynomial*. It was introduced in [7] and some of its basic properties were established there. There are, however, many open questions about this polynomial. For example, for ordinary (generating) matching polynomials [8, 16] we know that their coefficients are log-concave. Is this valid also for maximal matching polynomials? We have computed maximal matching polynomials explicitly for several families of graphs, and we have enumerated maximal matchings in several other families. So far, no counterexample has been found, but the proof still eludes us.

Another interesting thing to do would be to look at the dynamic aspect of the problem, emulating the approach of Flory [9].

Finally, it would be interesting to extend our results on other classes of graphs, such as rotagraphs, branching polymers, composite graphs and finite portions of various lattices.

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