

Matching Polynomials of Regular Chain-Type Graphs

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Abstract

In this article we describe an algorithm that allows us to recursively construct the matching polynomials of what we call “regular chain-type graphs”. These graphs are obtained from a fixed base graph by linking several copies in a linear fashion, the links being obtained by joining two consecutive copies at prescribed vertices. Loops obtained by closing these chains are also studied. Finally, a method to compute the growth rate of the Hosoya index is presented. The proposed methods are applicable to chain-type molecular structures, providing insights into their chemical properties.

1 Introduction

In graph theory, a matching is formally defined as a subset of edges in which no two edges are incident to a common vertex. Among the various algebraic tools developed to study the structure of graphs, the matching

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polynomial stands out as a significant invariant due to its capacity to capture complex combinatorial structures [13, 14, 16]. This polynomial serves not only as a generating function for enumerating matchings of different sizes but also reflects deeper structural properties of the graph, such as independence and connectivity patterns among edge subsets [11]. The matching polynomial holds a fundamental role in both theoretical graph theory and its diverse applications [2–4, 6, 9, 12]. As an example in chemical graph theory, the matching polynomial is employed to evaluate molecular stability through resonance structures, linking combinatorial properties to chemical phenomena [1, 17]. Furthermore, a significant algebraic property of the matching polynomial is that all its roots are real for any graph, a fact that facilitates spectral analysis and contributes to stability assessments in complex network models [13, 21].

The Hosoya index is the total number of matchings in the graph (of any size). It was introduced by H. Hosoya to describe the branching structures and connectivity arrangements of chemical compounds [18].

Determining the Hosoya index in arbitrary graphs is a #P-complete problem, a complexity class that encompasses counting problems which are computationally at least as hard as NP-complete decision problems and are widely regarded as intractable [25]. Due to the intrinsic computational complexity, the matching polynomial serves as an essential indirect approach for the analysis and approximation of these quantities, thereby enabling the examination of enumerations that are otherwise computationally infeasible [21].

In this paper we study regular chain-type graphs, where an arbitrary starting graph forms a chain by adding a new copy of the graph (in a regular pattern) at each step. Two kinds of attachment patterns are considered; in the first two graphs attach each other at a vertex, and in the other two vertices are joined by an edge. Such graphs are common in both nature and mathematics because of their simple and fundamental structure. Representing linear structures, these graphs find applications across many theoretical and practical fields. For example, in chemical graph theory, chain-type graphs are frequently used to model linear alkanes and polymers. By serving as a baseline, they enable the study of branching

effects through comparison with more complex, branched molecular structures. This simplicity makes them invaluable for exploring how molecular connectivity influences chemical properties [24]. In this paper we use the self-similar structure of regular chain-type graphs to develop recursive methods for computing their matching numbers.

There have been several recent advances in the techniques that allow the computation of the Hosoya indices (or matching numbers) of complicated graphs from those of the simpler ones. In [23] a very general theoretical framework for graphs with self-similar structure is discussed, but one generally needs a tailored approach to get concrete results for specific classes of graphs. For example, from a chemical point of view, graphs formed by attaching regular n -gons along edges are of special interest. In [10, 19, 20] the authors have studied the computation of Hosoya indices in various benzenoid chains, corresponding to hexagonal blocks, whereas in [7] matching numbers are computed for (octagonal) cyclooctatetraene chains. These works make use of tools such as transfer-matrices, Hosoya vectors and k -matching vectors. Very recently [15] has proposed a general transfer matrix method to compute matching numbers for graphs formed by amalgamating a sequence of graphs at one or two vertices at a time. This setting includes the regular chain-type graphs considered in this paper; but we have a more focused approach which produces extra information not given in [15].

In particular, we do not use matrix methods and work with what we call “partial matching polynomials”, employing another commonly-used idea in the literature. These are polynomials taking into account matchings conditioned on certain vertices being matched or not. They can be said to be analogous to the k -matching vectors which encode matching information of sub-graphs excluding certain vertices. For our particular setting, this preference leads to a certain simplification that allows us to easily compute the growth rate of the Hosoya index as a function of the chain length. We remark that in [5] and [8] a similar style was employed to study Sierpinski-type self-similar graphs. Finally, in Section 2.2 we explain how our methods can be adapted to study regular chains which close into loop-shaped graphs.

2 The method

We first begin by introducing our terminology. A (*undirected*) *graph* is simply a pair $G = (V, E)$ where V is a nonempty set whose elements are called *vertices* and E is a set of unordered vertex pairs $\{u, v\}$, called *edges* (the vertices u and v are called the *endpoints* of the edge). A graph is typically visualized by representing vertices with points and edges with arcs joining the two associated vertices.

Matching polynomials are considered for graphs that are *finite*, *simple* and *connected*. That is, (i) the sets V and E are finite, (ii) for any vertices $u, v \in V$ there is at most one edge with endpoints u and v , (iii) loops (edges from a vertex to itself) are not allowed, (iv) for any pair of distinct vertices u, v there is a sequence of edges $(\{u_i, u_{i+1}\})_{i=1}^k$ where $u_1 = u$ and $u_{k+1} = v$. Since the study of matching polynomials is limited to this context, the standing assumption in this article is that the conditions above hold for all the graphs considered. We nevertheless remark that the proofs given do not make use of any of these conditions.

Definition 1. A *matching* in a graph $G = (V, E)$ is a collection of edges where no two edges are adjacent (that is, where no two edges share a common endpoint). The *size* of a matching is the number of edges in the matching. By a k -matching we will mean a matching of size k . We will say that a vertex v is *matched* in a matching if v belongs to some edge of that matching.

It is evident from the definition of a matching that there can be no matching of size greater than $\lfloor \frac{|V|}{2} \rfloor$.

Definition 2. The number of k -matchings in a graph G is denoted by $m_k(G)$. The *matching polynomial* of a graph $G = (V, E)$ is defined as

$$M(x) := M(G; x) = \sum_{k=0}^{\infty} m_k(G) x^k = \sum_{k=0}^{\lfloor |V|/2 \rfloor} m_k(G) x^k.$$

The number

$$H(G) := M(1) = \sum_{k=0}^{\lfloor |V|/2 \rfloor} m_k(G)$$

is called the *Hosoya index* of G .

In a connected graph of n vertices there are at least $n - 1$ edges, hence at least $C(n - 1, k)$ edge subsets of size k . A brute-force algorithm to calculate $m_k(G)$ would be to simply make a search through these subsets to check whether they form a matching or not. The extremely rapid growth of $C(n, k)$ as $n \rightarrow \infty$ makes this approach prohibitively expensive even for small values of n . Therefore, methods that allow fast computations of these numbers are desirable from both theoretical and computational points of view.

Next we explain the graphs of interest of this study. We first define what we mean by joining two graphs at a pair of vertices. An illustration is in Figure 1.

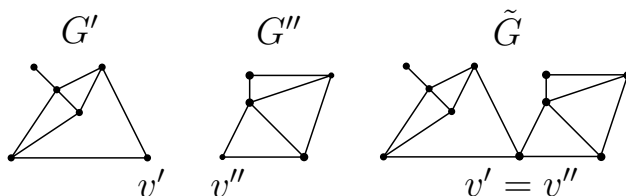


Figure 1. Joining graphs at vertices.

Definition 3. Let $G' = (V', E')$ and $G'' = (V'', E'')$ be two graphs and let $v' \in V'$, $v'' \in V''$. The graph $\tilde{G}$ obtained from G' and G'' by joining them at vertices v' and v'' is the graph whose vertex set is $\tilde{V} := (V' \cup V'')/\sim$ where $\sim$ is the equivalence relation identifying v' and v'' , and whose edge set is $\tilde{E} := E' \cup E''$.

Next, we define chains obtained by joining several copies of a graph:

Definition 4. Let G be a graph with vertex set $V = \{v_1, \dots, v_l\}$ and $l \geq 2$. Fix two distinct vertices v^L and v^R from V . For each $n = 1, 2, \dots$, let $G^{(n)}$ be an isomorphic copy of G . Let v_n^L and v_n^R be the vertices of $G^{(n)}$ corresponding to v^L and v^R , respectively, under this isomorphism. Define $G_1 := G$ and for $n \geq 1$ let G_{n+1} be the graph obtained by joining G_n and $G^{(n+1)}$ at the vertices v_n^R (regarded as a vertex of G_n) and v_{n+1}^L .

We will say that G_n is a chain-type graph obtained from the generating triple $\mathcal{G} = (G, v^L, v^R)$ with chain length n .

Any graph which is of the form above will be called a chain-type graph. Note that a chain-type graph may have more than one generating triple.

We now define some polynomials which will serve as intermediate devices to compute the matching polynomials.

Definition 5. Given a generating triple $\mathcal{G} = (G, v^L, v^R)$, let $P_B = P_B(\mathcal{G})$ be the “partial” matching polynomial of G given by

$$P_B(x) = \sum_{k=0}^{\lfloor |V|/2 \rfloor} m_{k,B}(\mathcal{G}) x^k$$

where $m_{k,B}(\mathcal{G})$ is the number of k -matchings of G in which the vertices v^L and v^R are both matched. We similarly define the polynomial P_L by considering the matchings which match vertex v^L but not v^R ; the polynomial P_R for matchings that match v^R but not v^L ; and finally the polynomial P_N for matchings which match neither vertex. The symbols $m_{k,R}(\mathcal{G})$, $m_{k,L}(\mathcal{G})$ and $m_{k,N}(\mathcal{G})$ are defined accordingly. Finally, we define P_n^+ and P_n^- as the partial matching polynomials of G_n corresponding to matchings where the vertex v_n^R is matched and not matched, respectively. Finally, we define P_n as the matching polynomial of G_n .

When we want to emphasize the dependence of these polynomials on the generating triple $\mathcal{G} = (G, v^L, v^R)$ we will write $P_L(\mathcal{G})$, $P_n^-(\mathcal{G})$, $m_{k,N}(\mathcal{G})$ etc., but when there is no risk of confusion we will drop $\mathcal{G}$ from the notation. From now on we fix our generating triple $\mathcal{G} = (G, v^L, v^R)$.

It is quite easy to see that the identities

$$\begin{aligned} M(G; x) &= P_B(x) + P_L(x) + P_R(x) + P_N(x) \\ P_n &= P_n^+ + P_n^- \end{aligned} \tag{1}$$

hold. The theorem below is the main result for the computation of matching polynomials:

Theorem 1. *Consider a chain-type graph sequence constructed from an arbitrary generating triple and their partial matching polynomials as given in Definition 4 and Definition 5. The following recursion relations hold for each $n \geq 1$:*

$$P_{n+1}^+ = P_n P_R + P_n^- P_B, \quad (2)$$

$$P_{n+1}^- = P_n P_N + P_n^- P_L. \quad (3)$$

Note that these recursive relations allow us to construct $P_n^\pm$ for all n , starting from the initial polynomials P_B , P_L , P_R and P_N . From this, using (1) we get the following immediate corollary about the matching polynomials:

Corollary 1. *For each $n \geq 1$ we have*

$$P_{n+1} = P_n(P_R + P_N) + P_n^-(P_B + P_L).$$

Therefore, to compute the matching polynomial of a chain-type graph, it is sufficient to compute the partial matching polynomials of its generating graph. For long chains, this method reduces the computation time drastically compared to the brute-force approach.

Proof of Theorem 1: Since (2) and (3) have similar proofs, we are going to prove only the former identity and leave the other to the reader.

First of all, note that using (1) we can rewrite (2) as

$$P_{n+1}^+ = P_n^+ P_R + P_n^- P_R + P_n^- P_B. \quad (4)$$

Now, we make a general observation about matchings of joined graphs: Suppose $\tilde{G} = (\tilde{V}, \tilde{E})$ is obtained by joining the graphs $G' = (V', E')$ and $G'' = (V'', E'')$ at their vertices v' and v'' , respectively. Let $\mathcal{E} \subseteq \tilde{E}$ be a k -matching of $\tilde{G}$. Then, $\mathcal{E}' := \mathcal{E} \cap E'$ and $\mathcal{E}'' := \mathcal{E} \cap E''$ are matchings of G' and G'' , respectively, with the following properties:

1. $|\mathcal{E}'| + |\mathcal{E}''| = k$,
2. $\mathcal{E}'$ and $\mathcal{E}''$ do not simultaneously match the vertices v' and v'' , respectively.

Conversely, given any pair $(\mathcal{E}', \mathcal{E}'')$ of matchings of G' and G'' , respectively, satisfying the conditions above, the set $\mathcal{E} = \mathcal{E}' \cup \mathcal{E}''$ is a k -matching of $\tilde{G}$.

So, let m_l^{n+} be the number of l -matchings of G_n that match the vertex v_n^R , and let m_l^{n-} denote the number of those not matching v_n^R . Then, each k -matching of G_{n+1} which matches v_{n+1}^R arises from a pair of matchings which belongs to one of the following three mutually exclusive categories, and there is a bijective correspondence with the union of these three sets:

- An l -matching of G_n which matches v_n^R and a $(k-l)$ -matching of $G^{(n+1)}$ which matches v_{n+1}^R but not v_{n+1}^L , $l = 0, 1, \dots, k$,
- An l -matching of G_n which does not match v_n^R and a $(k-l)$ -matching of $G^{(n+1)}$ which matches v_{n+1}^R but not v_{n+1}^L , $l = 0, 1, \dots, k$,
- An l -matching of G_n which does not match v_n^R and a $(k-l)$ -matching of $G^{(n+1)}$ which matches both v_{n+1}^L and v_{n+1}^R , $l = 0, 1, \dots, k$.

Since $G^{(n+1)}$ is isomorphic to G with $v_{n+1}^L \leftrightarrow v^L$ and $v_{n+1}^R \leftrightarrow v^R$, the number of pairs in the first case is

$$\sum_{l=0}^k m_l^{n+} \cdot m_{k-l,R}. \quad (5)$$

But since

$$P_n^+(x) = \sum_{i=0}^{\infty} m_i^{n+} x^i \quad \text{and} \quad P_R(x) = \sum_{j=0}^{\infty} m_{j,R} x^j,$$

it is readily seen that (5) is the coefficient of the degree k term of the product polynomial $P_n^+ P_R$. Similarly, the number of pairs in the second category is the degree k coefficient in $P_n^- P_R$, and the same holds for the polynomial $P_n^- P_B$ in the third case. Therefore, $m_k^{(n+1)+}$ is the sum of these three numbers, proving the identity (4).

Example 1. Let T be a triangle, that is, a complete graph with 3 vertices. One can form a generating triple $\mathcal{T}$ from T by selecting any two vertices (and the choice does not matter by symmetry). In [22], chain-type graphs constructed from $\mathcal{T}$ were considered and it was claimed that the Hosoya

index of the chain T_n is given by $H(T_n) = 4 \cdot 3^{n-1}$ for all $n \geq 1$. The proof in the given article leaves some details unexplained, but a direct computation of $m_k(T_n)$ is plausible since any k -matching of T_n can contain at most one edge from each triangular copy. We can nevertheless confirm the claim easily with our method presented above. Indeed, fixing any two vertices in T as v^L and v^R , it is easily seen that the partial matching polynomials for T are

$$P_B(x) = P_L(x) = P_R(x) = x, \quad P_N(x) = 1. \quad (6)$$

We now make the claim that $P_n^+(1) = P_n^-(1) = 2 \cdot 3^{n-1}$ and hence $P_n(1) = P_n^+(1) + P_n^-(1) = 4 \cdot 3^{n-1}$ for all $n \geq 1$. This is easily verified for $n = 1$. Now, using the inductive assumption for n , the relations (2), (3) and the polynomials in (6), we get that

$$P_{n+1}^+(1) = P_{n+1}^-(1) = P_n(1) + P_n^-(1) = 4 \cdot 3^{n-1} + 2 \cdot 3^{n-1} = 2 \cdot 3^n.$$

This proves our claim.

The computation of the Hosoya index for chains can also be made using a matrix representation as explained in the following theorem. As a consequence, the asymptotic growth rate of $H(G_n)$ can be derived.

Theorem 2. *Define the 2×2 matrix A by*

$$A = \begin{bmatrix} (P_N + P_L)(1) & P_N(1) \\ (P_R + P_B)(1) & P_R(1) \end{bmatrix}$$

and let $r = \begin{bmatrix} (P_N + P_L)(1) \\ (P_R + P_B)(1) \end{bmatrix}$. Then

$$H(G_n) = s^- + s^+$$

where

$$\begin{bmatrix} s^- \\ s^+ \end{bmatrix} = A^{n-1}r.$$

Proof. We observe that (3) and (2) are equivalent to

$$\begin{aligned} P_{n+1}^- &= P_n^- P_N + P_n^+ P_N + P_n^- P_L = (P_N + P_L)P_n^- + P_N P_n^+, \\ P_{n+1}^+ &= P_n^+ P_R + P_n^- P_R + P_n^- P_B = (P_R + P_B)P_n^- + P_R P_n^+. \end{aligned}$$

Using matrices with polynomial entries, this can be formulated as

$$\begin{bmatrix} P_{n+1}^- \\ P_{n+1}^+ \end{bmatrix} = \begin{bmatrix} P_N + P_L & P_N \\ P_R + P_B & P_R \end{bmatrix} \begin{bmatrix} P_n^- \\ P_n^+ \end{bmatrix}, \quad (7)$$

immediately implying that

$$\begin{bmatrix} P_{n+1}^- \\ P_{n+1}^+ \end{bmatrix} = \begin{bmatrix} P_N + P_L & P_N \\ P_R + P_B & P_R \end{bmatrix}^n \begin{bmatrix} P_1^- \\ P_1^+ \end{bmatrix}. \quad (8)$$

Now simply observe that $P_1^- = P_N + P_L$ and $P_1^+ = P_R + P_B$. Computing all polynomials at $x = 1$, we get the desired result. $\blacksquare$

Corollary 2. *The Hosoya index $H(G_n)$ of a regular chain-type graph grows asymptotically with exponential speed. More precisely,*

$$\lim_{n \rightarrow \infty} \frac{\ln H(G_n)}{n} = \lambda$$

where λ is the leading eigenvalue of the matrix A above. The same growth law also holds for $P_n^-(1)$ and $P_n^+(1)$.

Proof. First, observe that $P_N(1) > 0$ since the polynomial P_N has constant term 1 (for the unique 0-matching in G). But $P_R(1) + P_B(1) > 0$ as well, because either G contains the edge $\{v^L, v^R\}$ (a 1-matching by itself), thus contributing a linear term to P_B , else any single edge attached to v^R contributes a linear term to P_R . Therefore, A is a 2×2 matrix whose off-diagonal entries are strictly positive. This means that A has distinct real eigenvalues (see Lemma 1 below), say λ and γ , where $\lambda > \gamma$. Since A has positive trace, we must have $\lambda > |\gamma| \geq 0$. Now, A can be diagonalized

into the form $J = \begin{bmatrix} \lambda & 0 \\ 0 & \gamma \end{bmatrix}$ via some conjugation $A = PJP^{-1}$. Suppose

$$P = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

With a little computation, we can see that

$$A^n = PJ^nP^{-1} = \frac{1}{\det P} \begin{bmatrix} ad\lambda^n - bc\gamma^n & ab(\gamma^n - \lambda^n) \\ cd(\lambda^n - \gamma^n) & ad\gamma^n - bc\lambda^n \end{bmatrix}. \quad (9)$$

Considering the case $n = 1$ and the strict positivity of the off-diagonal entries, we get that $ab \neq 0$ and $cd \neq 0$. Hence, all entries of P must be nonzero. From what was said above, the entries of the column matrix r in Theorem 2 are strictly positive as well. Then, since each entry in (9) is positive and has a dominant term of magnitude $C\lambda^n$ ($C > 0$), the same applies to the two entries of the column vector $A^n r$. ■

For completeness, we prove the following easy fact used above:

Lemma 1. *If A is a real 2×2 matrix whose off-diagonal entries have a positive product, then A has two distinct real eigenvalues.*

Proof. Let $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. Then the characteristic polynomial is $p(\lambda) = (\lambda - a)(\lambda - d) - bc = \lambda^2 - (a + d)\lambda + ad - bc$. The discriminant of this polynomial is

$$\Delta = (a + d)^2 - 4(ad - bc) = (a - d)^2 + 4bc > 0$$

since we assume $bc > 0$. ■

2.1 Edge-linked chains

The initial motivation for studying matching polynomials was related to the study of chemical compounds [18]. In this context, vertices correspond to the atoms in the compound and the edges represent bonds. Our linking procedure above identifies vertices from two given graphs, but this form of

connection does not correspond to chemical bonding in the sense described above. To keep the analogy, we now link two graphs by drawing an edge between the selected vertices, rather than collapsing them into a single vertex. This could simulate certain cases of polymer formation where a base molecule forms chains by bonding to one or two other molecules at specified locations. The formal definition is below.

Definition 6. Let $G = (V', E')$ and $G'' = (V'', E'')$ be two graphs and let $v' \in V'$, $v'' \in V''$. The graph $\tilde{G}$ obtained from G' and G'' by linking the vertices v' and v'' is the graph $\tilde{G} = (\tilde{V}, \tilde{E})$ where $\tilde{V} = V' \cup V''$ and $\tilde{E} = E' \cup E'' \cup \{\{v', v''\}\}$.

Since the construction procedure below is similar to the chain-type graphs introduced above, we will avoid repeating the formalism there for sake of brevity. We again start with a generating triple $\mathcal{G} = (G, v^L, v^R)$ where $G = (V, E)$ and $v^L, v^R \in V$ are two distinct vertices. Given the isomorphic copies $G^{(n)}$, $n \geq 1$, we define $GL_1 := G^{(1)}$ and we form GL_{n+1} by linking vertex v_n^R of GL_n to vertex v_{n+1}^L of $G^{(n+1)}$. Our purpose is to compute the matching polynomial PL_n of GL_{n+1} .

To this end, we consider a new base graph $B = (V_B, E_B)$ obtained by extending G from vertex v^R by a single new edge. Formally, let v^{RR} be an element not in V , and set $V_B = V \cup \{v^{RR}\}$, $E_B = E \cup \{\{v^R, v^{RR}\}\}$. Let B_n be the chain-type graph generated by $\mathcal{B} = (B, v^L, v^{RR})$ and for $n \geq 1$ define the polynomials

$$Q_n^- := P_n^-(\mathcal{B}) \quad \text{and} \quad Q_n^+ := P_n^+(\mathcal{B}),$$

as well as $Q_N := P_L(\mathcal{B})$, $Q_L := P_L(\mathcal{B})$, $Q_R := P_R(\mathcal{B})$ and $Q_B := P_B(\mathcal{B})$.

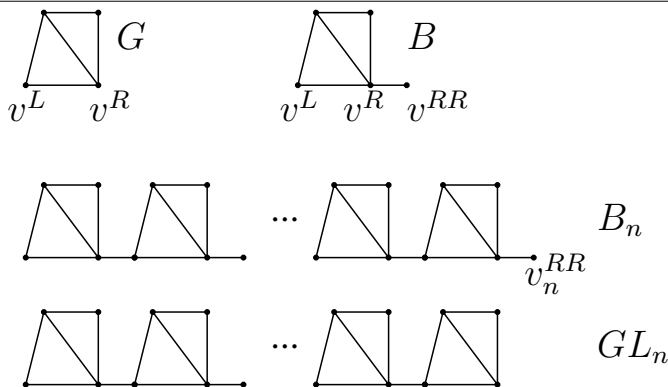


Figure 2. The chain graphs B_n and GL_n .

Theorem 3. *We have for all $n \geq 1$*

$$M(GL_n, x) = Q_n^-(x).$$

Proof. The vertex set of B_n is that of GL_n , plus the extra vertex v_n^{RR} . Similarly, the edge set of B_n is precisely the edge set of GL_n plus the single edge $\{v_n^R, v_n^{RR}\}$ (cf. Figure 2). Since this is the only edge in B_n connected to v_n^{RR} , for each $k \geq 0$ there is a bijection between the k -matchings of GL_n and the k -matchings of B_n which do not match the vertex v_n^{RR} . The cardinality of the former is the coefficient of x^k in $M(GL_n, x)$, whereas that of the latter is the same in $Q_n^-(x)$. ■

Since we are able to compute Q_n^- and Q_n^+ recursively, we have also solved the problem for edge-linked chains. Also, for the base-case polynomials, we have the following relations between those of $\mathcal{B}$ and $\mathcal{G}$:

Lemma 2. *We have the relations*

$$\begin{aligned} Q_N &= P_N(\mathcal{G}) + P_R(\mathcal{G}), \quad Q_L = P_L(\mathcal{G}) + P_B(\mathcal{G}), \\ Q_R &= xP_N(\mathcal{G}), \quad Q_B = xP_R(\mathcal{G}). \end{aligned}$$

Proof. Since $\{v^R, v^{RR}\}$ is the only edge in B attached to v^{RR} , the k -matchings of B which match neither v^L nor v^{RR} are in bijection with the k -matchings of G not matching v^L (with no restriction on the matching

status of v^R). This proves the first equality. For the second, note that k -matchings of B which match v^L but not v^{RR} are in bijection with the k -matchings of G that match v^L (with no restriction on the matching status of v^R). Next, each k -matching of B that matches v^{RR} but not v^L contains the edge $\{v^R, v^{RR}\}$, therefore these are in bijection with the $(k-1)$ -matchings of G which match neither v^L nor v^R . This justifies the third equality and the last one is dealt with similarly. ■

Example 2. Let T be the triangular graph as in Example 1 and let TL_n be the edge-linked chain of length n constructed from T . In [22], it was claimed that $H(GL_n) = 4 \cdot 5^{n-1}$, but the proof again has gaps. Here we provide a proof with our method. For this case, we claim that

$$Q_n^-(1) = 4 \cdot 5^{n-1}, \quad Q_n^+(1) = 2 \cdot 5^{n-1}$$

for all $n \geq 1$. The result will follow from Theorem 3. The base-case polynomials are $Q_N(x) = 1 + x$, $Q_L(x) = 2x$, $Q_R(x) = x$ and $Q_B(x) = x^2$. Evaluating the polynomials at $x = 1$, from (7) we get

$$\begin{aligned} Q_{n+1}^-(1) &= 4Q_n^-(1) + 2Q_n^+(1), \\ Q_{n+1}^+(1) &= 2Q_n^-(1) + Q_n^+(1). \end{aligned}$$

Combining this with $Q_1^-(1) = Q_N(1) + Q_L(1) = 4$ and $Q_1^+(1) = Q_R(1) + Q_B(1) = 2$, we get the result by induction on n .

Corollary 3. $H(GL_n)$ has asymptotic exponential growth as $n \rightarrow \infty$.

Proof. This directly follows from Corollary 2 and Theorem 3. Note that the exponent is related to the dominant eigenvalue of the matrix A corresponding to $\mathcal{B}$, rather than to $\mathcal{G}$. ■

2.2 Loops from chains

In this subsection we briefly consider the variant where the chain graphs are closed onto loops by identifying vertices from the first and last copies.

Definition 7. Consider the construction given in Definition 4. We define

LG_n to be the graph obtained from G_n by identifying the vertices v_1^L and v_n^R .

Clearly, a k -matching of G_n remains a matching for LG_n if and only if the two identified vertices are not both matched in that matching. Conversely, any k -matching of LG_n is converted into a k -matching of G_n when we “cut” the graph at the identified vertices, and the resulting matching does not match the two vertices simultaneously. This correspondence is clearly a bijection.

Therefore, counting the matchings of LG_n amount to counting the matchings of G_n which do not match v_1^L and v_n^R simultaneously. The construction above, via the polynomials P_n^+ and P_n^- , has kept track of the matchings that matches (or not) the vertex v_n^R . If we also wish to categorize according to the matching status of v_1^L then we must consider the cases at the start of the construction.

Indeed, if we want to count the matchings where v_1^L is not matched, then we must only allow matchings of G_1 in which v_1^L are unused. But it is evident that once started from this base case, generation of the next-generation matching polynomials follows the same recursive scheme, since they depend only on the configuration schemes at the identified vertex pairs. Therefore, equation (8) is still valid, but the base case is different.

Thus, if we want to count the matchings of GL_1 where both v_1^L and v_n^R are matched, the base case is given by $\begin{bmatrix} P_L \\ P_B \end{bmatrix}$ instead of $\begin{bmatrix} P_N + P_L \\ P_R + P_B \end{bmatrix}$. Therefore, the partial matching polynomial counting these matchings is the second entry of

$$\begin{bmatrix} P_N + P_L & P_N \\ P_R + P_B & P_R \end{bmatrix}^{n-1} \begin{bmatrix} P_L \\ P_B \end{bmatrix}.$$

Excluding these from all the matchings of GL_n , we arrive at the cases which correspond to the matchings of LG_n . We can summarize the result in the following statement.

Theorem 4. Consider the polynomial matrix $M = \begin{bmatrix} P_N + P_L & P_N \\ P_R + P_B & P_R \end{bmatrix}$.

Then, the matching polynomial of LG_n is

$$P_n - \begin{bmatrix} 0 & 1 \end{bmatrix} M^{n-1} \begin{bmatrix} P_L \\ P_B \end{bmatrix} = \begin{bmatrix} 1 & 1 \end{bmatrix} M^{n-1} \begin{bmatrix} P_N + P_L \\ P_R + P_B \end{bmatrix} - \begin{bmatrix} 0 & 1 \end{bmatrix} M^{n-1} \begin{bmatrix} P_L \\ P_B \end{bmatrix}.$$

We finally remark that the same reasoning can be applied to loops obtained from GL_n by identifying v_1^L and v_n^{RR} (this would amount to combining n copies of G into a loop by joining them by edges). Using the notation of the previous subsection, one just applies the theorem above to the chain B_n (instead of G_n).

3 Conclusion

In this paper, we present a recursive formula for computing the matching polynomials and the Hosoya indices of regular chain-type graphs. We present a novel method to compute the precise rate of growth of the Hosoya index as a function of the chain length, given that the matching numbers of the basic chain element are known. The proposed methods extend to the analysis of loop-shaped graphs obtained by closing the regular chains at the two ends. These results contribute to the mathematical understanding of chain-type molecular structures, which are common in chemical and biological systems.

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