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The Permanental Polynomials of Certain Graphs^{*}

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Abstract

In this paper we consider the computation of permanental polynomials of some graphs. By orienting even cycles oddly, explicit expressions for the permanental polynomials of some basic graphs including a path and a cycle are obtained in terms of roots. For hexagonal systems, based on reduction procedures, the permanental polynomials of hexagonal chains and a type of pericondensed hexagonal system are deduced from product of matrices of order 5. Meanwhile, the permanental polynomial of a general polygonal chain is also derived.

1 Introduction

This paper deals with the computation of permanental polynomials of some graphs. Suppose G = (V, E) is a finite and simple graph on n vertices. The permanental polynomial of G is defined as

$$\pi(G, x) = per(xI - A(G)) = \sum_{k=0}^{n} b_k x^{n-k},$$

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where I is the identity matrix of order n, A(G) is the adjacency matrix of G and the permanent $per(\widetilde{A})$ of a matrix $\widetilde{A} = (a_{ij})_{n \times n}$ is given as [18]

$$\operatorname{per}(\widetilde{A}) = \sum_{\sigma \in \Lambda_n} \prod_{i=1}^n a_{i\sigma(i)}$$

with Λ_n denoting the set of all the permutations of $\{1, 2, \dots, n\}$. For the permanental polynomial of a bipartite graph with an even number of vertices, one has $b_{2i+1} = 0$ and $b_{2i} = \sum_{H} \operatorname{per}(A(H)) = \sum_{H} M^2(H)$, where the summation extends over all induced subgraphs H with 2i vertices of G and M(H) is the number of perfect matchings of H [4, 17, 24]. Obviously, the value of the last coefficient is the square of the number of perfect matchings of G.

As is well known, computing the permanent of a matrix is a #P-complete problem [23]. So computing the permanental polynomial of a graph is difficult. In the literature, Merris et al. [17] proved that the coefficient of the permanental polynomial satisfies that

$$(-1)^{i}b_{i} = \sum_{H} 2^{k(H)},\tag{1}$$

where the sum ranges over all subgraphs H on i vertices whose components are single edges or cycles, and k(H) is the number of cycles. Based on this result, similarly to the technique of computing the characteristic polynomial of a graph in terms of subgraphs [20], Borowiecki and Jóźwiak [5] studied the relationship between the permanental polynomial of a dimultigraph (resp. a muligraph) and certain subgraphs. Recently, Belardo et al. extended these results to characteristic and permanental polynomials of weighted graphs and matrices in [2] and [3], respectively. For the permanental polynomials of chemical graphs, in [7] by generating all the coefficients of the permanental polynomial of fullerenes up through C_{36} , the zeros of these polynomials were dealt with by Cash. It was shown that of the independent zeros, ten are nearly constant within an isomer series of constant N, while the remaining (N/2 - 10) zeros vary greatly with structure. This indicates that the permanental polynomial encodes a variety of structure information. To determine the coefficients of a permanental polynomial, Gutman and Cash [13] considered the relation between the permanental polynomial and the characteristic polynomial of hexagonal systems and fullerenes, and established a formula on a part of coefficients of these two polynomials. Later by focusing on the orientation graph of a bipartite graph containing no even subdivision of $K_{2,3}$, Yan and Zhang [25] proved that the permanental polynomial of such a bipartite graph can be computed by the characteristic polynomial of a skew adjacency matrix. Furthermore, in [26] we obtained that only the permanental polynomials of bipartite graphs containing no even subdivision of $K_{2,3}$ can be computed in this way, and a characterization of this kind of graphs is given. For more studies on the permanental polynomials in chemistry and mathematics, see [4, 6, 8, 9, 14, 15, 16, 22] and related references.

To overcome the difficulty of computing permanents, it is reasonable to convert the computation of permanental polynomials to the computation of matrices and determinants. Motivated by this idea, in this work, we first pay attentions to some basic graphs, such as a path and a cycle. Instead of computing the permanental polynomials directly, we assign orientations to graphs, and compute the characteristic polynomials of the corresponding skew adjacency matrices. Then we turn to some chemical graphs including some types of hexagonal systems, which is a natural graph representation of benzenoid hydrocarbons. The corresponding polynomials are produced by the product of matrices.

The organization of this paper is as follows. In Section 2 we give explicit expressions of the permanental polynomials of a path, an even cycle, an even *n*-sun graph and one subgraph of an *n*-sun graph. Under these formulas, the roots of the corresponding polynomials follow immediately. Applying the reduction procedures, in Section 3 we obtain the permanental polynomials of a general polygonal chain G_n and a kind of pericondensed system H_n by multiplications of matrices. According to this, the permanental polynomial of a hexagonal chain is provided. As special cases, explicit formulas on the permanental polynomials of a linear chain, zigzag chain and helix chain are obtained.

2 Explicit expressions for the permanental polynomials of some basic graphs

In this section, we will compute the permanental polynomials of a path, an even cycle, an even *n*-sun graph and the subgraph of an *n*-sun graph. Throughout this paper we denote by P_n a path on *n* vertices, C_n a cycle on *n* vertices and S_n an *n*-sun graph. An *n*-sun graph is the graph on 2n vertices obtained by attaching a pendant edge to each vertex of a cycle C_n [1]. Particularly, we call C_n (resp. S_n) an even cycle (resp. even *n*-sun graph) if *n* is even.

Using the results of matching polynomials on paths and cycles [11] and formula (1), it is easy to check that the permanental polynomials of a path and a cycle given as

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

and

$$\pi(C_n, x) = \sum_{k=0}^{\left\lceil \frac{n}{2} \right\rceil - 1} \frac{n}{n-k} \binom{n-k}{k} x^{n-2k} + b(C_n),$$
(3)

where $b(C_n) = 4$ if n is even, and $b(C_n) = -2$ if n is odd. Here by computing the characteristic polynomial of the skew adjacency matrix of an orientation graph, we will derive the explicit expressions of the permanental polynomials of a path and an even cycle in terms of roots. We begin by introducing a few definitions and lemmas.

A graph G is an *even subdivision* of a graph H if G is obtained from H by replacing the edges of H by internally disjoint paths, each containing an even number of vertices and at least one edge.

For a graph G, an even cycle C is said to be *nice* if G - V(C) has a perfect matching. Let G^e be an orientation of G. An even cycle is said to be *oddly oriented* in G^e if the number of edges pointing in each direction is odd. Under an orientation G^e , the *skew adjacency matrix* $A(G^e) = (a'_{ij})_{n \times n}$ is defined as

$$a'_{ij} = \begin{cases} 1 & \text{if } (v_i, v_j) \text{ is a directed edge from } v_i \text{ to } v_j, \\ -1 & \text{if } (v_j, v_i) \text{ is a directed edge from } v_j \text{ to } v_i, \\ 0 & \text{if no edges connect } v_i \text{ and } v_j. \end{cases}$$

Theorem 2.1. [24] Let G be a bipartite graph containing no even subdivision of $K_{2,3}$. Then there exists an orientation G^e of G such that

$$\pi(G, x) = \det(xI - A(G^e)).$$

Moreover, each cycle of G^e is oddly oriented.



Figure 1: Orientations P_n^e and C_n^e of P_n and C_n , respectively.

Lemma 2.2. [21] Define $n \times n$ matrices U_n and U_n^{-1} with components $1 \le k, k' \le n$:

$$(U_n)_{k,k'} = \sqrt{\frac{2}{n+1}} i^k \sin(\frac{kk'\pi}{n+1}), \qquad (U_n^{-1})_{k,k'} = \sqrt{\frac{2}{n+1}} (-i)^{k'} \sin(\frac{kk'\pi}{n+1}).$$
Let Q_n be the $n \times n$ matrix $\begin{pmatrix} 0 & 1 & & \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \\ & & & & -1 & 0 \end{pmatrix}$. Then the matrix $\widetilde{Q}_n = U_n^{-1} Q_n U_n$

has the element $(\widetilde{Q}_n)_{k,k'} = \delta_{k,k'} \cdot 2i \cos \frac{k\pi}{n+1}$ for $1 \le k, k' \le n$ and $i^2 = -1$.

Theorem 2.3. The permanental polynomial of a path P_n is

$$\pi(P_n, x) = \prod_{t=1}^n (x + 2i\cos\frac{t\pi}{n+1}).$$
(4)

Proof. By Theorem 2.1 and according to the orientation P_n^e of P_n shown in Figure 1(a), $\pi(P_n, x) = \det(xI - A(P_n^e)) = \det(xI_n + Q_n)$ holds. Following the result of Lemma 2.2, conjugate the matrix $(xI_n + Q_n)$ by U_n to obtain $U_n^{-1}(xI_n + Q_n)U_n = \operatorname{diag}(x+2i\cos\frac{\pi}{n+1}, x+2i\cos\frac{2\pi}{n+1}, \cdots, x+2i\cos\frac{n\pi}{n+1})$. So $\pi(P_n, x) = \prod_{t=1}^n (x+2i\cos\frac{t\pi}{n+1})$ is got. \Box

Remark 2.4. Combining the formula for the characteristic polynomial of a path P_n [20]

$$\phi(P_n,x) = \prod_{t=1}^n (x-2\cos\frac{t\pi}{n+1}) = \prod_{t=1}^n (x+2\cos\frac{t\pi}{n+1})$$

and the theorem presented in [4], the same result as (4) can be obtained.

Lemma 2.5. [25] Define $n \times n$ matrices V_n and V_n^{-1} with components $1 \le t, j \le n$:

$$(V_n)_{t,j} = \sqrt{\frac{1}{n}} e^{i\frac{(2j-1)t\pi}{n}}, \qquad (V_n^{-1})_{t,j} = \sqrt{\frac{1}{n}} e^{-i\frac{(2t-1)j\pi}{n}}.$$
Let Y_n be the $n \times n$ matrix $\begin{pmatrix} 0 & 1 & & 1 \\ -1 & 0 & 1 & & \\ & -1 & 0 & 1 & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ -1 & & & -1 & 0 \end{pmatrix}$. Then the matrix $\widetilde{Y}_n = V_n^{-1} Y_n V_n$
has the element $(\widetilde{Y})_{k,j} = \delta$. Sign $(2t-1)\pi$ for $1 \le t$ is $\le n$ and $i^2 = -1$.

has the element $(\widetilde{Y}_n)_{t,j} = \delta_{t,j} \cdot 2i \sin \frac{(2t-1)\pi}{n}$ for $1 \le t, j \le n$ and $i^2 = -1$.

Theorem 2.6. The permanental polynomial of an even cycle C_n is

$$\pi(C_n, x) = \prod_{t=1}^n (x + 2i\sin\frac{(2t-1)\pi}{n}).$$
(5)

Proof. An orientation C_n^e of C_n referring to Figure 1(b) is oddly oriented when n is even. The matrix $xI - A(C_n^e)$ takes the form R_n , where

$$R_n = \begin{pmatrix} x & 1 & & & 1 \\ -1 & x & 1 & & \\ & -1 & x & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & x & 1 \\ -1 & & & & -1 & x \end{pmatrix}.$$
 (6)

Conjugating $R_n = xI_n + Y_n$ by V_n , we obtain that $\det(R_n) = \det(V_n^{-1}R_nV_n) = \det(\operatorname{diag}(x+2i\sin\frac{\pi}{n}, x+2i\sin\frac{3\pi}{n}, \cdots, x+2i\sin\frac{(2n-1)\pi}{n}))$. So $\pi(C_n, x) = \prod_{t=1}^n (x+2i\sin\frac{(2t-1)\pi}{n})$ holds.

Remark 2.7. For n = 4k + 2, using the characteristic polynomial of a cycle C_n [20]

$$\phi(C_n, x) = \prod_{t=1}^n (x - 2\cos\frac{2t\pi}{n}) = \prod_{t=1}^n (x + 2\sin\frac{(3n - 4t)\pi}{2n})$$

and the theorem presented in [4], the same result as (5) can be also obtained. For other values of n, $\pi(C_n, x)$ cannot be get in this way.

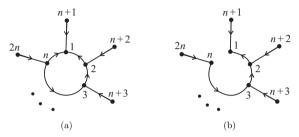


Figure 2: The *n*-sun graph S_n^e and the graph $S_n^e - \vec{n1}$.

Theorem 2.8. The permanental polynomial of an even n-sun graph S_n is

$$\pi(S_n, x) = \prod_{t=1}^n (x^2 + x^2 i \sin \frac{(2t-1)\pi}{n} + 1).$$
(7)

Proof. Figure 2(a) gives an orientation S_n^e of an even *n*-sun graph S_n with the only cycle being oddly oriented. Following the labeling of vertices and the orientation graph S_n^e in Figure 2(a), the matrix $xI - A(S_n^e)$ takes the form $\begin{pmatrix} R_n & I_n \\ -I_n & xI_n \end{pmatrix}$. Since $R_n(-I_n) = (-I_n)R_n$, it follows that $\det(xI - A(S_n^e)) = \det(R_n(xI_n) - (-I_n)I_n) = \det(D_n)$, where the matrix R_n takes the form shown in (6) and

$$D_n = \begin{pmatrix} x^2 + 1 & x & & & x \\ -x & x^2 + 1 & x & & & \\ & -x & x^2 + 1 & x & & \\ & & \ddots & \ddots & \ddots & \\ & & & -x & x^2 + 1 & x \\ -x & & & -x & x^2 + 1 \end{pmatrix}$$

By Lemma 2.5, conjugate $D_n = (x^2 + 1)I_n + xY_n$ by V_n to obtain

$$V_n^{-1}D_nV_n = \operatorname{diag}(x^2 + 1 + x^2i\sin\frac{\pi}{n}, x^2 + 1 + x^2i\sin\frac{3\pi}{n}, \cdots, x^2 + 1 + x^2i\sin\frac{(2n-1)\pi}{n}).$$

Then according to Theorem 2.1, $\pi(S_n, x) = \det(xI - A(S_n^e)) = \det(D_n) = \prod_{t=1}^n (x^2 + 1 + 2xi \sin \frac{(2t-1)\pi}{n})$ is obtained with $i = \sqrt{-1}$.

For an edge e of a graph G, G-e is the graph resulting from the remove of e. Choosing an edge e belonging to the cycle of S_n , the resulting graph $S_n - e$ takes the form shown in Figure 2(b). By Lemma 2.2 and the discussion in the proof of Theorem 2.8, we have

Theorem 2.9. Let e be an edge belonging to the cycle of an n-sun graph. Then

$$\pi(S_n - e, x) = \prod_{t=1}^n (x^2 + x^{2t} \cos \frac{t\pi}{n+1} + 1).$$
(8)

Remark 2.10. By the equations $x^2 + x2i\sin\frac{(2t-1)\pi}{n} + 1 = 0$ and $x^2 + x2i\cos\frac{t\pi}{n+1} + 1 = 0$, the roots of $\pi(S_n, x)$ and $\pi(S_n - e, x)$ can be obtained, respectively.

3 Recursive expressions for the permanental polynomials of some kinds of graphs

3.1 Identities for permanental polynomials

In [5] Borowiecki and Jóźwiak proved an identity on the permanental polynomial, which is described in Theorem 3.1.

Theorem 3.1. [5] Let e = (u, v) be an edge of a graph G and $\mathscr{C}_e(G)$ the set of cycles containing e. Then

$$\pi(G, x) = \pi(G - e, x) + \pi(G - u - v, x) + 2\sum_{C \in \mathscr{C}_e(G)} (-1)^{|V(C)|} \pi(G - V(C), x).$$
(9)

Formula (9) provides a general connection between the permanental polynomial of a graph and the permanental polynomials of its subgraphs. With the help of Theorems 2.3 and 2.6, a different expression comparing with (3) appears immediately.

Theorem 3.2. The permanental polynomial of a cycle C_n on n vertices is

$$\pi(C_n, x) = \begin{cases} \prod_{t=1}^n (x + 2i \sin \frac{(2t-1)\pi}{n}), & \text{if } n \text{ is even,} \\ \prod_{t=1}^n (x + 2i \cos \frac{t\pi}{n+1}) + \prod_{t=1}^{n-2} (x + 2i \cos \frac{t\pi}{n-1}) - 2, & \text{if } n \text{ is odd.} \end{cases}$$

Let u_1, v_1 (resp. u_2, v_2) be a pair of vertices of a graph G_1 (resp. G_2). Then the bridge graph $G_1 \diamond G_2$ of G_1 and G_2 through e_1 and e_2 is the graph obtained by joining edges e_1 between u_1 and u_2 and e_2 between v_1 and v_2 . See Figure 3 for an illustration.

Corollary 3.3. For the bridge graph $G = G_1 \diamond G_2$ through $e_1 = (u_1, u_2)$ and $e_2 = (v_1, v_2)$, the following result holds.

$$\begin{aligned} \pi(G,x) = &\pi(G_1,x)\pi(G_2,x) + \pi(G_1 - u_1,x)\pi(G_2 - u_2,x) + \pi(G_1 - v_1,x)\pi(G_2 - v_2,x) \\ &+ \pi(G_1 - u_1 - v_1,x)\pi(G_2 - u_2 - v_2,x) + 2\sum_{C \in \mathscr{C}_{e_1}(G)} (-1)^{|V(C)|} \pi(G - V(C),x). \end{aligned}$$

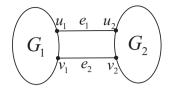


Figure 3: The bridge graph $G_1 \diamond G_2$.

Proof. Using Theorem 3.1, we obtain that

$$\begin{aligned} \pi(G,x) &= \pi(G-e_1,x) + \pi(G-u_1-u_2,x) + 2\sum_{C \in \mathscr{C}_{e_1}(G)} (-1)^{|V(C)|} \pi(G-V(C),x) \\ &= \pi(G-e_1-e_2,x) + \pi(G-e_1-v_1-v_2,x) + \pi(G-u_1-u_2-e_2,x) \\ &+ \pi(G-u_1-u_2-v_1-v_2,x) + 2\sum_{C \in \mathscr{C}_{e_1}(G)} (-1)^{|V(C)|} \pi(G-V(C),x) \\ &= \pi(G_1,x) \pi(G_2,x) + \pi(G_1-v_1,x) \pi(G_2-v_2,x) + \pi(G_1-u_1,x) \pi(G_2-u_2,x) \\ &+ \pi(G_1-u_1-v_1,x) \pi(G_2-u_2-v_2,x) + 2\sum_{C \in \mathscr{C}_{e_1}(G)} (-1)^{|V(C)|} \pi(G-V(C),x). \end{aligned}$$

3.2 The permanental polynomial of a general polygonal chain

Inspired by the idea given in [19], we now deduce the permanental polynomial of a general polygonal chain by a recursive procedure. To derive our main results, we give some definitions and notations.

A general polygonal chain is a polygonal system satisfying (a) each of the two end polygons has exactly one adjacent polygon and any other polygon has two adjacent polygons; (b) the intersection of any two adjacent polygons is a path whose internal vertices are of degree two; (c) no three polygons have a vertex in common.

For simple, a general polygonal chain with n polygons (each polygon has at least six vertices) is denoted by G_n . For the *i*-th polygon in G_n , $i \in \{1, 2, 3, \dots, n\}$, two root vertices u_i and v_i are prescribed, which are joined by a path P_{l_i} of internal vertices of degree two. In the i + 1-th polygon, the edge with u_i as an endvertex is marked by e_{i+1} . The path in the *i*-th polygon joining u'_i (the neighbor of u_{i-1}) and v'_i (the neighbor of v_{i-1}) is denoted by P_{r_i} , and the path connecting u'_i (resp. v'_i) and u_i (resp. v_i) is denoted by P_{s_i} (resp. P_{t_i}). See Figure 4. In addition, we denote by $\mathscr{C}_{V(H)}(G)$ the set of cycles of G containing the vertices of the subgraph H and $\mathscr{C}_e(G)$ the set of cycles in G including the edge e.

Theorem 3.4. For a general polygonal chain G_{n+1} , let $\alpha(G_n)$ be the column vector $(\pi(G_n, x), \pi(G_n - u_n, x), \pi(G_n - v_n, x), \pi(G_n - V(P_{l_n}), x), \sum_{C \in \mathscr{C}_{V(P_1-})(G_n)} (-1)^{|V(C)|} \pi(G_n - U(P_{l_n}), x)$

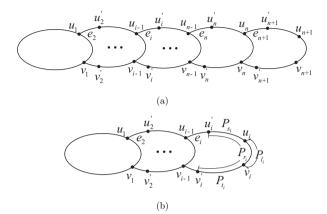


Figure 4: Polygonal chains G_{n+1} and G_i .

 $V(C), x))^{\mathrm{T}}$. Then the permanental polynomial of G_{n+1} satisfies the recurrence

$$\alpha(G_{n+1}) = A_{n+1} \cdot \alpha(G_n),\tag{11}$$

$$\begin{split} & \text{where } A_n \text{ is } a \ 5 \times 5 \ \text{matrix whose } i\text{-th row vector is } l_n^i \text{ for } 1 \le i \le 5. \ \text{Explicitly}, \\ & l_n^1 = (\pi(P_{r_n}, x), \pi(P_{r_n-1}, x), \pi(P_{r_n-1}, x), \pi(P_{r_n-2}, x)\pi(P_{l_{n-1}-2}, x) + 2(-1)^{r_n+l_{n-1}}, \\ & 2(-1)^{r_n+l_{n-1}}\pi(P_{l_{n-1}-2}, x)), \\ & l_n^2 = (\pi(P_{s_n-1}, x)\pi(P_{t_n}, x), \pi(P_{s_n-2}, x)\pi(P_{t_n}, x), \pi(P_{s_n-1}, x)\pi(P_{t_{n-1}}, x), \pi(P_{s_{n-2}}, x)\pi(P_{t_{n-1}}, x) \\ & \pi(P_{l_{n-1}-2}, x), 0), \\ & l_n^3 = (\pi(P_{s_n}, x)\pi(P_{t_{n-1}}, x), \pi(P_{s_{n-1}}, x)\pi(P_{t_{n-1}}, x), \pi(P_{s_n}, x)\pi(P_{t_{n-2}}, x), \pi(P_{t_{n-2}}, x)\pi(P_{t_{n-2}}, x)) \\ & \pi(P_{l_{n-1}-2}, x), 0), \\ & l_n^4 = (\pi(P_{s_n-1}, x)\pi(P_{t_{n-1}}, x), \pi(P_{s_{n-2}}, x)\pi(P_{t_{n-1}}, x), \pi(P_{s_{n-1}}, x)\pi(P_{t_{n-2}}, x), \pi(P_{s_{n-2}}, x)) \\ & \pi(P_{t_{n-2}}, x)\pi(P_{t_{n-1}-2}, x), 0), \ and \\ & l_n^5 = (0, 0, 0, (-1)^{r_n+l_{n-1}}, (-1)^{r_n+l_{n-1}}\pi(P_{l_{n-1}-2}, x)). \\ & Consequently, \end{split}$$

$$\alpha(G_n) = A_n \cdot A_{n-1} \cdots A_1 \cdot \alpha(G_0), \tag{12}$$

where $\alpha(G_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

Proof. We can see that the general polygonal chain G_{n+1} is the bridge graph of G_n and the path $P_{r_{n+1}}$. Then by Corollary 3.3,

$$\pi(G_{n+1}, x) = \pi(G_n, x)\pi(P_{r_{n+1}}, x) + \pi(G_n - u_n, x)\pi(P_{r_{n+1}-1}, x) + \pi(G_n - v_n, x)\pi(P_{r_{n+1}-1}, x) + \pi(G_n - V_{P_{l_n}}, x)\pi(P_{r_{n+1}-2}, x)\pi(P_{l_n-2}, x) + 2\sum_{C \in \mathscr{C}_{e_{n+1}}(G_{n+1})} (-1)^{|V(C)|}\pi(G_{n+1} - V(C), x).$$
(13)

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As the internal vertices of $P_{r_{n+1}}$ are of degree two, a cycle containing e_{n+1} in G_{n+1} must pass through the path $P_{r_{n+1}}$. So it follows that

$$\sum_{C \in \mathscr{C}_{e_{n+1}}(G_{n+1})} (-1)^{|V(C)|} \pi(G_{n+1} - V(C), x)$$

= $(-1)^{r_{n+1}+l_n} \pi(G_n - V_{P_{l_n}}, x)$
+ $(-1)^{r_{n+1}+l_n} \pi(P_{l_n-2}, x) \sum_{C \in \mathscr{C}_{V(P_{l_n})}(G_n)} (-1)^{|V(C)|} \pi(G_n - V(C), x).$ (14)

From (13) and (14), we have

$$\begin{aligned} \pi(G_{n+1},x) &= \pi(G_n,x)\pi(P_{r_{n+1}},x) + \pi(G_n - u_n,x)\pi(P_{r_{n+1}-1},x) + \pi(G_n - v_n,x)\pi(P_{r_{n+1}-1},x) \\ &+ \pi(G_n - V_{P_{l_n}},x)[\pi(P_{r_{n+1}-2},x)\pi(P_{l_{n-2}},x) + 2(-1)^{r_{n+1}+l_n}] \\ &+ 2(-1)^{r_{n+1}+l_n}\pi(P_{l_{n-2}},x)\sum_{C\in\mathscr{C}_V(P_{l_n})(G_n)}(-1)^{|V(C)|}\pi(G_n - V(C),x). \end{aligned}$$

Thus, $\pi(G_{n+1}, x) = l_n^1 \cdot \alpha(G_n).$

Similarly, we also have $\pi(G_{n+1} - u_{n+1}, x) = l_n^2 \cdot \alpha(G_n), \ \pi(G_{n+1} - v_{n+1}, x) = l_n^3 \cdot \alpha(G_n)$ and $\pi(G_{n+1} - u_{n+1} - v_{n+1}, x) = l_n^4 \cdot \alpha(G_n)$.

Since

$$\sum_{\substack{C \in \mathscr{C}_{V(P_{l_{n+1}})}(G_{n+1})}} (-1)^{|V(C)|} \pi(G_{n+1} - V(C), x)$$

= $(-1)^{r_{n+1}+l_n} \pi(G_n - V(P_{l_n}), x)$
+ $(-1)^{r_{n+1}+l_n} \pi(P_{l_n-2}, x) \sum_{\substack{C \in \mathscr{C}_{V(P_{l_n})}(G_n)}} (-1)^{|V(C)|} \pi(G_n - V(C), x)$

we get that $\sum_{C \in \mathscr{C}_{V(P_{l_{n+1}})}(G_{n+1})} (-1)^{|V(C)|} \pi(G_{n+1} - V(C), x) = l_n^5 \cdot \alpha_n.$

By now

$$\alpha(G_{n+1}) = A_{n+1} \cdot \alpha(G_n)$$

is established.

For a general polygonal chain, the starting step G_0 is an edge (u_0, v_0) . Given this, we obtain that $\alpha(G_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$. So equation (12) follows.

Remark 3.5. It needs to point out that $\pi(P_0, x) = 1$ and $\pi(P_{-1}, x) = 0$.

As a special case of a general polygonal chain, a *polygonal chain* is a connected series of polygons arranged in a linear form satisfying the intersection of two adjacent polygons is an edge and no three polygons have a vertex in common. For a polygonal chain with at least six vertices on each polygon (denoted by G'_n), we have the following corollary. **Corollary 3.6.** For a polygonal chain G'_{n+1} , let $\alpha(G'_n)$ be the column vector $(\pi(G'_n, x), \pi(G'_n - u_n, x), \pi(G'_n - v_n, x), \pi(G'_n - u_n - v_n, x), \sum_{C \in \mathscr{C}_{(u_n, v_n)}(G'_n)} (-1)^{|V(C)|} \pi(G'_n - V(C), x))^{\mathrm{T}}$. Then

$$\alpha(G'_{n+1}) = A'_{n+1} \cdot \alpha(G'_n), \tag{15}$$

where A'_n is the matrix obtained from A_n with $l_{n-1} = 2$ and $\pi(P_{l_{n-1}-2}, x) = 1$. Furthermore,

$$\alpha(G'_n) = A'_n \cdot A'_{n-1} \cdots A'_1 \cdot \alpha(G'_0) \tag{16}$$

with $\alpha(G'_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

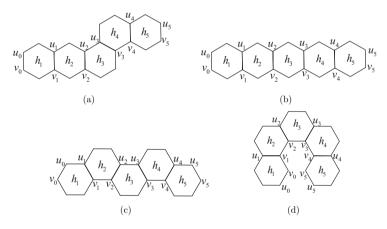


Figure 5: (a) a hexagonal chain F_5 , (b) a linear chain L_5 , (c) a zigzag chain Z_5 and (d) a helix chain T_5 .

A hexagonal system is a finite connected plane graph without cut vertices in which each interior region is surrounded by a regular hexagon of side length one. A catacondensed hexagonal system corresponds to those hexagonal system with no internal vertices, and a pericondensed hexagonal system has at least one internal vertex. A hexagonal chain is a catacondensed hexagonal system satisfying each hexagon has at most two adjacent hexagons and only each of two end hexagons has one adjacent hexagon (refer to Figure 5(a)). For more about hexagonal systems, see [12] and related references.

As an important special case, a hexagonal chain is a polygonal chain with all polygons being hexagons. Before presenting the permanental polynomial of a hexagonal chain, we introduce three types of hexagons. A hexagon h_i in a hexagonal chain is of *type-I* if the minimum length of the path joining u_{i-1} and u_i in h_i is two, and of *type-II* (resp. *type-III*) if the minimum length of the corresponding path is three (resp. one). As shown

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in Figure 5(a), the hexagons h_1 , h_2 and h_5 are of type-I, h_3 is of type-III and h_4 is of type-II. According to the matrix A'_n in Corollary 3.6, we define three matrices Γ_1 , Γ_2 and Γ_3 as follows

$$\Gamma_{1} = \begin{pmatrix} x^{4} + 3x^{2} + 1 & x^{3} + 2x & x^{3} + 2x & x^{2} + 3 & 2 \\ x^{3} + x & x^{2} + 1 & x^{2} & x & 0 \\ x^{3} + x & x^{2} & x^{2} + 1 & x & 0 \\ x^{2} & x & x & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$
$$\Gamma_{2} = \begin{pmatrix} x^{4} + 3x^{2} + 1 & x^{3} + 2x & x^{3} + 2x & x^{2} + 3 & 2 \\ x^{3} + x & x^{2} & x^{2} + 1 & x & 0 \\ x^{3} + 2x & x^{2} + 1 & 0 & 0 & 0 \\ x^{2} + 1 & x & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}$$

and

$$\Gamma_3 = \begin{pmatrix} x^4 + 3x^2 + 1 & x^3 + 2x & x^3 + 2x & x^2 + 3 & 2 \\ x^3 + 2x & 0 & x^2 + 1 & 0 & 0 \\ x^3 + x & x^2 + 1 & x^2 & x & 0 \\ x^2 + 1 & 0 & x & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \end{pmatrix}.$$

Corollary 3.7. Let F_n be a hexagonal chain with hexagons h_1, h_2, \dots, h_n . Then

$$\alpha(F_n) = W(h_n) \cdot W(h_{n-1}) \cdots W(h_1) \cdot \alpha(F_0),$$

where

$$W(h_i) = \begin{cases} \Gamma_1, & \text{if } h_i \text{ is of type-I}, \\ \Gamma_2, & \text{if } h_i \text{ is of type-II}, \\ \Gamma_3, & \text{if } h_i \text{ is of type-III}, \end{cases}$$
(17)

and $\alpha(F_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

Following Corollary 3.7, for the hexagonal chain F_5 in Figure 5(a), we have that $\alpha(F_5) = \Gamma_1 \cdot \Gamma_2 \cdot \Gamma_3 \cdot \Gamma_1^2 \cdot (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$. By a simple computation with MAPLE, it gives that

$$\begin{aligned} \pi(F_5,x) = & x^{22} + 26x^{20} + 287x^{18} + 1770x^{16} + 6757x^{14} + 16708x^{12} + 27173x^{10} + 28855x^8 + \\ & 19391x^6 + 7720x^4 + 1592x^2 + 121. \end{aligned}$$

Now we focus on some special hexagonal chains. If all the hexagons in a hexagonal chain are of type-I, then we call such a hexagonal chain a *linear chain* (see Figure 5(b)). **Corollary 3.8.** Let L_n be a linear chain with n hexagons. Then

$$\alpha(L_n) = \Gamma_1^n \cdot \alpha(L_0)$$

with $\alpha(L_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

$\pi(L_1, x) =$	$x^6 + 6x^4 + 9x^2 + 4$
$\pi(L_2, x) =$	$x^{10} + 11x^8 + 41x^6 + 65x^4 + 43x^2 + 9$
$\pi(L_3, x) =$	$x^{14} + 16x^{12} + 98x^{10} + 296x^8 + 473x^6 + 392x^4 + 148x^2 + 16$
$\pi(L_4, x) =$	$x^{18} + 21x^{16} + 180x^{14} + 822x^{12} + 2192x^{10} + 3510x^8 + 3321x^6 + 1731x^4 + $
	$415x^2 + 25$
$\pi(L_5, x) =$	$x^{22} + 26x^{20} + 287x^{18} + 1768x^{16} + 6725x^{14} + 16498x^{12} + 26429x^{10} + 27292x^8 + 2729x^8 + 27$
	$17399x^6 + 6230x^4 + 1009x^2 + 36$

Table 1: The permanental polynomials of linear chain L_n for n = 1, 2, 3, 4, 5.

We compute the permanental polynomials of L_n for n = 1, 2, 3, 4, 5 as exhibited in Table 1. The permanental polynomials in Tables 1-4 are all determined with MAPLE using the built-in MatrixVector-Multiply function.

If the hexagons in a hexagonal chain appear with type-II and type-III alternately, then it is said to be a *zigzag chain*. An illustration is given in Figure 5(c).

Corollary 3.9. For the zigzag chain Z_n with hexagons h_1, h_2, \dots, h_n ,

$$\alpha(Z_n) = \begin{cases} (\Gamma_2 \cdot \Gamma_3)^{\frac{n-1}{2}} \cdot \Gamma_2 \cdot \alpha(Z_0), & \text{ if } h_1 \text{ and } h_n \text{ are both of type-II,} \\ (\Gamma_3 \cdot \Gamma_2)^{\frac{n-1}{2}} \cdot \Gamma_3 \cdot \alpha(Z_0), & \text{ if } h_1 \text{ and } h_n \text{ are both of type-III,} \\ (\Gamma_3 \cdot \Gamma_2)^{\frac{n}{2}} \cdot \alpha(Z_0), & \text{ if } h_1 \text{ is of type-II and } h_n \text{ is of type-III,} \\ (\Gamma_2 \cdot \Gamma_3)^{\frac{n}{2}} \cdot \alpha(Z_0), & \text{ if } h_1 \text{ is of type-III and } h_n \text{ is of type-II,} \end{cases}$$

where $\alpha(Z_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

For the zigzag chains Z_n with the starting hexagon h_1 of type-III, we show their permanental polynomials for n = 1, 2, 3, 4, 5 in Table 2.

$\pi(Z_1, x) =$	$x^6 + 6x^4 + 9x^2 + 4$
$\pi(Z_2, x) =$	$x^{10} + 11x^8 + 41x^6 + 65x^4 + 43x^2 + 9$
$\pi(Z_3, x) =$	$x^{14} + 16x^{12} + 98x^{10} + 297x^8 + 479x^6 + 407x^4 + 166x^2 + 25$
$\pi(Z_4, x) =$	$x^{18} + 21x^{16} + 180x^{14} + 824x^{12} + 2214x^{10} + 3605x^8 + 3533x^6 + 1990x^4 + $
	$577x^2 + 64$
$\pi(Z_5, x) =$	$x^{22} + 26x^{20} + 287x^{18} + 1771x^{16} + 6773x^{14} + 16812x^{12} + 27538x^{10} + 29618x^8 + 286x^{10} + 286$
	$20364x^6 + 8453x^4 + 1886x^2 + 169$

Table 2: The permanental polynomials of zigzag chain Z_n for n = 1, 2, 3, 4, 5.

We call a hexagonal chain whose hexagons are all of type-II a *helix chain* [10]. An example is provided in Figure 5(d). The same analysis as above, we obtain that

Corollary 3.10. For the helix chain T_n ,

$$\alpha(T_n) = \Gamma_2^n \cdot \alpha(T_0),$$

where $\alpha(T_0) = (x^2 + 1, x, x, 1, 0)^{\mathrm{T}}$.

We list the permanental polynomials of T_n for n = 1, 2, 3, 4, 5 in Table 3.

$\pi(T_1, x) =$	$x^6 + 6x^4 + 9x^2 + 4$
$\pi(T_2, x) =$	$x^{10} + 11x^8 + 41x^6 + 65x^4 + 43x^2 + 9$
$\pi(T_3, x) =$	$x^{14} + 16x^{12} + 98x^{10} + 297x^8 + 479x^6 + 407x^4 + 166x^2 + 25$
$\pi(T_4, x) =$	$x^{18} + 21x^{16} + 180x^{14} + 824x^{12} + 2213x^{10} + 3599x^8 + 3518x^6 + 1972x^4 + 2213x^{10} + 3598x^8 + 3518x^6 + 1972x^4 + 2213x^{10} + 3598x^8 + 3518x^6 + 1972x^4 + 2213x^{10} + 359x^8 + 3518x^6 + 1972x^8 + 3518x^6 + 1972x^8 + 3518x^6 + 1972x^8 + 3518x^6 + 1972x^8 + 3518x^6 + 350x^8 + 3518x^6 + 350x^8 + 350$
	$568x^2 + 64$
$\pi(T_5, x) =$	$x^{22} + 26x^{20} + 287x^{18} + 1771x^{16} + 6771x^{14} + 16791x^{12} + 27450x^{10} + 29427x^8 + 26x^{10} + 29427x^{10} + 2947x^{10} + 2947x^{10} + 2947x^{10} + 2947x^{$
	$20138x^6 + 8318x^4 + 1856x^2 + 169$

Table 3: The permanental polynomials of helix chain T_n for n = 1, 2, 3, 4, 5.

3.3 The permanental polynomial of a pericondensed system

Figure 6 illustrates a pericondensed system denoted by H_n . As the labeling of vertices, H_{n+1} is the bridge graph of H_n and H_1 through $e_n^1 = (u_n^2, u_{n+1}^1)$ and $e_n^2 = (v_n^2, v_{n+1}^1)$. Let H_n^* be the graph obtained from H_n by adding an edge e_n^* joining u_n^2 and v_n^2 . Now, we devote ourselves to computing the permanental polynomial of H_n in a recursive technique.

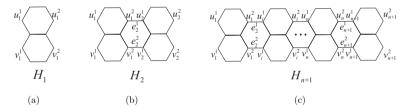


Figure 6: The pericondensed systems H_1 , H_2 and H_{n+1} .

Theorem 3.11. Let $\beta(H_n)$ be the column vector $(\pi(H_n, x), \pi(H_n - u_n^2, x), \pi(H_n - v_n^2, x), \pi(H_n - u_n^2, x), \pi(H_n - u_n^2, x), \sum_{C \in \mathscr{C}_*(H_*^*)} (-1)^{|V(C)|} \pi(H_n^* - V(C), x))^{\mathrm{T}}$. Then

$$\beta(H_{n+1}) = B \cdot \beta(H_n),$$

 $\begin{array}{l} \text{where } B \ \text{is the } 5 \times 5 \ \text{matrix with row vectors } y_1, y_2, y_3, y_4 \ \text{and } y_5. \ \text{More precisely}, \\ y_1 = (\omega_1, \omega_2, \omega_2, \omega_3, -2(\pi(P_7, x) + 2\pi(P_3, x) + x)), \\ y_2 = (\omega_2, \pi(C_6, x)\pi(P_2, x), \pi(P_8, x), \pi(P_5, x)\pi(P_2, x), -2\pi(P_2, x) - 2\pi(P_4, x)\pi(P_2, x)), \\ y_3 = (\omega_2, \pi(P_8, x), \pi(C_6, x)\pi(P_2, x), \pi(P_5, x)\pi(P_2, x), -2\pi(P_2, x) - 2\pi(P_4, x)\pi(P_2, x)), \\ y_4 = (\omega_3, \pi(P_5, x)\pi(P_2, x), \pi(P_5, x)\pi(P_2, x), \pi^3(P_2, x), -2x\pi^2(P_2, x)) \ \text{and} \\ y_5 = (-(\pi(P_7, x) + 2\pi(P_3, x) + x), -(\pi(P_2, x) + \pi(P_2, x)\pi(P_4, x)), -(\pi(P_2, x) + \pi(P_2, x)\pi(P_4, x)), \\ -x\pi^2(P_2, x), 2\pi^2(P_2, x) - \pi(P_2, x)), \end{array}$

where $\omega_1 = x^{10} + 11x^8 + 41x^6 + 65x^4 + 43x^2 + 9$, $\omega_2 = x^9 + 9x^7 + 26x^5 + 29x^3 + 11x$ and $\omega_3 = x^8 + 7x^6 + 14x^4 + 8x^2$.

Thus

$$\beta(H_n) = B^{n-1} \cdot \beta(H_1) \tag{18}$$

with $\beta(H_1) = (\omega_1, \omega_2, \omega_2, \omega_3, -\pi(P_7, x) - 2\pi(P_3, x) - x)^{\mathrm{T}}.$

Proof. The result of Corollary 3.3 derives

$$\pi(H_{n+1}, x) = \pi(H_n, x)\pi(H_1, x) + \pi(H_n - u_n^2, x)\pi(H_1 - u_1^1, x) + \pi(H_n - v_n^2, x)\pi(H_1 - v_1^1, x) + \pi(H_n - u_n^2 - v_n^2, x)\pi(H_1 - u_1^1 - v_1^1, x) + 2\sum_{C \in \mathscr{C}_{e_{n+1}^1}(H_{n+1})} (-1)^{|V(C)|} \pi(H_{n+1} - V(C), x),$$
(19)

A cycle C using e_{n+1}^1 in H_{n+1} must contain e_{n+1}^2 , $C' - e_n^*$ (C' is a cycle belonging to $\mathscr{C}_{e_n^*(H_n^*)}$) and the path induced by the bold edges as shown in Figure 7. So it implies

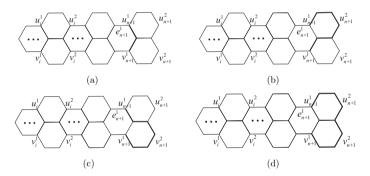


Figure 7: The cases of a part of a cycle containing e_{n+1}^1 in H_{n+1} .

$$\sum_{\substack{C \in \mathscr{C}_{e_{n+1}^1}(H_{n+1})}} (-1)^{|V(C)|} \pi(H_{n+1} - V(C), x)$$

= $[\pi(P_7, x) + 2\pi(P_3, x) + x][-\sum_{\substack{C \in \mathscr{C}_{e_n^*}(H_n^*)}} (-1)^{|V(C)|} \pi(H_n^* - V(C), x)],$ (20)

A series of computation leads to

$$\pi(H_1, x) = \omega_1, \pi(H_1 - u_1^1, x) = \pi(H_1 - v_1^1, x) = \omega_2 \text{ and } \pi(H_1 - u_1^1 - v_1^1, x) = \omega_3.$$
(21)

Based on these results, we get that $\pi(H_{n+1}, x) = y_1 \cdot \beta(H_n)$.

The same analysis as above, $\pi(H_{n+1} - u_{n+1}^2, x) = y_2 \cdot \beta(H_n), \ \pi(H_{n+1} - v_{n+1}^2, x) = y_3 \cdot \beta(H_n),$ and $\pi(H_{n+1} - u_{n+1}^2 - v_{n+1}^2, x) = y_4 \cdot \beta(H_n)$ are got.

Now we consider the cycle containing e_{n+1}^* in H_{n+1}^* . The following formula is derived.

$$\sum_{C \in \mathscr{C}_{e_{n+1}^*}(H_{n+1}^*)} (-1)^{|V(C)|} \pi(H_{n+1}^* - V(C), x)$$

= $-\pi(H_{n+1}', x) - \pi(H_n^1, x) - \pi(H_n^2, x) - x\pi(H_n, x)$
 $-\pi(P_2, x) \sum_{C \in \mathscr{C}_{e_n^*}(H_n^*)} (-1)^{|V(C)|} \pi(H_n^* - V(C), x),$ (22)

where the graph H'_n is the one obtained from H_n by deleting the path of length three joining u_n^2 and v_n^2 , and H_n^1 (resp. H_n^2) is the coalescence of H_n and P_4 with u_n^2 (resp. v_n^2) as the coalesced vertex. Refer to Figure 8.

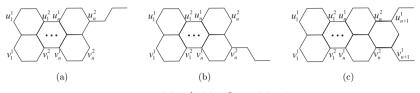


Figure 8: (a) H_n^1 , (b) H_n^2 and (c) H'_{n+1} .

By Theorem 3.1,

$$\pi(H_n^1, x) = \pi(H_n, x)\pi(P_3, x) + \pi(H_n - u_n^2, x)\pi(P_2, x),$$

$$\pi(H_n^2, x) = \pi(H_n, x)\pi(P_3, x) + \pi(H_n - v_n^2, x)\pi(P_2, x).$$
(23)

Using Corollary 3.3 to $\pi(H'_{n+1}, x)$, we have

$$\pi(H'_{n+1}, x) = \pi(H_n, x)\pi(P_7, x) + \pi(H_n - u_n^2, x)\pi(P_2, x)\pi(P_4, x) + \pi(H_n - v_n^2, x)\pi(P_2, x)\pi(P_4, x) + \pi(H_n - u_n^2 - v_n^2, x)\pi^2(P_2, x)x - 2\pi^2(P_2, x) \sum_{C \in \mathscr{C}_{e_n^*}(H_n^*)} (-1)^{|V(C)|} \pi(H_n^* - V(C), x).$$
(24)

The substitution of (23) and (24) into (22) yields

$$\begin{split} &\sum_{C \in \mathscr{C}_{e_{n+1}}(H_{n+1}^*)} (-1)^{|V(C)|} \pi(H_{n+1}^* - V(C), x) = \\ &- [x + 2\pi(P_3, x) + \pi(P_7, x)] \pi(H_n, x) - [\pi(P_2, x) + \pi(P_2, x)\pi(P_4, x)] \pi(H_n - u_n^2, x) \\ &- [\pi(P_2, x) + \pi(P_2, x)\pi^2(P_4, x)] \pi(H_n - v_n^2, x) - x\pi^2(P_2, x)\pi(H_n - u_n^2 - v_n^2, x) \\ &+ [2\pi^2(P_2, x) - \pi(P_2, x)] \sum_{C \in \mathscr{C}_{e_n^*}(H_n^*)} (-1)^{|V(C)|} \pi(H_n^* - V(C), x). \end{split}$$

According to this, $\sum_{C \in \mathscr{C}_{e_{n+1}^*}(H_{n+1}^*)} (-1)^{|V(C)|} \pi(H_{n+1}^* - V(C), x) = y_5 \cdot \beta(H_n)$ is obtained. By the discussions above, $\beta(H_{n+1}) = B \cdot \beta(H_n)$ follows. On the other hand, by (21) and a direct calculation, it gives that $\beta(H_1) = (\omega_1, \omega_2, \omega_2, \omega_3, -\pi(P_7, x) - 2\pi(P_3, x) - x)^{\mathrm{T}}$. Thus equation (18) is established.

In Table 4 we list some $\pi(H_n, x)$ explicitly by the method provided in Theorem 3.11.

Table 4: The permanental polynomials of H_n for n = 1, 2, 3, 4.

$\pi(H_1, x) =$	$x^{10} + 11x^8 + 41x^6 + 65x^4 + 43x^2 + 9$
$\pi(H_2, x) =$	$x^{20} + 24x^{18} + 240x^{16} + 1314x^{14} + 4350x^{12} + 9066x^{10} + 11993x^8 + 9882x^6 + 98$
	$4791x^4 + 1178x^2 + 81$
$\pi(H_3, x) =$	$x^{30} + 37x^{28} + 608x^{26} + 5878x^{24} + 37338x^{22} + 164826x^{20} + 521531x^{18} + $
	$1202331x^{16} + 2032192x^{14} + 2512170x^{12} + 2244727x^{10} + 1414603x^8 +$
	$600378x^6 + 156878x^4 + 20677x^2 + 729$
$\pi(H_4, x) =$	$\frac{600378x^6 + 156878x^4 + 20677x^2 + 729}{x^{40} + 50x^{38} + 1145x^{36} + 15954x^{34} + 151566x^{32} + 1042672x^{30} + 5384511x^{28} + 1042672x^{30} + 538451x^{30} + 538451x^{30} + 538451x^{30} + 53845x^{30} + 53845x^{3$
$\pi(H_4, x) =$	
$\pi(H_4, x) =$	$x^{40} + 50x^{38} + 1145x^{36} + 15954x^{34} + 151566x^{32} + 1042672x^{30} + 5384511x^{28} + 1042672x^{30} + 538451x^{30} + 538451x^{30} + 1042672x^{30} + 538451x^{30} + 53845x^{30} + 1042672x^{30} + 53845x^{30} + 53845x^{30} + 1042672x^{30} + 53845x^{30} + 1042672x^{30} + 53845x^{30} +$
$\pi(H_4, x) =$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$

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