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Matchings and Independent Sets in Polyphenylene Chains

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Abstract

We investigate enumerative properties of unbranched polyphenylene chains. In particular, we find exact formulas for the numbers of matchings and independent sets of given cardinalities in three types of uniform chains. Further, we show that two of those three types are extremal with respect to the number of considered structures among all chains of a given length. The paper also presents some results on polyphenylene dendrimers.

1 Introduction

A **phenylene** is any of divalent aromatic radicals obtained from a benzene molecule by removing two hydrogen atoms. Any of numerous polymers in which the basic building block is a phenylene is called a **polyphenylene**. Polyphenylenes make an important class of compounds that serve as precursors to many scientifically and commercially interesting materials, such as, e.g., polyphenylene oxide and polyphenylene sulfide. Unbranched polyphenylenes appear in the context of low-dimensional organic conductors [3], while their dendrimer-like counterparts play an important role in synthesizing large graphene molecules [4].

Polyphenylenes share many structural similarities with benzenoid compounds. As a consequence, both classes of compounds can be efficiently modeled by closely related classes of graphs. However, while the study of benzenoid compounds has been followed (and in many cases preceded) by the study of benzenoid graphs, the graphs representing polyphenylene

compounds remain largely unexplored. The main purpose of this paper is to investigate structural and enumerative aspects of some chemically relevant concepts such as, e.g., matchings and independent sets, in graphs that represent unbranched polyphenylene chains. Among other results, we present explicit formulas for the number of matchings (i.e., the Hosoya index) and for the number of independent sets (the Merrifield-Simmons index) of three types of uniform chains. We also find the chains extremal with respect to the considered indices. At the end, we briefly comment on branched polyphenylenes and on some possible further developments.

The present paper follows the approach developed recently in a paper concerned by chain hexagonal cacti [1]. For the reader's convenience, we tried to make this paper reasonably self-contained by presenting all necessary definitions and technical background and by providing details of crucial proofs. However, we will refer the reader to the mentioned reference for all details that do not offer any insight specific to the class of graphs we consider here.

2 Definitions, conjectures, and preliminary results

We start by defining the basic terms. For the general graph-theoretic terminology we refer the reader to any of standard monographs, such as, e. g., [7] or [10].

All graphs considered here are finite and simple. For a given graph G, the set of its vertices is denoted by $V(G)$ and the set of its edges by $E(G)$. For a vertex $u \in V(G)$ by $G - u$ we denote the graph induced by $V(G) - \{u\}$. For an edge $e \in E(G)$ we denote by $G - e$ the graph obtained from G by deleting the edge e, while $G\backslash e$ denotes the graph obtained by deleting e and both its end-vertices. The closed neighborhood of a vertex v is denoted by $N[v]$.

A **cactus graph** is a connected graph in which no edge is contained in more than one cycle. Hence, each block of a cactus graph is either a cycle or an edge. A cactus graph in which all blocks are cycles of the same size m is called m-uniform cactus graph. A **hexagonal cactus** is a 6-uniform cactus. An example is shown in Fig. 1.

A **polyphenylene** is a graph obtained from a hexagonal cactus by expanding each of its cut-vertices to an edge. The polyphenylene corresponding to the hexagonal cactus from Fig. 1 is shown in Fig. 2.

A polyphenylene in which no hexagon has more than two cut-vertices is called a **polyphe-**

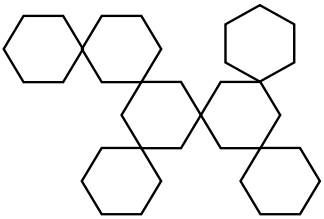

Figure 1: A hexagonal cactus.

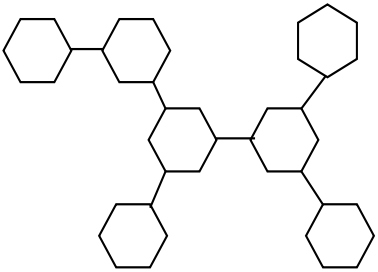

Figure 2: A polyphenylene.

nylene chain. Obviously, each polyphenylene chain contains exactly two hexagons with only one cut-vertex. Those hexagons are called **terminal**; all other hexagons are **internal**. The number of hexagons in a given polyphenylene chain is called its **length**. A polyphenylene chain of length 6 is shown in Fig. 3.

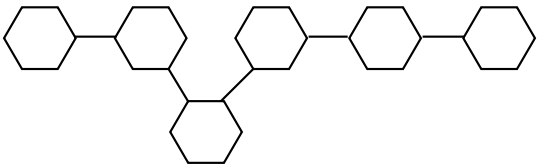

Figure 3: A polyphenylene chain of length 6.

An internal hexagon is called **ortho-hexagon**, **meta-hexagon**, or **para-hexagon** if its cut-vertices are at distance 1, 2, or 3, respectively. The terminology is inherited from chemistry, where it is used to describe the relative position of two atoms in the benzene molecule. (See Fig. 4.) If all internal hexagons in a polyphenylene chain are of the same type, say ortho, the chain is an **ortho-chain**. The meta- and para-chains are defined analogously. We denote an ortho-, a meta-, and a para-chain of length n by O_n, M_n, and L_n, respectively. (We reserve P_n for the path on n vertices.) The three types of uniform

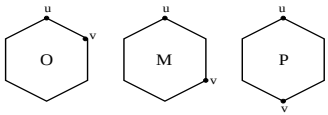

Figure 4: Ortho-, meta-, and para-positions of atoms in benzene.

chains are shown in Fig. 5. The cut-vertex u of the rightmost hexagon and the cut-edge

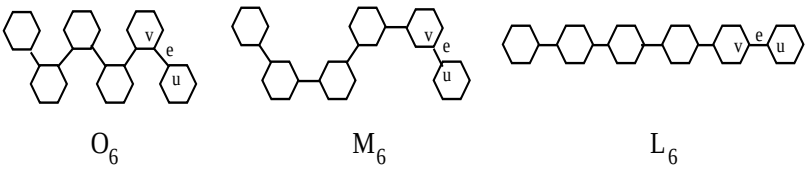

Figure 5: Polyphenylene chains of length 6.

$e = \{u, v\}$ incident to it will play special roles in our computations. We call them the **critical vertex** and the **critical edge**, respectively. Three auxiliary graphs that appear as components of $G \backslash e$ and $G - N[u]$ are shown in Fig. 6. For a polyphenylene chain G_n,

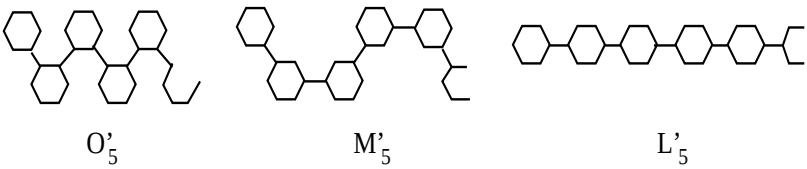

Figure 6: The three types of auxiliary graphs.

its auxiliary graph is denoted by G'_n, where G stands for O, M, or L.

Clearly, polyphenylene chains of a given length are in a bijective correspondence with cactus chains of the same length. That fact enables us to enumerate all polyphenylene chains of a given length. We refer the reader to [1] for the proof of the following result.

Theorem 1

There are $\frac{1}{2}\left(3^{n-2} + 3^{\lfloor \frac{n-1}{2} \rfloor}\right)$ different polyphenylene chains of length n. ■

In the rest of this section we define the basic concepts related to matchings and independent sets.

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**. The cardinality of any maximum

matching in G is called the **matching number** of G and denoted by $\nu(G)$. If a matching in G is not a subset of a larger matching of G, it is called a **maximal matching**. The size of any smallest maximal matching in G is called the **saturation number** of G and denoted by $s(G)$. Obviously, any maximum matching is also maximal, while the opposite claim is generally not valid. A vertex u incident with an edge from a matching M is said to be **covered** by M. The number of vertices of G not covered by a matching M is the **defect** of M. We denote the number of matchings of defect d in G by $N_d(G)$. The matchings with defect zero are called **perfect**.

Let us denote by $\Phi_k(G)$ the number of matchings of size k in G. Obviously, $\Phi_0(G) = 1$, $\Phi_1(G) = |E(G)|$, and $\Phi_k(G) = 0$ for $k > \nu(G)$. A compact way to treat all numbers $\Phi_k(G)$ as a single entity is to combine them into a matching polynomial.

The **matching polynomial** of G is defined as

$$m(G;x) = \sum_{k=0}^{\nu(G)} \Phi_k(G) x^k,$$

where x is a formal variable. For the sake of brevity, we will often write $m(G)$ instead of $m(G;x)$ when there is no possibility of confusion.

By evaluating $m(G;x)$ at $x = 1$ we obtain the total number of matchings in G. We denote this quantity by $\Phi(G)$. In chemical literature $\Phi(G)$ is often denoted by $Z(G)$ and called Hosoya Z-index of G.

There are two common forms of matching polynomials. The one considered here is sometimes called the **matching generating polynomial**, as opposed to the matching defect polynomial, also known as the acyclic polynomial [5]. We refer the reader to Chapter 8.5 in [9] and to [2] for more information on the general theory of matching polynomials.

The following two results belong to the mathematical folklore.

Theorem M1 Let G be a graph and e an edge of G. Then

$$m(G;x) = m(G-e;x) + x \cdot m(G\backslash e;x)\ . \qquad \blacksquare$$

Theorem M2 Let G be a graph with components $G_1, \ldots, G_k$. Then

$$m(G;x) = m(G_1;x) \cdot \ldots \cdot m(G_k;x)\ . \qquad \blacksquare$$

Starting from the two quoted theorems and the fact $m(K_1;x) = 1$, one can compute the matching polynomial of any graph by recursively reducing it to trivial components.

The matching polynomials of paths and cycles on n vertices are given by following formulas:

$$m(P_n;x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n-k}{k} x^k ,$$

$$m(C_n;x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n}{n-k} \binom{n-k}{k} x^k .$$

From them it follows that the total numbers of matchings in P_n and C_n are given by the Fibonacci and Lucas numbers F_{n+1} and L_n, respectively. We will find the above formulas useful since both paths and cycles will appear as fragments of polyphenylene chains under the decomposition procedure.

A set $S \subseteq V(G)$ of vertices of G is an **independent set** in G if no two vertices of S are adjacent. An independent set of the largest possible size is called a **maximum independent set**. The cardinality of any maximum independent set in G is called the **independence number** (or the **stability number**) of G and denoted by $\alpha(G)$. An independent set in G that cannot be extended to a larger independent set is called **maximal**.

The **independence polynomial** of a graph G is defined by

$$i(G;x) = \sum_{k=0}^{\alpha(G)} \Psi_k(G) x^k,$$

where x is a formal variable, and $\Psi_k(G)$ denotes the number of independent sets in G with k vertices. Obviously, $\Psi_0(G) = 1$ and $\Psi_1(G) = |V(G)|$. Again, setting $x = 1$ in $i(G;x)$ yields the total number of independent sets in G; we denote it by $\Psi(G)$. In chemical literature $\Psi(G)$ is known as the Merrifield-Simmons index. When there is no possibility of confusion, we will omit x and write simply $i(G)$. The independence polynomial was introduced by Gutman and Harary in 1983 [6]. For a recent survey on independence (and other) polynomials we refer the reader to [8].

The following properties of independence polynomials are analogous to the properties of matching polynomials from Theorems M1 and M2, and play a similar role in the computations.

Theorem I1 Let G be a graph and u a vertex in G. Then

$$i(G;x) = i(G-u;x) + x \cdot i(G-N[u];x) . \qquad \blacksquare$$

Theorem I2 Let G be a graph consisting of the components G_1, G_2, ..., G_k. Then

$$i(G;x) = i(G_1;x)i(G_2;x)\cdot\ldots\cdot i(G_k;x)\ . \qquad \blacksquare$$

It is a simple exercise to verify that the independence polynomials of paths and cycles are given by the following formulas:

$$i(P_n;x) = \sum_{k=0}^{\lfloor\frac{n+1}{2}\rfloor} \binom{n+1-k}{k} x^k;$$

$$i(C_n;x) = \sum_{k=0}^{\lfloor n/2\rfloor} \frac{n}{n-k}\binom{n-k}{k} x^k.$$

From them one can see that the number of independent sets in cycles is equal to the number of matchings, while in paths it exceeds the number of matchings by F_n.

3 Main results

3.1 Matchings in polyphenylene chains

Here we investigate structural and enumerative aspects of matchings in polyphenylene chains. The structural aspects do not present any challenge; it is easy to see that all polyphenylene chains have a perfect matching. Furthermore, it is easy to see using the parity arguments that no cut-edge can participate in a perfect matching of a polyphenylene chain. Hence we have the following observation.

Proposition 2

Let G_n be a polyphenylene chain of length n. Then $\nu(G_n) = 3n$. Furthermore, G_n contains exactly 2^n different perfect matchings. $\blacksquare$

Proposition 3

Let G_n be a polyphenylene chain of length n and $s(G_n)$ its saturation number. Then $s(G_n) = 2n$.

Proof

It is easy to exhibit a maximal matching that leaves uncovered exactly two vertices in each hexagon of G_n. Hence $s(G_n) \geq 2n$. Let us assume that there is a maximal matching M of smaller cardinality. Then there are at least $2n+2$ vertices uncovered by M. By the pigeonhole principle, at least one hexagon must contain at least three of those vertices. From the maximality of M it follows that those three vertices must form an independent

set, and this further implies that the remaining three vertices in the hexagon must be covered by an edge of M not lying in the hexagon. Hence all three of them must be cut-vertices, and this is a contradiction with the definition of polyphenylene chains. ■

From the parity arguments it follows that G_n has a defect-d matching for all even d between 0 and $6n = V(G_n)$.

Now we turn our attention to the enumerative problems. For short lengths, $n = 1$ and 2, there is no difference between ortho-, meta-, and para-chains. Their matching polynomials are easily obtained by direct application of Theorems M1 and M2.

$$m(G_1; x) = m(C_6; x) = 1 + 6x + 9x^2 + 2x^3;$$

$$m(G_2; x) = 1 + 13x + 62x^2 + 134x^3 + 129x^4 + 45x^5 + 4x^6.$$

We are now ready for computing the matching polynomials of ortho-, meta- and para-phenylene chains. In all three cases we proceed by deriving a recurrence relation by decomposing all matchings into those that do and those that do not contain the critical edge. We work out the ortho- case in some detail; the remaining two cases follow along the same lines.

Lemma 4

$$m(O_n) = m(C_6)m(O_{n-1}) + x \cdot m(P_5)m(O'_{n-2});$$

$$m(O'_n) = m(P_5)m(O_n) + x \cdot m(P_4)m(O'_{n-1}).$$

■

Theorem 5

The matching polynomials of O_n, $n \geq 2$, are given by

$$m(O_n) = (1 + 7x + 12x^2 + 3x^3)m(O_{n-1}) - x^2(1 + 6x + 11x^2 + 6x^3 + 2x^4)m(O_{n-2}).$$

Proof

The result follows by plugging in the second expression of Lemma 4 into the first, taking into account the explicit expressions for matching polynomials of paths and cycles and simplifying the resulting expressions. ■

By putting $x = 1$ into the recurrence for $m(O_n)$ we can obtain the explicit formula for the number of all matchings in O_n. The recurrence for $\Phi(O_n)$ has the form

$$\Phi(O_n) = 23\Phi(O_{n-1}) + 26\Phi(O_{n-2}),$$

with the initial conditions $\Phi(O_1) = 18$, $\Phi(O_2) = 388$. The generating function for $\Phi(O_n)$ is given by $g_o(x) = \frac{1-5x}{1-23x+26x^2}$, and the explicit formula is then readily obtained by solving the characteristic equation $1-23x+26x^2 = 0$ and taking into account the initial conditions.

Theorem 6

$$\Phi(O_n) = \left(\frac{13+5\sqrt{17}}{10\sqrt{17}}\right)\left(\frac{23+5\sqrt{17}}{2}\right)^n + \left(\frac{-13+5\sqrt{17}}{10\sqrt{17}}\right)\left(\frac{23-5\sqrt{17}}{2}\right)^n .$$

■

The leading term of the above expression behaves asymptotically as 21.8078^n.

Now we present, omitting the details, the results for meta- and para- phenylene chains.

Lemma 7

$$m(M_n) = m(C_6)m(M_{n-1}) + x \cdot m(P_5)m(M'_{n-2})$$

$$m(M'_n) = m(P_5)m(M_n) + x \cdot m(P_3)m(M'_{n-1}).$$

■

Theorem 8

The matching polynomials of M_n, $n \geq 2$, are given by

$$m(M_n) = (1 + 7x + 11x^2 + 2x^3)m(M_{n-1}) + x^3(1 + 4x + 5x^2)m(M_{n-2}).$$

■

Theorem 9

$$\Phi(M_n) = \left(\frac{15+\sqrt{481}}{2\sqrt{481}}\right)\left(\frac{21+\sqrt{481}}{2}\right)^n + \left(\frac{-15+\sqrt{481}}{2\sqrt{481}}\right)\left(\frac{21-\sqrt{481}}{2}\right)^n .$$

■

We can conclude from the above expression that $\Phi(M_n) \sim 21.4659^n$ for large values of n.

Lemma 10

$$m(L_n) = m(C_6)m(L_{n-1}) + x \cdot m(P_5)m(L'_{n-2})$$

$$m(L'_n) = m(P_5)m(L_n) + x \cdot m(P_2)^2 m(L'_{n-1}).$$

■

Theorem 11

The matching polynomials of L_n, $n \geq 2$, are given by

$$m(L_n) = (1 + 7x + 11x^2 + 3x^3)m(L_{n-1}) - 2x^4(1 + x)^2 m(L_{n-2}) \ .$$ ■

Theorem 12

$$\Phi(L_n) = \left(\frac{7+\sqrt{113}}{2\sqrt{113}}\right)(11+\sqrt{113})^n + \left(\frac{-7+\sqrt{113}}{2\sqrt{113}}\right)(11-\sqrt{113})^n.$$

■

Asymptotic behavior of the above expression is given by 21.6301^n.

We observe that the number of matchings in a para-polyphenylene chain of a given length falls between the numbers of matchings in ortho- and meta- chains of the same length. We proceed by showing that the ortho- and meta- chains are indeed extremal with respect to the number of matchings among all chains.

Theorem 13

Let G_n be a polyphenylene chain of length n. Then

$$\Phi(M_n) \leq \Phi(G_n) \leq \Phi(O_n).$$

Proof

Let S_1 and S_2 be two polyphenylene chains whose lengths add to $n-1$. There are three ways to insert a hexagon between them and forming a chain of length n. The inserted hexagon becomes an ortho-, a meta-, or a para-hexagon of the resulting chains. The three possibilities are shown in Fig. 7. Let us denote the cut-vertices of the inserted hexagon by

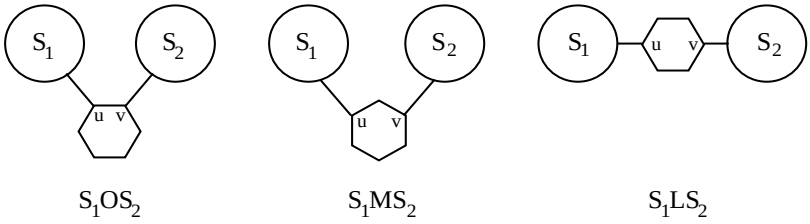

Figure 7: Three ways of inserting a hexagon.

u and v. By $\Phi_u(G)$ we denote the number of matchings that cover vertex u, and similarly for vertex v. By considering and counting the matchings that cover vertices u and v we arrive at six auxiliary graphs shown in Fig. 8. By applying the decomposition procedure we obtain following expressions.

$$\begin{aligned}\Phi(S_1OS_2) &= \Phi_u(S_1 \sim u)\Phi(S_2') + \Phi(S_1)\Phi(C_6 \sim S_2) \\ &= \Phi_u(S_1 \sim u)[\Phi(P_4)\Phi(S_2 \sim v) + \Phi(P_5)\Phi(S_2)] + \Phi(S_1)\Phi(C_6 \sim S_2);\end{aligned}$$

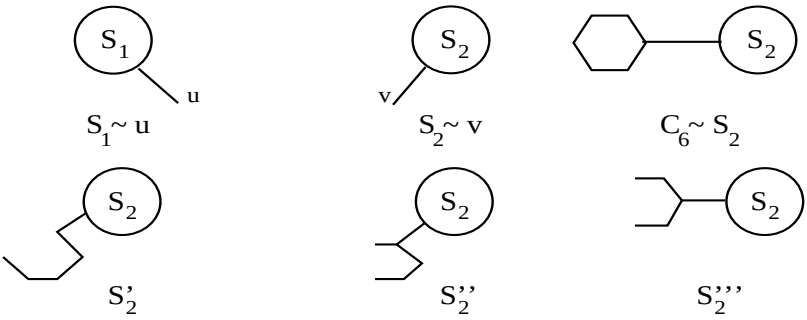

Figure 8: The six auxiliary graphs.

$$\begin{aligned}\Phi(S_1MS_2) &= \Phi_u(S_1 \sim u)\Phi(S_2'') + \Phi(S_1)\Phi(C_6 \sim S_2)\\ &= \Phi_u(S_1 \sim u)[\Phi(P_1)\Phi(P_3)\Phi_v(S_2 \sim v) + \Phi(P_5)\Phi(S_2)] + \Phi(S_1)\Phi(C_6 \sim S_2);\end{aligned}$$

$$\begin{aligned}\Phi(S_1PS_2) &= \Phi_u(S_1 \sim u)\Phi(S_2''') + \Phi(S_1)\Phi(C_6 \sim S_2)\\ &= \Phi_u(S_1 \sim u)[\Phi(P_2)^2\Phi_v(S_2 \sim v) + \Phi(P_5)\Phi(S_2)] + \Phi(S_1)\Phi(C_6 \sim S_2);\end{aligned}$$

Now we pairwise subtract the above expressions.

$$\Phi(S_1OS_2) - \Phi(S_1PS_2) = \Phi_u(S_1 \sim u)\Phi_v(S_2 \sim v)[\Phi(P_4) - \Phi(P_2)^2] > 0;$$

$$\Phi(S_1PS_2) - \Phi(S_1MS_2) = \Phi_u(S_1 \sim u)\Phi_v(S_2 \sim v)[\Phi(P_2)^2 - \Phi(P_3)] > 0.$$

Hence, a polyphenylene chain with maximum number of matchings cannot contain meta- and para-hexagons. The same argument implies that a polyphenylene chain with minimum number of matchings cannot contain ortho- and para-hexagons. ■

We conclude this section by computing the expected size of a matching in each of the considered chains. We start by computing the bivariate generating functions from the recurrences for matching polynomials. The bivariate generating functions are denoted as follows.

$$O(x,y) = \sum_{n\geq 0}\sum_{k\geq 0}\Phi_k(O_n)x^n y^k;$$

$$M(x,y) = \sum_{n\geq 0}\sum_{k\geq 0}\Phi_k(M_n)x^n y^k;$$

$$L(x,y) = \sum_{n\geq 0}\sum_{k\geq 0}\Phi_k(L_n)x^n y^k.$$

It is obvious from the definition that the coefficients of x^n are exactly our computed generating polynomials (just taken in variable y). We introduce compact notation for the polynomials appearing in the recurrences for matching polynomials:

$$\begin{aligned} o_1(y) &= 1 + 7y + 12y^2 + 3y^3; \\ o_2(y) &= -y^2(1 + 6y + 11y^2 + 6y^3 + 2y^4); \\ m_1(y) &= 1 + 7y + 11y^2 + 2^3; \\ m_2(y) &= y^3(1 + 4y + 5y^2); \\ l_1(y) &= 1 + 7y + 11y^2 + 3y^3; \\ l_2(y) &= -2y^4(1 + y)^2. \end{aligned}$$

The matching polynomials of three shortest chains we denote by

$$\begin{aligned} m_0(x, y) &= 1; \\ m_1(x, y) &= x(1 + 6y + 11y^2 + 6y^3 + 2y^4); \\ m_2(x, y) &= x^2(1 + 13y + 62y^2 + 134y^3 + 129y^4 + 45y^5 + 4y^6). \end{aligned}$$

Now the recurrence for matching polynomials can be written as

$$m(G_n) = g_1(y)m(G_{n-1}) + g_2(y)m(G_{n-2}),$$

where G stands for O, M, and L, and g stands for o, m, and l, respectively. The bivariate generating functions are now obtained in the usual way, by multiplying the recurrences through by x^n and summing over all $n \geq 2$. The result is a linear equation in the unknown generating function $G(x, y)$

$$G(x, y) - m_0(x, y) - m_1(x, y) = xg_1(y)[G(x, y) - m_0(x, y)] + x^2 g_2(y)G(x, y).$$

The equation is readily solved, yielding the explicit formula for the bivariate generating function.

$$G(x, y) = \frac{m_0(x, y)[1 - xg_1(y)] + m_1(x, y)}{1 - xg_1(y) - x^2 g_2(y)}.$$

By substituting the pairs (O, o), (M, m), and (L, l) for (G, g) in the obtained formula, we get the explicit formulas for desired bivariate generating functions.

Theorem 14

$$O(x,y) = \frac{1 - xy - 3x^2y + x^3y}{1 - xo_1(y) - x^2o_2(y)};$$
$$M(x,y) = \frac{-1 + xy + 2xy^2}{1 - xm_1(y) - x^2m_2(y)};$$
$$L(x,y) = \frac{-1 + xy + 2xy^2 + xy^3}{1 - xl_1(y) - x^2l_2(y)}.$$

■

By setting $y = 1$ in the above expressions we recover the univariate generating functions for the number of matchings in the three types of polyphenylene chains.

Corollary 15

$$O(x) = \frac{1 - 5x}{1 - 23x + 26x^2};$$
$$M(x) = \frac{1 - 3x}{1 - 21x - 10x^2};$$
$$L(x) = \frac{1 - 4x}{1 - 22x + 8x^2}.$$

■

Now the expected number of edges in a random matching is obtained in the standard way, by using the fact that $\frac{\partial G}{\partial y}(x,y)\Big|_{y=1}$ is the generating function for the total number of edges in all matchings and by dividing the total number of edges by the total number of matchings. (See [11] for more on bivariate generating functions.) We present only the leading term, leaving out the computational details.

Theorem 16

Let $\overline{k}(G_n)$ be the expected number of edges in a random matching in G_n. Then

$$\overline{k}(O_n) \sim 1.7045n;$$
$$\overline{k}(M_n) \sim 1.6893n;$$
$$\overline{k}(L_n) \sim 1.7004n.$$

■

3.2 Independent sets in polyphenylene chains

Now we present the results on structural and enumerative properties of independent sets in polyphenylenes. Again, the structural properties are not difficult to obtain, due to the very special structure of our chains.

Proposition 17

The stability number of any polyphenylene chain is given by $\alpha(G_n) = 3n$. The smallest maximal independent set in G_n has the cardinality of $2n$. ■

The results concerning the enumerative properties are derived much in the same way as for the case of matchings. Hence we restrict ourselves to presenting them in a very concise form, omitting all computational details. We start with the recurrences for the independence polynomials.

Theorem 18

$$i(O_n) = (1 + 6x + 9x^2 + 2x^3)i(O_{n-1}) - x^2(1 + 3x + x^2)^2 i(O_{n-2});$$

$$i(M_n) = (1 + 6x + 8x^2 + x^3)i(M_{n-1}) + x^3(1 + 4x + 5x^2 + x^3)i(M_{n-2});$$

$$i(L_n) = (1 + 6x + 8x^2 + 2x^3)i(L_{n-1}) - x^4(2 + 4x + x^2)i(L_{n-2}).$$

■

Theorem 19

$$\Psi(O_n) = \frac{9 + 2\sqrt{14}}{4\sqrt{14}}(9 + 2\sqrt{14})^n - \frac{9 - 2\sqrt{14}}{4\sqrt{14}}(9 - 2\sqrt{14})^n;$$

$$\Psi(M_n) = \frac{2 + \sqrt{3}}{2\sqrt{3}}(8 + 5\sqrt{3})^n + \frac{-2 + \sqrt{3}}{2\sqrt{3}}(8 - 5\sqrt{3})^n;$$

$$\Psi(L_n) = \frac{19 + 3\sqrt{29}}{6\sqrt{29}}\left(\frac{17 + 3\sqrt{29}}{2}\right)^n + \frac{-19 + 3\sqrt{29}}{6\sqrt{29}}\left(\frac{17 - 3\sqrt{29}}{2}\right)^n.$$

■

The leading terms for $\Psi(O_n)$, $\Psi(M_n)$ and $\Psi(L_n)$ are 16.4833^n, 16.6603^n, and 16.5777^n, respectively. We observe that M_n is richer than L_n, and that one is in turn richer than O_n with respect to the total number of independent sets. By using the same approach as in the case of matchings it can be shown that the ortho- and the meta-chain are extremal among all chains of a given length.

Theorem 20

Let G_n be a polyphenylene chain on n hexagons. Then

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

■

We notice that the richest chains with respect to independent sets are the poorest ones with respect to matchings, and vice versa. This is consistent with the behavior of other types of chains, such as hexagonal cacti or benzenoid chains.

The meta-chain is also the richest one in terms of maximum independent sets; while O_n and L_n contain $n+1$ independent set of cardinality $3n$, the meta-chain contains F_{n+2} maximum independent sets. The result can be verified by simple combinatorial reasoning and we omit the details.

We close this section by reporting the asymptotic behavior of the expected size of a random independent set in the three types of chains. We denote that quantity by $\overline{i}(G_n)$, where G stands for O, M, and L. The computations involved are completely analogous to the ones for matchings.

Theorem 21

$$\overline{i}(O_n) \sim 1.5991n;$$

$$\overline{i}(M_n) \sim 1.6166n;$$

$$\overline{i}(L_n) \sim 1.6062n.$$

■

We observe that M_n keeps its primacy also with respect to the size of a random independent set.

4 Further developments

In this section we report some preliminary results on polyphenylene dendrimers. An example is shown in Fig. 9. In order to keep the presentation reasonably short we will

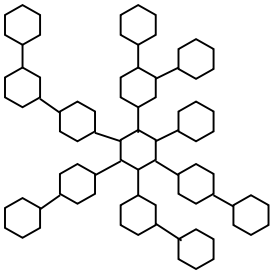

Figure 9: A polyphenylene dendrimer.

consider only the case in which six polyphenylene chains of the same type and the same length are attached to a central hexagon. We denote the generic chain by G_n and the graph with all six chains attached by $S_{n,6} = S_6$. The auxiliary graphs that have k chains

of length n attached to k consecutive vertices of a hexagon we denote by S_k for $0 \leq k \leq 5$. (We suppress n for sake of notational brevity.) Another type of auxiliary graphs formed by attaching k chains of length n to k consecutive vertices of P_5 we denote by S'_k for $0 \leq k \leq 5$. (The k vertices on P_5 where the chains are attached include a terminal vertex.) Finally, G'_n denotes an auxiliary graph of the type shown in Fig. 6, where G can be O, M, or L. Examples are shown in Fig 10.

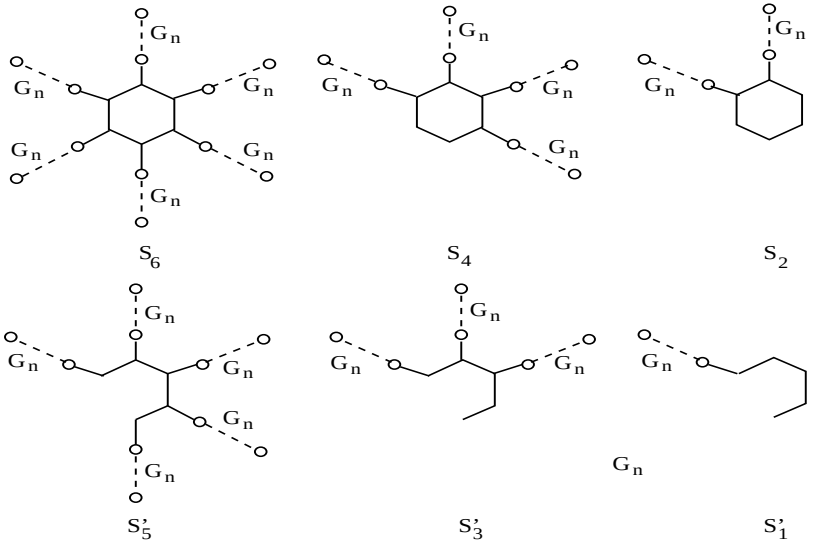

Figure 10: Auxiliary graphs for star-like polyphenylene dendrimer.

Label the edges between the copies of G_n and the central hexagon by $e_1, \ldots, e_6$. By applying iteratively Theorems M1 and M2 to S_6, we obtain the following expression for $m(S_6)$.

$$\begin{aligned} m(S_6) &= m(S_6 - e_1) + x \cdot m(S_6 \backslash e_1) = m(G_n)m(S_5) + x \cdot m(G'_{n-1})m(S'_5) \\ &= m(G_n)[m(S_5 - e_2) + x \cdot m(S_5 \backslash e_2)] + x \cdot m(G'_{n-1})m(S'_5) \\ &= m(G_n)^2 m(S_4) + x \cdot m(G'_{n-1})m(G_n)m(S'_4) + x \cdot m(G'_{n-1})m(S'_5) \\ &\vdots \\ &= m(G_n)^6 m(C_6) + x \cdot m(G'_{n-1})[m(S'_5) + m(G_n)m(S'_4) + \ldots + m(G_n)^5 m(S'_0)]. \end{aligned}$$

Now we take a closer look at the edges of the central hexagon. Applying the decomposing

procedure to them will result in graphs consisting of paths of length m for $1 \leq m \leq 5$ with a chain of length n attached to each vertex. We denote such graphs by H_m. The graph obtained by attaching a chain of length n to each internal vertex and only one of the terminal vertices is denoted by H'_m. Now the generating function for matching polynomials of H_m is obtained by starting from the coupled recurrences

$$m(H_m) = m(H'_{m-1})m(G_n) + x \cdot m(H_{m-1})m(G'_{n-1})$$
$$m(H'_{m-1}) = m(H_{m-1}) + x \cdot m(H_{m-2})m(G_n).$$

That results in a recurrence for $m(H_m)$ of the form

$$m(H_m) = m(H_1)m(H_{m-1}) + [m(H_2) - m(H_1)^2]m(H_{m-2}),$$

with the initial conditions

$$m(H_1) = m(G_n) + x \cdot m(G'_{n-1})$$
$$m(H_2) = m(H_1)^2 + x \cdot m(G_n)^2.$$

Now the generating function $H(z) = \sum_{m\geq 1} m(H_m)z^m$ is readily obtained as

$$H(z) = \frac{1}{1 - [m(G_n) + x \cdot m(G'_{n-1})]z - x \cdot m(G_n)^2 z^2} - 1.$$

It remains to find the matching polynomials of G'_n. From previous Lemmas we know that

$$m(G'_n) = m(P_5)m(G_n) + x \cdot \alpha_G \cdot m(G'_{n-1}),$$

where $\alpha_O = m(P_4)$, $\alpha_M = m(P_3)$, and $\alpha_L = m(P_2)^2$. Now the generating function $K(x, y) = \sum_{n\geq 0} m(G'_n; x)y^n$ is given by

$$K(x, y) = \frac{m(P_5)(1 + G(x, y))}{1 - x \cdot \alpha_G \cdot y}.$$

Now we have all necessary elements for writing down the explicit formula for the matching polynomial of the star-like dendrimer.

Theorem 22

$$\begin{aligned} m(S_n) = {} & (1 + 6x + 9x^2 + 2x^3)m(G_n)^6 + 6x(1 + 4x + 3x^2)m(G_n)^5 m(G'_{n-1}) \\ & + 3x^2(5 + 12x + 3x^2)m(G_n)^4 m(G_{n-1})^2 + 4x^3(5 + 6x)m(G_n)^3 m(G'_{n-1})^3 \\ & + 3x^4(5 + 2x)m(G_n)^2 m(G'_{n-1})^4 + 6x^5 m(G_n)m(G'_{n-1})^5 + x^6 m(G'_{n-1})^6 \ . \end{aligned}$$

■

We have compared the number of matchings in three types of stars and found out that the relative order of the three types of chains is preserved: there are about $2.40668 \cdot 10^{33}$, $1.78317 \cdot 10^{33}$, and $2.0624 \cdot 10^{33}$ matchings, respectively, in stars with 6 ortho-, meta-, and para-chains of length 4. We have also compared the number of matchings in the three types of stars with the number of matchings in the corresponding chains on the same number of hexagons and found that the stars are richer in the number of matchings.
The methods developed here can be also used to compute the matchings and independent sets related invariants for dendrimers with lower symmetries.

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