Chain hexagonal cacti: Matchings and independent sets

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A B S T R A C T

In this paper we consider three classes of chain hexagonal cacti and study their matching and independence related properties. Explicit recurrences are derived for their matching and independence polynomials, and explicit formulae are presented for the number of matchings and independent sets of certain types. Bivariate generating functions for the number of matchings and independent sets of certain types are also computed and then used to deduce the expected size of matchings and independent sets in chains of given length. It is shown that the extremal chain hexagonal cacti with respect to the number of matchings and of independent sets belong to one of the considered types. Possible directions of further research are discussed.

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1. Introduction

The objects nowadays known as cactus graphs appeared in the scientific literature more than half a century ago under the name of Husimi trees. Their introduction was motivated by papers of Husimi [12] and Riddell [16] dealing with cluster integrals in the theory of condensation in statistical mechanics [19]. Besides statistical mechanics, where Husimi trees and their generalizations serve as simplified models of real lattices [14,18], the concept has also found applications in the theory of electrical and communication networks [23] and in chemistry [11,21].

The enumerative aspects of Husimi trees were elucidated soon after their appearance in a series of papers by Harary, Uhlenbeck and Norman [10,8], and summarized twenty years later in the classical monograph on graph enumeration by Harary and Palmer [9]. Later the Husimi trees became known in the mathematical literature as cactus graphs. In recent times, they attracted some attention when it was found out that some NP-hard facility allocation problems can be solved in polynomial time for the cactus graphs [1,22]. Also, certain invariants of a closely related class of block-cactus graphs have been studied recently [2,24].

The present paper was motivated by an article of E.J. Farrell on matchings in hexagonal cacti [4], where he presented recurrences and/or explicit formulae for a number of matching-related invariants in certain classes of hexagonal cacti. We take further the line of research of the above reference by deriving analogous results for several classes of graphs not considered there. Further, we investigate and determine the extremal graphs with respect to the matching-related properties studied in both papers. Then we extend the results to the context of independent sets. In particular, we derive explicit recurrences for the independence polynomials in the considered classes of cacti, and we show that certain configurations are extremal with respect to the number of independent sets. For both matchings and independent sets we establish explicit bivariate generating functions and use them to find the expected size of random matchings and independent sets. We also report some non-enumerative results, such as the matching number and the independence number for the considered graphs.

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Theorem 2.1. There are \( \frac{1}{2} \left( 3^n - 2 + 3^{\left\lfloor \frac{n}{2} \right\rfloor} \right) \) different chain hexagonal cacti of length \( n \).
A chain hexagonal cactus $G_n$ is an ortho-chain if all its internal hexagons are ortho-hexagons. The meta-chain and para-chain are defined in a completely analogous manner. These three types of chains are the main protagonists of the present paper.

The ortho-chain of length $n$ is denoted by $O_n$, and the meta-chain is denoted by $M_n$. The para-chain of length $n$ will be denoted by $L_n$, in order to avoid confusion with the standard notation $P_n$ for a path on $n$ vertices. Also, $L_n$ was the notation for para-chains (called linear hexagonal cacti there) in the paper by Farrell mentioned in the Introduction.

Ortho-, meta-, and para-chains of length 6 are shown in Fig. 3.

In the course of our computations in the subsequent sections we will need to deal with some auxiliary graphs that arise from chain hexagonal cacti by various processes of vertex and/or edge removal. We tried to develop and adhere to a consistent, self-explaining system of notation. The auxiliary graphs for the ortho-, meta-, and para-chains are illustrated in Figs. 4–6, respectively.

Let us now introduce the basic concepts relevant for 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.

The interest in counting matchings in graphs was first sparked by an observed correlation between the (chemical) stability of benzenoid compounds and the number of perfect matchings in the corresponding graphs. The subject later acquired a life of its own in mathematical literature and became a well established discipline. We refer the reader to the classical monograph by Lovász and Plummer [13] for a thorough introduction to the topic.

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 neat 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 the 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. Both polynomials are special forms of general matching polynomials introduced by Farrell in [3]. We refer the reader to Chapter 8.5 in [13] for more information on the general theory of matching polynomials.

We quote without proof the following two results.

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

$$m(G; x) = m(G - e; x) + x \cdot m(G \setminus e; x).$$

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

$$m(G; x) = m(G_1; x) \cdot \cdots \cdot m(G_k; x).$$

The two quoted theorems, together with the fact $m(K_1; x) = 1$, enable us to 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 formulae:

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

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

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.

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 the 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 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

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

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

$$i(G; x) = i(G_1; x)i(G_2; x) \cdots i(G_k; x).$$

The reader can easily verify that the independence polynomials of paths and cycles are given by following formulae:

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

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

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 $F_n$. 

**Theorem I1.** Let $G$ be a graph and $e$ an edge of $G$. Then

$$m(G; x) = m(G - e; x) + x \cdot m(G \setminus e; x).$$

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

$$m(G; x) = m(G_1; x) \cdot \cdots \cdot m(G_k; x).$$

The two quoted theorems, together with the fact $m(K_1; x) = 1$, enable us to 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 formulae:

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

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

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.

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

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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 the 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 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

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

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

$$i(G; x) = i(G_1; x)i(G_2; x) \cdots i(G_k; x).$$

The reader can easily verify that the independence polynomials of paths and cycles are given by following formulae:

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

$$i(C_n; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n - k}{k} x^k.$$
3. Matchings in chain hexagonal cacti

In this section we investigate the enumerative aspects of matchings in three families of chain hexagonal cacti introduced in Section 2. For two of them, ortho- and meta-chains, we derive the explicit recurrences for their matching polynomials in the fashion of Farrell’s paper [4], and determine the number of matchings in them with certain properties. The Farrell’s results are quoted for the sake of completeness. Afterwards we proceed by showing that ortho- and meta-chains are extremal among all chain cacti with respect to the total number of matchings. At the end of this section we bring also the para-chains into consideration by deriving the bivariate generating functions for the numbers of matchings of a given size in all three types of chains, and by calculating the expected number of edges in a random matching in a chain.

For $n = 0, 1, 2$ the matching polynomials of $O_n, M_n,$ and $L_n$ are all equal:

- $m(O_0) = m(M_0) = m(L_0) = 1$
- $m(O_1) = m(M_1) = m(L_1) = 1 + 6x + 9x^2 + 2x^3$
- $m(O_2) = m(M_2) = m(L_2) = 1 + 12x + 50x^2 + 88x^3 + 61x^4 + 12x^5$

We will first establish an explicit recurrence for the matching polynomial of the ortho-chain, $O_n.$ In doing so, we need two simple lemmas that are easily obtained by applying the decomposition procedure and using Theorems M1 and M2.

**Lemma 3.1.** For $n \geq 1,$ $m(O''_n) = m(P_3)m(O_n) + x \cdot m(P_4)m(O''_{n-1}).$ □

**Lemma 3.2.** For $n \geq 1,$ $m(O''_n) = m(P_4)m(O_n) + x \cdot m(P_5)m(O''_{n-1}).$ □

**Theorem 3.3.** The matching polynomials of $O_n, n \geq 2,$ are given by

$$m(O_n) = (1 + 5x + 5x^2)m(O_{n-1}) + (x + 6x^2 + 11x^3 + 6x^4 + 2x^5)m(O_{n-2}).$$

**Proof.** By applying the reduction process to $O_n, n \geq 2,$ deleting the edge $uv$ (see Fig. 3), we get

$$m(O_n) = m(O'_{n-1}) + x \cdot m(P_4)m(O''_{n-2}).$$

After substitution for $m(O'_{n-1})$ using Lemma 3.1 we have

$$m(O_n) = m(P_3)m(O_{n-1}) + 2x \cdot m(P_4)m(O''_{n-2}).$$

For the case $n = 2$ the theorem can be established by calculating the right-hand side. For $n \geq 3,$ substituting for $m(O''_{n-2})$ using Lemma 3.2 yields

$$m(O_n) = m(P_5)m(O_{n-1}) + 2x \cdot m(P_4)^2m(O_{n-2}) + 2x^2 \cdot m(P_3)m(P_4)m(O''_{n-3}).$$

Then, by substituting for $2x \cdot m(P_4)m(O''_{n-3})$ using Eq. (1), we get

$$m(O_n) = (x \cdot m(P_3) + m(P_5))m(O_{n-1}) + (2x \cdot m(P_4)^2 - x \cdot m(P_3)m(P_5))m(O_{n-2}).$$ □

This recurrence is not only useful in itself, but will also be used in establishing other matching properties of the ortho-chain.

The degree of the matching polynomial of a graph $G$ is the number of edges in a maximum matching of $G,$ so we obtain the following corollary by applying Theorem 3.3 recursively, using the fact that $\deg (m(O_n)) = 0$ and $\deg (m(O_1)) = 3.$

**Corollary 3.4.** The matching number of $O_n, n \geq 0,$ is $\nu(O_n) = (5n + 1)/2$ if $n$ is odd, and $\nu(O_n) = 5n/2$ if $n$ is even. □

Since a matching covers an even number of vertices and $|V(O_n)| = 5n + 1,$ $O_n$ has no defect-$d$ matching when $d$ and $n$ have same parities. The smallest possible defect of a matching of $O_n$ is $5n + 1 - 2\nu(O_n),$ with $\nu(O_n)$ as given in the above corollary. Together with the fact that for any matching of defect $d,$ an edge can be removed to get a matching of defect $d + 2,$ we therefore have the following theorem.

**Theorem 3.5.** The chain $O_n, n \geq 0,$ has a defect-$d$ matching if and only if $0 \leq d \leq 5n + 1$ and $d$ has opposite parity of $n.$ □

From this result, we observe that $O_n$ has a perfect matching if and only if $n$ is odd.

The next lemma can be used to find explicit formulae for coefficients of the matching polynomial of $O_n.$ We will use it to find the number of maximum matchings.

**Lemma 3.6.** If $O_n, n \geq 2,$ has a defect-$d$ matching, then it has a total of

$$N_d(O_n) = N_{d-5}(O_{n-1}) + 5N_{d-3}(O_{n-1}) + 5N_{d-1}(O_{n-1}) + 6N_{d-6}(O_{n-2}) + 6N_{d-2}(O_{n-2}) + 11N_{d-4}(O_{n-2}) + 6N_{d-2}(O_{n-2}) + 2N_d(O_{n-2})$$

defect-$d$ matchings.
Consider $O_n, n \geq 2$. The number of edges in a defect-$d$ matching is $k$, where $2k = 5n + 1 - d$. Therefore, the number of defect-$d$ matchings of $O_n$ is $\Phi_{\frac{5n+1-d}{2}}(O_n)$. By Theorem 3.3 we see that

$$
\Phi_{\frac{5n+1-d}{2}}(O_n) = \Phi_{\frac{5n+1-d}{2}}(O_{n-1}) + 5\Phi_{\frac{5n+1-d}{2}-1}(O_{n-1}) + 5\Phi_{\frac{5n+1-d}{2}-2}(O_{n-1}) + \Phi_{\frac{5n+1-d}{2}-1}(O_{n-2}) + 6\Phi_{\frac{5n+1-d}{2}-2}(O_{n-2}) + 11\Phi_{\frac{5n+1-d}{2}-3}(O_{n-2}) + 6\Phi_{\frac{5n+1-d}{2}-4}(O_{n-2}) + 2\Phi_{\frac{5n+1-d}{2}-5}(O_{n-2})
$$

which after rewriting yields the result. \qed

Theorem 3.7. The number of maximum matchings of $O_n, n \geq 0$, is $\Phi_{\frac{5n+1}{2}}(O_n) = 2^{(n+1)/2}$ when $n$ is odd and $\Phi_{\frac{5n}{2}}(O_n) = (5n + 2)^2(2^{(n-2)/2})$ when $n$ is even.

Proof. From Theorem 3.5 we know that a maximum matching has defect 0 when $n$ is odd and defect 1 when $n$ is even. Suppose $n \geq 3$ is odd. By putting $d = 0$ in Lemma 3.6 and then applying it recursively we obtain

$$
N_0(O_n) = 2N_0(O_{n-2}) = 2^2N_0(O_{n-4}) = \cdots = 2^{(n-1)/2}N_0(O_1) = 2^{(n+1)/2}.
$$

For the case when $n$ is even, setting $d = 1$ yields

$$
N_1(O_n) = 5N_0(O_{n-1}) + 2N_1(O_{n-2}) = 5 \cdot 2^{n/2} + 2N_1(O_{n-2}),
$$

which by recursion gives the result. \qed

We now give an explicit formula for the number of matchings of $O_n$. Later in the text we will prove that $O_n$ is an extremal hexagonal chain cactus in this regard.

Theorem 3.8. The chain $O_n, n \geq 0$, has a total of

$$
\Phi(O_n) = \frac{4}{3} \cdot 13^n - \frac{1}{3} \cdot (-2)^n
$$

matchings.

Proof. From Theorem 3.3 we see that for $n \geq 2$

$$
\Phi(O_n) = 11\Phi(O_{n-1}) + 26\Phi(O_{n-2})
$$

by setting $x = 1$. The characteristic equation is $r^2 - 11r - 26 = 0$, which has the roots $r_1 = 13$ and $r_2 = -2$, so the solution of the recurrence has the form $c_1r_1^n + c_2r_2^n$. Solving for $c_1$ and $c_2$ using the initial values $\Phi(O_2) = 224$ and $\Phi(O_3) = 2932$ yields $c_1 = 4/3$ and $c_2 = -1/3$. \qed

We will now proceed with the meta-chain, $M_n$, finding an explicit recurrence for the matching polynomial and establishing matching properties in an analogous way to what we did for the ortho-chain.

To obtain a recurrence for the matching polynomial of $M_n$ we will use two lemmas. We omit their proofs since they are very similar to the proofs of the two lemmas used for the ortho-chains.

Lemma 3.9. For $n \geq 1$, $m(M_n') = m(P_5)m(M_n) + x \cdot m(P_4)m(M_{n-1})$. \qed

Lemma 3.10. For $n \geq 1$, $m(M_n'') = m(P_5)m(M_n) + (m(P_2) + m(P_3))x \cdot m(M_{n-1}'')$. \qed

Theorem 3.11. The matching polynomials of $M_n, n \geq 2$, are given by

$$
m(M_n) = (1 + 6x + 6x^2)m(M_{n-1}) - (x^2 + 4x^3 + 5x^4)m(M_{n-2}).
$$

Proof. Apply the reduction process to $M_n, n \geq 2$, by deleting the edge $uv$ (see Fig. 3). This yields

$$
m(M_n) = m(M_{n-1}') + x \cdot m(P_4)m(M_{n-2}'').
$$

By substituting for $m(M_{n-1}')$ using Lemma 3.9, we get

$$
m(M_n) = m(P_5)m(M_{n-1}) + 2x \cdot m(P_4)m(M_{n-2}). \quad (2)
$$

For the case $n = 2$, the theorem can be established by calculating the right-hand side. For $n \geq 3$, we substitute for $m(M_{n-2}')$ using Lemma 3.10 and get

$$
m(M_n) = m(P_5)m(M_{n-1}) + 2x \cdot m(P_4)m(M_{n-2}) + 2x^2 \cdot (m(P_2) + m(P_3))m(P_4)m(M_1').
$$

Substituting for $2x \cdot m(P_4)m(M_{n-2}')$ using Eq. (2) yields

$$
m(M_n) = ((m(P_2) + m(P_3))x + m(P_5))m(M_{n-1}) + (2 \cdot m(P_2)m(P_4) - (m(P_2) + m(P_3)))x \cdot m(M_{n-2}). \quad \Box
$$

This theorem will be used in finding matching properties of $M_n$, in a similar way to what we did for $O_n$. By applying it recursively, we see that the highest power of $x$ occurring in $m(M_n)$ is $2n + 1$, so we have the following corollary.
Theorem 3.13. The chain $M_n$, $n \geq 2$, has a defect-$d$ matching if and only if $n - 1 \leq d \leq 5n + 1$ and $d$ has the opposite parity of $n$. □

From the above theorem, we see that the meta-chain of length $n$ has no perfect matching for $n \geq 2$.

As for $O_n$, we will use a lemma in order to find the number of maximum matchings.

Lemma 3.14. If $M_n$, $n \geq 2$, has a defect-$d$ matching, then it has a total of

$$N_d(M_n) = N_{d-s}(M_{n-1}) + 6N_{d-s}(M_{n-1}) + 6N_{d-1}(M_{n-1}) - N_{d-6}(M_{n-2}) - 4N_{d-4}(M_{n-2}) - 5N_{d-2}(M_{n-2})$$

defect-$d$ matchings.

Proof. Consider $M_n$, $n \geq 2$. Since a matching of defect $d$ has $k$ edges, where $2k = 5n + 1 - d$, the number of defect-$d$ matchings of $M_n$ is $\Phi^{2n+1-d}(M_n)$. By Theorem 3.11 we see that

$$\Phi^{2n+1-d}(M_n) = \Phi^{2n+1-d}(M_{n-1}) + 6\Phi^{2n+1-d-1}(M_{n-1}) + 6\Phi^{2n+1-d-2}(M_{n-1}) - \Phi^{2n+1-d-3}(M_{n-2}) - 5\Phi^{2n+1-d-4}(M_{n-2}).$$

which is the same as the claim of the lemma. □

Theorem 3.15. The chain $M_n$, $n \geq 2$, has $\nu(M_n) = \frac{1}{2} \cdot 5^n - \frac{1}{2}$ maximum matchings.

Proof. Let $n \geq 2$. Since a maximum matching of $M_n$ has defect $n - 1$, $\Phi_{\nu(M_n)}(M_n) = N_{n-1}(M_n)$. From Lemma 3.14, it follows that

$$N_{n-1}(M_n) = N_{n-6}(M_{n-1}) + 6N_{n-4}(M_{n-1}) + 6N_{n-2}(M_{n-1}) - N_{n-7}(M_{n-2}) - 4N_{n-5}(M_{n-2}) - 5N_{n-3}(M_{n-2}).$$

Looking at the parities, using Theorem 3.13, we see that all terms on the right-hand side but two equal zero, so the expression simplifies to

$$N_{n-1}(M_n) = 6N_{n-2}(M_{n-1}) - 5N_{n-3}(M_{n-2}),$$

which can be rewritten as

$$\Phi_{\nu(M_n)}(M_n) = 6\Phi_{\nu(M_{n-1})}(M_{n-1}) - 5\Phi_{\nu(M_{n-2})}(M_{n-2}).$$

The characteristic equation of this recurrence is $r^2 - 6r + 5 = 0$ with roots $r_1 = 1$ and $r_2 = 5$, so it has solutions of the form $c_1 + c_2 n^2$. Solving for $c_1$ and $c_2$ using the initial values $\Phi(M_2) = 12$ and $\Phi(M_3) = 62$ yields $c_1 = -1/2$ and $c_2 = 1/2$. □

Theorem 3.16. The chain $M_n$, $n \geq 2$ has a total of

$$\left(\frac{1}{2} + \frac{23}{2\sqrt{129}}\right)^n \left(\frac{13 + \sqrt{129}}{2}\right)^n + \left(\frac{1}{2} - \frac{23}{2\sqrt{129}}\right)^n \left(\frac{13 - \sqrt{129}}{2}\right)^n$$

matchings.

Proof. By setting $x = 1$ in Theorem 3.11, we see that

$$\Phi(M_n) = 13\Phi(M_{n-1}) - 10\Phi(M_{n-2}).$$

The characteristic equation of this recurrence is $r^2 - 13r + 10 = 0$, which has the roots $r_1 = \frac{13+\sqrt{129}}{2}$ and $r_2 = \frac{13-\sqrt{129}}{2}$, and solutions of the form $\Phi(M_n) = c_1 r_1^n + c_2 r_2^n$. By solving for $c_1$ and $c_2$ using the initial values $\Phi(M_2) = 224$ and $\Phi(M_3) = 2732$ we get $c_1 = \frac{13+\sqrt{129}}{2}$ and $c_2 = \frac{13-\sqrt{129}}{2}$. □

Matchings of the para-chain, $L_n$, was studied in [4]. For the sake of completeness, we list some of the results here, in the same form as for the ortho- and the meta-chains.

Theorem 3.17. The matching polynomial of $L_n$, $n \geq 2$, is given by

$$m(L_n) = (1 + 6x + 5x^2)m(L_{n-1}) + (2x^3 + 4x^4 + 2x^5)m(L_{n-2}).$$

Corollary 3.18. The matching number of $L_n$, $n \geq 2$, is $\nu(L_n) = (5n + 1)/2$ if $n$ is odd, and $\nu(L_n) = 5n/2$ if $n$ is even. □

We note that $\nu(L_n) = \nu(O_n)$.

Theorem 3.19. $L_n$, $n \geq 2$, has a defect-$d$ matching if and only if $0 \leq d \leq 5n + 1$ and $d$ has opposite parity of $n$. □

From the above theorem, we see that $L_n$ has a defect-$d$ matching if and only if the same is true for $O_n$. 
Lemma 3.20. If \( L_n \), \( n \geq 2 \), has a defect-\( d \) matching, then it has a total of
\[
N_d(L_n) = N_{d-5}(L_{n-1}) + 6N_{d-3}(L_{n-1}) + 5N_{d-1}(L_{n-1}) + 2N_{d-4}(L_{n-2}) + 4N_{d-2}(L_{n-2}) + 2N_d(L_{n-2})
\]
defect-\( d \) matchings. □

Theorem 3.21. The number of maximum matchings of \( L_n, n \geq 2 \), is \( \Phi_{\nu(L_n)}(L_n) = 2^{(n+1)/2} \) when \( n \) is odd and \( \Phi_{\nu(L_n)}(L_n) = (5n + 2)2^{(n-2)/2} \) when \( n \) is even. □

We observe that \( \Phi_{\nu(L_n)}(L_n) = \Phi_{\nu(0_n)}(O_n) \).

Theorem 3.22. The chain \( L_n, n \geq 2 \), has a total of
\[
\Phi(L_n) = \frac{3\sqrt{11} - 7}{8\sqrt{11}}(6 + 2\sqrt{11})^{n+1} + \frac{3\sqrt{11} + 7}{8\sqrt{11}}(6 - 2\sqrt{11})^{n+1}
\]
matchings. □

(The above theorem is a corrected version of Theorem 13 in [4], in which there is a sign error.)

By comparing the explicit formulae for the total number of matchings we can see that an ortho-chain of length \( n \) contains more matchings than a para-chain, which, in turn, is richer in matchings than a meta-chain of the same length. Hence,
\[
\Phi(M_n) \leq \Phi(L_n) \leq \Phi(O_n).
\]
This double inequality remains valid even if \( L_n \) is replaced by any other chain \( G_n \in e_n \).

Theorem 3.23. Let \( G_n \) be a chain hexagonal cactus of length \( n \). Then
\[
\Phi(M_n) \leq \Phi(G_n) \leq \Phi(O_n).
\]

Proof. Let \( S_1 \) and \( S_2 \) be two chain hexagonal cacti such that their lengths add to \( n - 1 \). There are three ways of inserting a hexagon between them and forming a chain of length \( n \). We denote by \( S_1OS_2, S_1MS_2, \) and \( S_1PS_2 \) the cases when the inserted hexagon is an ortho-, a meta, and a para-hexagon in the resulting chain. These three possibilities are shown in Fig. 7.

The four auxiliary graphs needed in the proof are shown in Fig. 8.

Let us denote by \( \Phi_c(G) \) the number of matchings in a graph \( G \) that cover vertex \( u \). By counting the matchings that do and those that do not cover the cut-vertices \( u \) and \( v \) in \( S_1OS_2 \) we obtain the following expression.
\[
\Phi(S_1OS_2) = \Phi_u(S_1)\Phi(S_2) + \Phi(S_1 - u)\Phi(C_6 \cdot S_2)
\]
\[
= \Phi_u(S_1)\left[5\Phi_v(S_2) + 8\Phi(S_2 - v)\right] + \Phi(S_1 - u)\left[8\Phi_v(S_2) + 18\Phi(S_2 - v)\right]
\]
\[
= 5\Phi_u(S_1)\Phi_v(S_2) + 8 \left[ \Phi_u(S_1)\Phi(S_2 - v) + \Phi(S_1 - u)\Phi_v(S_2) \right] + 18 \Phi(S_1 - u)\Phi(S_2 - v).
\]
Here we used the facts that \( \Phi(P_4) = 5, \Phi(P_5) = 8, \) and \( \Phi(C_6) = 18 \). In a similar way we obtain the expressions for \( \Phi(S_1MS_2) \) and \( \Phi(S_1PS_2) \).

\[
\Phi(S_1MS_2) = \Phi_u(S_1)\Phi(S_2) + \Phi(S_1 - u)\Phi(C_6 \cdot S_2)
\]
\[
= 3\Phi_u(S_1)\Phi_v(S_2) + 8 \left[ \Phi_u(S_1)\Phi(S_2 - v) + \Phi(S_1 - u)\Phi_v(S_2) \right] + 18 \Phi(S_1 - u)\Phi(S_2 - v).
\]

\[
\Phi(S_1PS_2) = \Phi_u(S_1)\Phi(S_2) + \Phi(S_1 - u)\Phi(C_6 \cdot S_2)
\]
\[
= 4\Phi_u(S_1)\Phi_v(S_2) + 8 \left[ \Phi_u(S_1)\Phi(S_2 - v) + \Phi(S_1 - u)\Phi_v(S_2) \right] + 18 \Phi(S_1 - u)\Phi(S_2 - v).
\]
Now we have
\[
\Phi(S_1OS_2) - \Phi(S_1PS_2) = \Phi(S_1PS_2) - \Phi(S_1MS_2) = \Phi_n(S_1)\Phi_n(S_2) \geq 0.
\]
Hence, a chain hexagonal cactus with the maximum possible number of matchings cannot contain a meta- or a para-hexagon. Similarly, a chain hexagonal cactus with the smallest possible number of matchings cannot contain an ortho- or a para-hexagon. □

Hence, we have established sharp lower and upper bounds on the total number of matchings for all chains from \( C_n \).

The explicit recurrences for the matching polynomials of the considered chains allow us to derive the full bivariate generating functions for the numbers \( \Phi_k(G_n) \), where \( G \) stands for \( O, M, \) and \( L \). The generating functions we denote as follows:

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

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

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

We refer the reader to [20] for more information on generating functions and their applications.

From the definition of the bivariate generating functions we see that the “coefficients” of \( x^n \) are exactly our matching polynomials for the respective graphs, written in the variable \( y \). We introduce the following notation for the polynomials that appear in the recurrences for the matching polynomials of chain hexagonal cacti in Theorems 3.3, 3.11 and 3.17.

\[
p_1(y) = 1 + 5y + 5y^2;
\]

\[
p_2(y) = y(1 + 6y + 11y^2 + 6y^3 + 2y^4);
\]

\[
q_1(y) = 1 + 6y + 6y^2;
\]

\[
q_2(y) = -y^2(1 + 4y + 5y^2);
\]

\[
r_1(y) = 1 + 6y + 5y^2;
\]

\[
r_2(y) = 2y^2(1 + y)^2.
\]

We also introduce a special notation for the matching polynomials of the three shortest chains.

\[
m_0(x, y) = 1;
\]

\[
m_1(x, y) = x(1 + 6y + 9y^2 + 2y^3);
\]

\[
m_2(x, y) = x^2(1 + 12y + 50y^2 + 88y^3 + 61y^4 + 12y^5).
\]

Now the recurrences for the matching polynomials of our three types of chains can be written in a unified manner.

\[
m(G_n) = g_1(y)m(G_{n-1}) + g_2(y)m(G_{n-2}).
\]

Here \( G \) stands for \( O, M, \) and \( L \) and \( g \) for \( p, q, \) and \( r \), respectively.

The above recurrence translates into the language of bivariate generating functions in the usual way, by multiplying it through by \( x^n \) and then summing over all \( n \geq 2 \). This results in a linear equation in the unknown generating function \( G(x, y) \).

\[
G(x, y) - m_0(x, y) - m_1(x, y) = x g_1(y)[G(x, y) - m_0(x, y)] + x^2 g_2(y)G(x, y).
\]

By solving this equation one gets the following explicit formula for the bivariate generating function of the sequence \( \Phi_k(G_n) \) for all \( k \geq 1 \):

\[
G(x, y) = \frac{m_0(x, y)[1 - x g_1(y)] + m_1(x, y)}{1 - x g_1(y) - x^2 g_2(y)}.
\]

By substituting the pairs \( (O, p), (M, q), \) and \( (L, r) \) for \( (G, g) \) in the above formula, we get the explicit formulae for the bivariate generating functions \( O(x, y), M(x, y), \) and \( L(x, y) \).

**Theorem 3.24.**

\[
O(x, y) = \frac{1 + xy(1 + 4y + 2y^2)}{1 - x(1 + 5y + 5y^2) - x^2y(1 + 6y + 11y^2 + 6y^3 + 2y^4)};
\]

\[
M(x, y) = \frac{1 + xy^2(3 + 2y)}{1 - x(1 + 6y + 6y^2) + x^2y^2(1 + 4y + 5y^2)};
\]

\[
L(x, y) = \frac{1 + 2xy^2(2 + y)}{1 - x(1 + 6y + 5y^2) - 2xy^2(1 + 2y + y^2)}.
\]

By setting \( y = 1 \) in the above formulae we get the ordinary generating functions for the total number of matchings in our three types of chains.
Corollary 3.25.

\[
O(x) = \frac{1 + 7x}{1 - 11x - 26x^2}; \\
M(x) = \frac{1 + 5x}{1 - 13x + 10x^2}; \\
L(x) = \frac{1 + 6x}{1 - 12x - 8x^2}. \quad \square
\]

Here we denoted \(O(x, 1)\) by \(O(x)\) and similarly for \(M(x)\) and \(L(x)\).

We conclude the section on matchings by determining the asymptotic behavior of the expected size of a random matching in each of our chains. Starting point is the fact that if \(G(x, y)\) is the bivariate generating function for the numbers \(\Phi_k(G_n)\), then \(\frac{\partial^2 G}{\partial y} (x, y) \mid_{y=1}\) is the generating function for the total number of edges in all matchings of \(G_n\) (see [20] or [17] for a more detailed explanation). From such a generating function we can find a recurrence for the total number of edges, solve it explicitly, and divide the leading term by the leading term of the total number of matchings. An alternative approach is to use Darboux’s theorem to find the asymptotic behavior of the coefficients of \(\frac{\partial^2 G}{\partial y} (x, y) \mid_{y=1}\) and \(G(x, y)\) and then to consider their quotient \([15]\). We state our results omitting the details.

Theorem 3.26. Let \(\bar{k}(G_n)\) denote the expected number of edges in a matching of \(G_n\). Then:

\[
\bar{k}(O_n) \sim \frac{55}{39} n \approx 1.41026n; \\
\bar{k}(M_n) \sim \left(\frac{17}{10} - \frac{41}{10\sqrt{129}}\right) n \approx 1.33902n; \\
\bar{k}(L_n) \sim \left(2 - \frac{2}{\sqrt{11}}\right) n \approx 1.39698n. \quad \square
\]

Hence, \(O_n\) is not only the richest in matchings, but its matchings are on average larger than the matchings in the other two chains.

4. Independent sets in chain hexagonal cacti

This section contains the results on the independent sets in ortho-, meta-, and para-chains. It is organized along the same lines as the previous one. As most of the results follow in a very similar way for all three types of chains, only the results for ortho-chains are worked out in full detail. The analogous results for the other two chains are then stated omitting the proofs.

The following formulae for the independence polynomials of short chains can be easily verified by direct calculations.

- \(i(O_0) = i(M_0) = i(L_0) = 1 + x\)
- \(i(O_1) = i(M_1) = i(L_1) = 1 + 6x + 9x^2 + 2x^3\)
- \(i(O_2) = i(M_2) = i(L_2) = 1 + 11x + 43x^2 + 73x^3 + 52x^4 + 13x^5 + x^6\).

We will now find explicit recurrences for the independence polynomials of the ortho-, meta- and para-chains, as well as establish some of their independence related properties; the independence number, the number of maximum independent sets and the total number of independent sets.

As we did for matchings, we start with the ortho-chain, \(O_n\).

Theorem 4.1. The independence polynomials of \(O_n, n \geq 3\), are given by

\[
i(O_n) = (1 + 4x + 3x^2)i(O_{n-1}) + x(1 + 3x + x^2)^2i(O_{n-2}).
\]

Proof. The independent sets in \(O_n\) that do not contain vertex \(u\) are counted by \(i(P_5)i(O''_{n-2})\), while those that contain \(u\) are counted by \(x \cdot i(P_3)^2i(O''_{n-3})\). This yields the relation

\[
i(O_n) = i(P_5)i(O''_{n-2}) + x \cdot i(P_3)^2i(O''_{n-3}).
\]

A similar reasoning yields the recurrence for the independence polynomials of \(O''_n, n \geq 2\):

\[
i(O''_n) = i(P_4)i(O''_{n-1}) + xii(P_3)^3i(O''_{n-2}).
\]

Hence, the matching polynomials of the auxiliary graphs \(O''_n\) satisfy a recurrence relation of length 2. But then the whole right-hand side of the recurrence for \(i(O_n)\) above satisfies the same recurrence, and then also the left-hand side of the equation must satisfy the same recurrence. \(\square\)
As in the case for the matching polynomials, the independence polynomials will turn out to be helpful in finding properties regarding independent sets.

**Theorem 4.2.** The independence number of \( O_n \), \( n \geq 0 \), is \( \alpha(O_n) = \frac{5n+2}{2} \), if \( n \) is even, and \( \alpha(O_n) = \frac{5n+1}{2} \), if \( n \) is odd.

**Proof.** Since \( \alpha(O_n) = \deg(i(O_n)) \), we can apply Theorem 4.1 recursively, using the fact that \( \deg(i(O_2)) = 1 \) and \( \deg(i(O_1)) = 3 \), to see that \( \deg(i(O_2)) = 6 \), \( \deg(i(O_3)) = 8 \), \( \deg(i(O_4)) = 11 \), \( \deg(i(O_5)) = 13 \), \ldots The claim of the theorem now follows by induction. \( \square \)

**Theorem 4.3.** The number of maximum independent sets of \( O_n \), \( n \geq 0 \), is \( \Psi_{\alpha(O_n)}(O_n) = 1 \), when \( n \) is even, and \( \Psi_{\alpha(O_n)}(O_n) = (3n + 1)/2 \), when \( n \) is odd.

**Proof.** First, consider the case when \( n \geq 2 \) is even. Note that then \( \alpha(O_n) = \frac{5n+2}{2} \). From Theorem 4.1, it follows that for \( n \geq 2 \)

\[
\Psi_{\frac{5n+2}{2}}(O_n) = \Psi_{\frac{5n+2}{2}}(O_{n-1}) + 4\Psi_{\frac{5n+2}{2}}(O_{n-2}) + 3\Psi_{\frac{5n+2}{2}}(O_{n-3}) + \Psi_{\frac{5n+2}{2}}(O_{n-4}) + 6\Psi_{\frac{5n+2}{2}}(O_{n-5})
\]

By Theorem 4.2, all terms on the right-hand side but one equal zero, so the expression simplifies to

\[
\Psi_{\frac{5n+2}{2}}(O_n) = \Psi_{\frac{5n+2}{2}}(O_{n-2}),
\]

which is the same as

\[
\Psi_{\alpha(O_n)}(O_n) = \Psi_{\alpha(O_n)}(O_{n-2}).
\]

Since \( \Psi_{\alpha(O_2)}(O_2) = 1 \), we see that \( \Psi_{\alpha(O_1)}(O_3) = 1 \), \( \Psi_{\alpha(O_2)}(O_4) = 1 \), \ldots

Now, consider the case when \( n \geq 3 \) is odd. By the same reasoning as above we get

\[
\Psi_{\alpha(O_n)}(O_n) = 3\Psi_{\alpha(O_{n-1})}(O_{n-1}) + \Psi_{\alpha(O_{n-2})}(O_{n-2}) = 3 + \Psi_{\alpha(O_{n-2})}(O_{n-2}).
\]

And since \( \Psi_{\alpha(O_2)}(O_3) = 2 \), it follows that \( \Psi_{\alpha(O_2)}(O_4) = 5 \), \( \Psi_{\alpha(O_2)}(O_5) = 8 \), \ldots \( \square \)

**Theorem 4.4.** The total number of independent sets of \( O_n \), \( n \geq 2 \), is

\[
\Psi(O_n) = \left(1 + \frac{5}{\sqrt{41}}\right)^{4 + \sqrt{41}} + \left(1 - \frac{5}{\sqrt{41}}\right)^{4 - \sqrt{41}}.
\]

**Proof.** By setting \( x = 1 \) in Theorem 4.1, we get for \( n \geq 2 \) the recurrence

\[
\Psi(O_n) = 8\Psi(O_{n-1}) + 25\Psi(O_{n-2}).
\]

Solving it, using the initial values \( \Psi(O_2) = 194 \) and \( \Psi(O_3) = 2002 \), yields the result. \( \square \)

We will now go on to study the meta-chain, \( M_n \). As promised, the results are stated without proofs.

**Theorem 4.5.** The independence polynomial of \( M_n \), \( n \geq 3 \), is given by

\[
i(M_n) = (1 + 5x + 5x^2 + x^3)i(M_{n-1}) - x^2(1 + 4x + 5x^2 + x^3)i(M_{n-2}). \quad \square
\]

From Fig. 3, it is easily seen that \( M_n \) has an independent set of \( 3n \) vertices, consisting of three vertices from each hexagon. Since a hexagon can give no more than three vertices to an independent set, we have the following result.

**Theorem 4.6.** The independence number of \( M_n \), \( n \geq 1 \), is \( \alpha(M_n) = 3n \). \( \square \)

The next result can also be observed from Fig. 3, or it can be obtained by recursion of Theorem 4.5.

**Theorem 4.7.** For \( n \geq 3 \), \( M_n \) has only \( \Psi_{\alpha(M_n)}(M_n) = 1 \) maximum independent set. \( \square \)

**Theorem 4.8.** The chain \( M_n \), \( n \geq 3 \), has a total of

\[
\Psi(M_n) = \frac{2}{5} + \frac{8}{5} \cdot 11^n
\]

independent sets. \( \square \)

We now proceed to the para-chain, \( L_n \).

**Theorem 4.9.** The independence polynomial of \( L_n \), \( n \geq 3 \), is given by

\[
i(L_n) = (1 + 5x + 4x^2)i(L_{n-1}) + x^3(2 + 4x + x^2)i(L_{n-2}). \quad \square
\]

**Theorem 4.10.** The independence number of \( L_n \), \( n \geq 1 \), is \( \alpha(L_n) = \frac{5n+1}{2} \) if \( n \) is odd, and \( \alpha(L_n) = \frac{5n+2}{2} \) if \( n \) is even. \( \square \)
Theorem 4.11. \( L_n, n \geq 3, \) has 1 maximum independent set when \( n \) is even and 2\( n \) maximum independent sets when \( n \) is odd. \( \square \)

Theorem 4.12. The chain \( L_n, n \geq 3, \) has a total of
\[
\Psi(L_n) = \left( 1 + \frac{1}{\sqrt{2}} \right) (5 + 4\sqrt{2})^n + \left( 1 - \frac{1}{\sqrt{2}} \right) (5 - 4\sqrt{2})^n
\]
independent sets. \( \square \)

As in the case of matchings, we see that the number of independent sets in a para-chain is sandwiched between the number of independent sets in an ortho- and a meta-chain, but with the opposite inequalities.
\[
\Psi(O_n) \leq \Psi(L_n) \leq \Psi(M_n).
\]

Again, it turns out that the ortho- and meta-chains provide the lower and upper bound for all chains in \( C_n, \) but the proof is a bit more complicated. We will need three more auxiliary graphs and a Lemma.

Lemma 4.13. Let \( G \) be a graph and \( \Psi_u(G) \) the number of independent sets in \( G \) that contain the vertex \( u. \) Then \( \Psi_u(G) \leq \Psi(G - u). \)

Proof. Let \( I \subseteq V(G) \) be an independent set in \( G \) that contains \( u. \) Then \( I - \{u\} \) is an independent set in \( G - u. \) Hence, to each independent set in \( G \) that contains \( u \) correspond an independent set in \( G - u. \) Since the correspondence is obviously injective, the claim of the lemma follows.

The three additional auxiliary graphs are shown in Fig. 9.

Now we can state and prove the result about the extremal chains with regard to the total number of independent sets.

Theorem 4.14. Let \( G_n \) be a chain hexagonal cactus of length \( n. \) Then
\[
\Psi(O_n) \leq \Psi(G_n) \leq \Psi(M_n).
\]

Proof. As in the proof of Theorem 3.23, take any two chains \( S_1 \) and \( S_2 \) whose lengths add to \( n - 1 \) and insert a hexagon between them connecting them into a chain of length \( n. \) Denote the resulting chain by \( S_1OS_2, S_1MS_2, \) or \( S_1PS_2 \) if the cut-vertices of the inserted hexagon are in ortho-, meta-, or para-position, respectively. By applying the reduction procedure to those cut-vertices one obtains the following expressions.
\[
\Psi(S_1OS_2) = \Psi(S_1)\Psi(S_2) + \Psi(S_1 - u)\Psi(S_2 - v)
\]
\[
= \Psi(S_1)[\Psi(S_1 + \Psi(S_2) + 5\Psi(S_2 - v)] + \Psi(S_1 - u)[5\Psi(S_2) + 8\Psi(S_2 - v)]
\]
\[
= 5[\Psi(S_1)\Psi(S_2 - v) + \Psi(S_1 - u)\Psi(S_2)] + 8\Psi(S_1 - u)\Psi(S_2 - v).
\]

Here we have used \( \Psi(P_3) = 5 \) and \( \Psi(P_4) = 8. \) Similarly we obtain
\[
\Psi(S_1MS_2) = \Psi(S_1)\Psi(S_2) + \Psi(S_1 - u)\Psi(S_2 - v)
\]
\[
= \Psi(S_1)[2\Psi(S_2) + 3\Psi(S_2 - v)] + \Psi(S_1 - u)[3\Psi(S_2) + 10\Psi(S_2 - v)]
\]
\[
= 2\Psi(S_1)\Psi(S_2) + 3[\Psi(S_1)\Psi(S_2 - v) + \Psi(S_1 - u)\Psi(S_2)] + 10\Psi(S_1 - u)\Psi(S_2 - v).
\]

Finally,
\[
\Psi(S_1PS_2) = \Psi(S_1)\Psi(S_2) + \Psi(S_1 - u)\Psi(S_2 - v)
\]
\[
= \Psi(S_1)[\Psi(S_2) + 4\Psi(S_2 - v)] + \Psi(S_1 - u)[4\Psi(S_2) + 9\Psi(S_2 - v)]
\]
\[
= \Psi(S_1)\Psi(S_2) + 4[\Psi(S_1)\Psi(S_2 - v) + \Psi(S_1 - u)\Psi(S_2)] + 9\Psi(S_1 - u)\Psi(S_2 - v).
\]

Now we can compute the differences:
\[
\Psi(S_1MS_2) - \Psi(S_1PS_2) = \Psi(S_1PS_2) - \Psi(S_1OS_2)
\]
\[
= \Psi(S_1)\Psi(S_2) - \Psi(S_1 - u)\Psi(S_2) - \Psi(S_1)\Psi(S_2 - v) + \Psi(S_1 - u)\Psi(S_2 - v)
\]
\[
= [\Psi(S_1 - u) - \Psi(S_1)]\Psi(S_2 - v) - \Psi(S_2).
\]
The terms in square brackets are nonnegative by Lemma 4.13 and hence
\[ \Psi(S_1O_2S_2) \leq \Psi(S_1P_2S_2) \leq \Psi(S_1M_2S_2). \]

Now the claim of theorem follows by the same reasoning as in the matching case. \( \square \)

Again, the lower and upper bound on \( \Psi(G_n) \) are sharp.

As in the previous section, we proceed by finding the bivariate generating functions for the two-indexed sequences \( (\Psi_k(G_n))_{n \geq 0, k \geq 0} \), where \( G = O, M, \) and \( L \). We denote them by \( OI(x, y) \), \( MI(x, y) \), and \( LI(x, y) \).

Now the three recurrences for the independence polynomials can be written as
\[
\begin{align*}
O_i &= i_0(x, y) + i_1(x, y) + i_2(x, y) = xg_1(y)[G(x, y) - i_0(x, y)] + x^2g_2(y)GI(x, y).
\end{align*}
\]

The resulting linear equation in the unknown function \( GI(x, y) \) is then solved to obtain the explicit formula.
\[
GI(x, y) = \frac{i_0(x, y)[1 - xg_1(y)] + i_1(x, y)}{1 - xg_1(y) - x^2g_2(y)}.
\]

As in the matching case, the particular expressions follow by substituting the pairs \((O, o), (M, m), \) and \((L, l)\) for \((G, g)\) in the above formula.

**Theorem 4.15.**

\[
\begin{align*}
OI(x, y) &= \frac{1 + y + xy(1 + 2y - y^2)}{1 - x(1 + 4y + 3y^2) - x^2y(1 + 3y + y^2)^2}; \\
MI(x, y) &= \frac{1 + y - xy^2(1 + 4y + y^2)}{1 - x(1 + 5y + 5y^2 + y^3) + x^2y^2(1 + 4y + 5y^2 + y^3)}; \\
LI(x, y) &= \frac{1 + y - 2xy^2}{1 - x(1 + 5y + 4y^2) - x^2y^3(2 + 4y + y^2)}. \quad \square
\end{align*}
\]

The ordinary generating functions for the total number of independent sets in our chains now follow by setting \( y = 1 \) in the above formulae.
Corollary 4.16.

\[ OI(x) = \frac{2 + 2x}{1 - 8x - 25x^2}; \]
\[ MI(x) = \frac{2 - 6x}{1 - 12x + 11x^2}; \]
\[ LI(x) = \frac{2 - 2x}{1 - 10x - 7x^2}. \]

\[ \square \]

By performing similar calculations to the ones needed for establishing Theorem 3.26 we obtain the asymptotic behavior of the expected size of a random independent set in the considered chains.

Theorem 4.17. Let \( j(G_n) \) denote the expected number of vertices in an independent set of \( G_n \). Then

\[ j(O_n) \sim \left( \frac{3}{2} - \frac{1}{\sqrt{41}} \right) n \approx 1.34383n; \]
\[ j(M_n) \sim \frac{159}{110} n \approx 1.44545n; \]
\[ j(L_n) \sim \frac{1}{28} (54 - 11\sqrt{2}) n \approx 1.37299n. \]

\[ \square \]

5. Miscellaneous

In this section we present some results concerning the independent sets and independence polynomials of a family of hexagonal cacti considered by Farrell, complementing the results on matchings in such cacti from [4]. Then we show that such graphs, the star hexagonal cacti, can be also viewed as a degenerate case of chains. The section ends by proposing a generalized setting that encompasses in a natural way both the cacti considered here and in a series of works by Farrell [5–7].

A star hexagonal cactus \( S_n \) is obtained by taking \( n \) copies of \( C_6 \) and splicing them all together in a single vertex \( u \) in a way shown in Fig. 10.

By decomposing \( S_n \) with respect to the cut-vertex \( u \) common to all hexagons we obtain an explicit formula for its independence polynomial.

Theorem 5.1. The independence polynomial of \( S_n, n \geq 0 \), is

\[ i(S_n) = (1 + 5x + 6x^2 + x^3)^n + x(1 + 3x + x^2)^n. \]

\[ \square \]

From this, we immediately get the following corollaries.

Corollary 5.2. The independence number of \( S_n, n \geq 1 \), is \( \alpha(S_n) = 3n. \)

Corollary 5.3. The star \( S_n, n \geq 0 \), has only \( \Psi_{\alpha(S_n)}(S_n) = 1 \) maximum independent set when \( n \) is even and \( \Psi_{\alpha(S_n)}(S_n) = 2n \) maximum independent sets when \( n \) is odd.

\[ \square \]

Corollary 5.4. The star \( S_n, n \geq 0 \), has \( \Psi(S_n) = 13^n + 5^n \) independent sets.

The numbers 13 and 5 in Corollary 5.4 come from the fact that the numbers of independent sets in paths are the Fibonacci numbers. Hence, it would be easy to extend the results concerning \( S_n \) to a wider class of star cacti made of \( n \) copies of \( C_m \) spliced together in a single vertex \( u \).

The star hexagonal cacti were given a separate treatment here since the results follow much easier than for the chain cacti of the previous two sections. However, star hexagonal cacti could be easily made to fit into the class of chains by...
allowing the two cut-vertices of all internal hexagons to coincide. Hence, a star hexagonal cactus is a chain hexagonal cactus whose cut-vertices are separated by a path of length 0. By abandoning our chemically motivated nomenclature and indexing the chains by an integer parameter specifying the distance between the cut-vertices, we obtain a uniform notation for all hexagonal cacti considered here: By \( C_n(6, k) \) we denote a chain hexagonal cactus whose cut-vertices are at the distance \( k \). Hence, \( C_n(6, 0) = S_n \), \( C_n(6, 1) = O_n \), \( C_n(6, 2) = M_n \), and \( C_n(6, 3) = L_n \).

The last step towards the general setting referred to at the beginning of this section now consists of dispensing with hexagons and considering instead the chain cacti \( C_n(m, k) \) made of \( n \) copies of \( m \)-gons whose cut-vertices are at the distance \( k \). Here we assume that \( k \leq \left\lfloor \frac{m}{2} \right\rfloor \).

It would be interesting to derive results for general \((m, k)\)-chains analogous to those presented here and in Refs. [5, 7, 6]. Some of those results could have neat expressions in terms of Fibonacci and Lucas numbers, and could turn out to be a source of interesting Fibonacci related identities and their proofs.

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