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On counting polynomials of certain polyomino chains

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A counting polynomial $C(G,x)$ is a sequence description of a topological property so that the exponents express the extent of its partitions while the coefficients are related to the occurrence of these partitions. Omega, Sadhana and Padmakar-Ivan polynomials are extensive examples of counting polynomials which play an important role in topological description of bipartite structures as well as counts equidistance and non-equidistance edges in graphs. These polynomials count the quasi orthogonal cut (qoc) strips in graphs generated from bipartite chemical structures. A qoc strip defined with respect to any edge in a graph $G(V,E)$, represents the smallest subset of edges closed under taking opposite edges on faces.

In this article, we focus on counting polynomials of polyomino chains of different possible shapes. We derive the exact formulas of omega, Sadhana and PI polynomials for 2-parametric 4-polyomino system P_n^k for $k \geq 3, n \geq 1$. An open problem is proposed for further research in this direction.

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INTRODUCTION AND PRELIMINARY RESULTS

A k*-polyomino system* is a finite 2-connected plane graph such that each interior face (also called cell) is surrounded by a regular $4k$-cycle of length one. In other words, it is an edge-connected union of cells [12].

Counting polynomials are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. A counting polynomial is defined as:

$$C(G,x) = \sum_c m(G,c)x^c \quad (1)$$

Where the coefficient $m(G,c)$ are calculable by various methods, techniques and algorithms. The expression (1) was found independently by Sachs, Harary, Milic′, Spialter, Hosoya, etc [5]. The corresponding topological index $P(G)$ is defined in this way:

$$C(G) = C'(G,x)|_{x=1} = \sum_c m(G,c) \times c$$

A *moleculer/chemical graph* is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. This is more important to say that the hydrogen atoms are often omitted in any molecular graph. A graph can be represented by a matrix, a sequence, a polynomial and a numeric number (often called a topological index) which represents the whole graph and these representations are aimed to be uniquely defined for that graph.

Two edges $e = uv$ and $f = xy$ in $E(G)$ are said to be *codistant*, usually denoted by $e\ co\ f$, if

$$d(x,u) = d(y,v)$$

and

$$d(x,v) = d(y,u) = d(x,u)+1 = d(y,v)+1$$

The relation "co" is reflexive as $e\ co\ e$ is true for all edges in G, also symmetric as if $e\ co\ f$ then $f\ co\ e$ for all $e, f \in E(G)$ but the relation "co" is not necessarily transitive. Consider

$$C(e) = \{ f \in E(G) : f\ co\ e \}$$

If the relation is transitive on $C(e)$ also, then $C(e)$ is called an *orthogonal cut* "co" of the graph

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G. Let $e = uv$ and $f = xy$ be two edges of a graph G, which are opposite or topological parallel, and this relation is denoted by $e\, op\, f$. A set of opposite edges, within the same face or ring, eventually forming a strip of adjacent faces/rings, is called an opposite edge strip ops, which is a quasi-orthogonal cut qoc (i.e. the transitivity relation is not necessarily obeyed). Note that "co" relation is defined in the whole graph while "op" is defined only in a face/ring.

In this article, G is considered to be simple connected graph with vertex set $V(G)$ and edge set $E(G)$, $m(G,c)$ be the number of ops of length c, $e = |E(G)|$ is the edge set cardinality of G.

The omega polynomial was introduced by *Diudea* et al. in 2006 on the ground of op strips. The omega polynomial is proposed to describe cycle-containing molecular structures, particularly those associated with nanostructures.

Definition 1.1. [1] Let G be a graph, then its omega polynomial denoted by $\Omega(G,x)$ in x is defined as

$$\Omega(G,x) = \sum_c m(G,c) \times x^c$$

The derivative of omega polynomial at $x = 1$ for any bipartite graph is equal to its edge set cardinality.

The Sadhana polynomial is defined based on counting opposite edge strips in any graph. This polynomial counts equidistant edges in G.

Definition 1.2. [6] Let G be a graph, then Sadhana polynomial denoted by $Sd(G,x)$ is defined as

$$Sd(G,x) = \sum_c m(G,c) \times x^{e-c}$$

The PI polynomial is defined based on counting opposite edge strips in any graph [10]. This polynomial counts non-equidistant edges in G.

Definition 1.3. [11] Let G be a graph, then PI polynomial denoted by $PI(G,x)$ is defined as

$$PI(G,x) = \sum_c m(G,c) \times c \times x^{e-c}$$

Ashrafi et al. computed Sadhana polynomial of V-phenylenic nanotube and nanotori.

Theorem 1.1. [2] Let G be the graph of V-phenylenic nanotube, then Sadhana polynomial of G is,

$$Sd(G,x) = 4\sum_{i=1}^{Max\{m,n\}-1} x^{|E(G)|-2i} + 2(|n-m|+1)x^{|E(G)|-2Min\{m,n\}} + nx^{|E(G)|-2m} + (m-1)x^{|E(G)|-2m} + (n-1)x^{|E(G)|-n}$$

All nanotubes are allotropes of carbon and are a type of fullerene. Imran et al. [9] computed omega and Sadhana polynomials of H-Naphtalenic nanotube.

Theorem 1.2. [9] The omega polynomial of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$ is:

$$\Omega(NPHX[m,n],x) = \begin{cases} \eta + 4\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{2i} + 2(n-2m+1)x^{4m}, & m \le \lfloor \frac{n}{2} \rfloor \\ \eta + 4\sum_{i=1}^{n-1} x^{2i} + 2(2m-n+1)x^{2n}, & m > \lfloor \frac{n}{2} \rfloor \end{cases}$$

where $\eta = nx^{3m} + mx^{2n} + (n-1)x^{2m}$.

The Sadhana polynomial of $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$ is.

$$Sd(NPHX[m,n],x) = \begin{cases} \eta + 4\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} x^{15mn-2m-2i} + 2(n-2m+1)x^{15mn-6m}, & m \le \lfloor \frac{n}{2} \rfloor \\ \eta + 4\sum_{i=1}^{n-1} x^{15mn-2m-2i} + 2(2m-n+1)x^{15mn-2m-2n}, & m > \lfloor \frac{n}{2} \rfloor \end{cases}$$

where

$$\eta = nx^{15mn-5m} + mx^{15mn-2m-2n} + (n-1)x^{15mn-4m}.$$

The preceding results are used to compute their corresponding topological indices which provides a good model correlating the certain physico-chemical properties of these carbon allotropes.

RESULTS AND DISCUSSION

In this paper, we compute omega, Sadhana and PI polynomials of polyomino chain system P_n^k for $k = 1,2,3,...,6$. By using these results, we present our main results of counting polynomials for polyomino chain system P_n^k for $k \ge 3, n \ge 1$. Imran et al. [8] studied some degree based topological indices of the polyomino chains. For further study of these polynomials their topological indices and various nanotubes, consult [3, 4, 9, 13, 14, 15]. These polynomials are used to predict various physico-chemical properties of certain chemical compounds.

Polyomino chains

A *polyomino system* is a finite 2-connected plane graph such that each interior face (or say a cell) is surrounded by a regular square of length one. In other words, it is an edge-connected union of cells in the planar square lattice. This polyomino system divides the plane into one infinite external region and a number of finite internal regions where all internal regions must be squares. A *polyomino chain* is a polyomino system, in which the joining of the centers of its adjacent cells (regular squares) forms a path $c_1, c_2, ..., c_n$, where c_i is the center of the i-th square. Such a polyomino chain is denoted as B_n. A square of a polyomino chain has either one or two neighboring squares. If a square has one neighboring square, it is called terminal, if it has two neighboring squares having no vertex of degree 2, it is called medial, and if it has two neighboring squares such that it has a vertex of degree 2, it is called kink. Every polyomino chain of dimension n has a unit such that it contains n number of units [16].

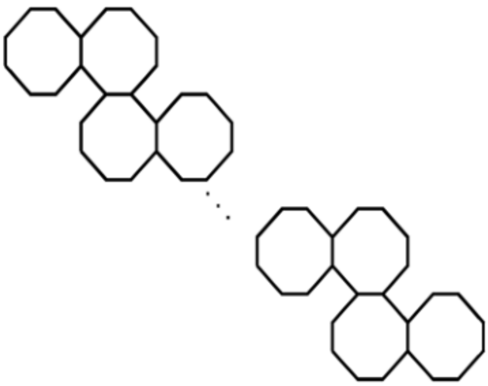

Fig. 1. A 2-polyomino system which is a zig-zag chain of 8-cycles.

Theorem 2.1.1. [7] Consider the graph of 2-polyomino system depicted in Figure 1. Then: $\Omega(x) = (4n - 1)\, x^3 + (8n + 2)\, x^2$ and $Sd(x) = (4n - 1)\, x^{28n-2} + (8n + 2)\, x^{28n-1}$.

We denote the polyomino chain system by P_n^k, and $k = k' + m + t$, where k' is the number of kinks, m is the number of medials and t is the number of terminals in a unit of polyomino chain. Figure 2 depicts the different polyomino chains with their units as dotted part. We call l_n, z_n, c_n, k_n, r_n and h_n the polyomino chains P_n^k for $k = 1,2,3,4,5$ and 6 respectively. Now we compute omega polynomial of these chemical graphs which count equidistance edges in these graphs.

Theorem 2.1.2. The omega polynomial of P_n^k for $k = 1,2,3,4,5,6$ is equal to:

$$\Omega(l_n, x) = x^{n+1} + nx^2$$

$$\Omega(z_n, x) = 2x^2 + (2n-1)x^3$$

$$\Omega(c_n, x) = (n+1)x^2 + (n+1)x^3 + (n-1)x^4$$

$$\Omega(k_n, x) = (2n+1)x^2 + nx^3 + x^4 + (n-1)x^5$$

$$\Omega(r_n, x) = (3n+1)x^2 + nx^3 + x^5 + (n-1)x^6$$

$$\Omega(h_n, x) = (4n+1)x^2 + nx^3 + x^6 + (n-1)x^7$$

Proof. **For** l_n

The polyomino chain l_n is a linear chain of squares as shown in Figure 2. The number of edges in this chain graph is $3n+1$. There are two types of ops in l_n, there are n qoc strips of length 2 and one strip of length $n+1$. Since

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(l_n, x) = nx^2 + x^{n+1}$$

For z_n ***:***

The chemical graph z_n is a zig-zag chain of squares as shown in Figure 2. The number of edges in this chain graph is $6n+1$. There are also two types of ops in z_n, there are 2 qoc strips of length 2 and $2n-1$ strips of length 3. Since

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(z_n, x) = 2x^2 + (2n-1)x^3$$

For c_n ***:***

The polyomino chain c_n is a polyomino chain P_n^k with $k = 3$ shown in Figure 2. The number of edges in this chain graph is $9n+1$. This chain of dimension n has three types of qoc strips in c_n, there are $n+1$ strips of length 2, $n+1$ strips of length 3 and $n-1$ strips of length 4. Now

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(c_n, x) = (n+1)x^2 + (n+1)x^3 + (n-1)x^4$$

For k_n ***:***

The number of edges in this chain graph is $12n+1$. This chain of dimension n has four types of qoc strips in k_n, there are $2n+1$ strips of length 2, n strips of length 3, one strip of length 4 and $n-1$ strips of length 5. Now

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(k_n, x) = (2n+1)x^2 + nx^3 + x^4 + (n-1)x^5$$

For r_n ***:***

In polyomino chain r_n, there are $15n+1$ edges and four types of strips. There are $3n+1$ strips of length 2, n strips of length 3, one strip of length 5 and $n-1$ strips of length 6. We know

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(r_n, x) = (3n+1)x^2 + nx^3 + x^5 + (n-1)x^6$$

For h_n **:**

The polyomino chain h_n contains $18n+1$ edges and four types of strips. There are $4n+1$ strips of length 2, n strips of length 3, one strip of length 6 and $n-1$ strips of length 7. We know

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(h_n, x) = (4n+1)x^2 + nx^3 + x^6 + (n-1)x^7$$

□

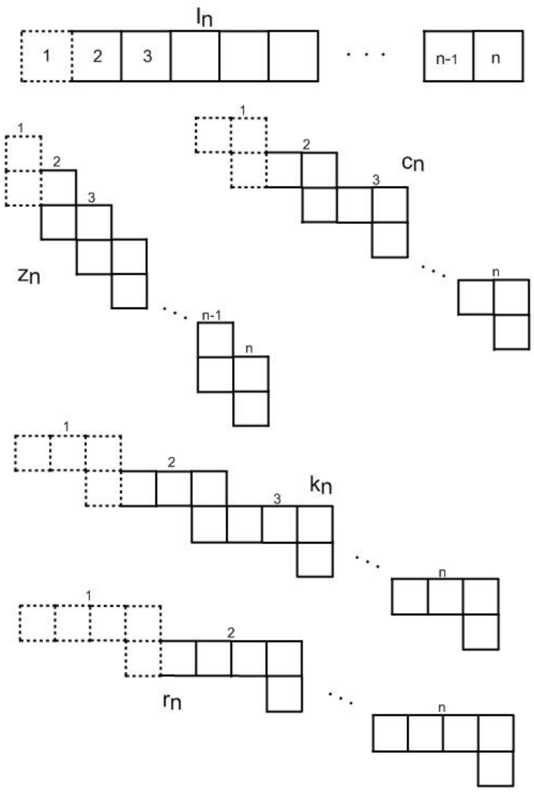

Fig. 2. Different polyomino chains.

In the following theorem, the Sadhana polynomial of P_n^k for $k = 1,2,3,4,5$ and 6 is computed.

Theorem 2.1.3. The Sadhana polynomial of P_n^k for $k = 1,2,3,4,5$ and 6 is as follows:

$$Sd(l_n, x) = nx^{3n-1} + x^{2n}$$

$$Sd(z_n, x) = 2x^{6n-1} + (2n-1)x^{6n-2}$$

$$Sd(c_n, x) = (n+1)x^{9n-1} + (n+1)x^{9n-2} + (n-1)x^{9n-3}$$

$$Sd(k_n, x) = (2n+1)x^{12n-1} + nx^{12n-2} + x^{12n-3} + (n-1)x^{12n-4}$$

$$Sd(r_n, x) = (3n+1)x^{15n-1} + nx^{15n-2} + x^{15n-4} + (n-1)x^{15n-5}$$

$$Sd(h_n, x) = (4n+1)x^{18n-1} + nx^{18n-2} + x^{18n-5} + (n-1)x^{18n-6}$$

The proof of this theorem is on the same lines as in case of omega polynomial, so we skip this proof.

Now we compute PI polynomial of P_n^k for $k = 1,2,3,4,5,6$.

Theorem 2.1.4. Consider the polyomino system P_n^k for $k = 1,2,3,4,5$ and 6. Then their PI polynomials are:

$$PI(l_n, x) = 2nx^{3n-1} + (n+1)x^{2n}$$

$$PI(z_n, x) = 4x^{6n-1} + (6n-3)x^{6n-2}$$

$$PI(c_n, x) = (2n+2)x^{9n-1} + (3n+3)x^{9n-2} + (4n-4)x^{9n-3}$$

$$PI(k_n, x) = (4n+2)x^{12n-1} + 3nx^{12n-2} + 4x^{12n-3} + (5n-5)x^{12n-4}$$

$$PI(r_n, x) = (6n+2)x^{15n-1} + 3nx^{15n-2} + 5x^{15n-4} + (6n-6)x^{15n-5}$$

$$PI(h_n, x) = (8n+4)x^{18n-1} + 3nx^{18n-2} + 6x^{18n-5} + (7n-7)x^{18n-6}$$

The proof of this result is also skipped due to similarity with proof of omega polynomial.

Polyomino chain system P_n^k

In this section, we deal with polyomino chain system P_n^k with two defining parameters k and n, where k is the sum of the number of kinks and number of terminals in a unit of any particular polyomino chain and n is the defining parameter of the chain i.e. dimension. Figure 3 shows the polyomino chain system P_n^k, with arbitrary defining parameters. The number of edges in P_n^k is $3kn+1$.

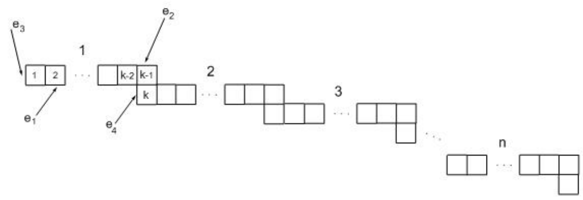

Fig. 3. General representation of P_n^k.

Table 1. Number of quasi-orthogonal strips in P_n^k for $k \geq 3$, $n \geq 1$.

Types of qoc's	Types of edges	Number of co-distant edges	No of qoc
C_1	e_1	2	*(kn-2n+1)*
C_2	e_2	3	*n*
C_3	e_3	*k*	*1*
C_4	e_4	*k*	*n-1*

There are four types of qoc strips in P_n^k shown in Table. In the following theorem, the omega polynomial of P_n^k is computed.

Theorem 2.2.1. The omega polynomial of P_n^k with $k \geq 3$, $n \geq 1$, is as follows:

$$\Omega(P_n^k, x) = (kn - 2n + 1)x^2 + nx^3 + x^k + (n-1)x^{k+1}$$

Proof. Let G be the graph of polyomino chain system P_n^k with $k \geq 3$, $n \geq 1$. Table 1 shows the number of co-distant edges and number of qoc in G. The quasi-orthogonal cuts and starting edges of strips are depicted in Fig 2. By using Table 1, the proof is mechanical. Now we apply formula and do some calculation to get our result.

$$\Omega(G, x) = \sum_c m(G, c) \times x^c$$

$$\Omega(G, x) = (kn - 2n + 1)x^2 + nx^3 + x^k + (n-1)x^{k+1}$$

□

Now we compute Sadhana polynomial of P_n^k for $k \geq 3$, $n \geq 1$. Following theorem shows the Sadhana polynomial for this family of polyomino chains.

Theorem 2.2.2. Consider the graph of P_n^k with $k \geq 3$, $n \geq 1$. Then its Sadhana polynomial is as follows:

$$Sd(P_n^k, x) = (kn - 2n + 1)x^{3kn-1} + nx^{3kn-2} + x^{3kn-k+1} + (n-1)x^{3kn-k}$$

Proof. Consider the graph of P_n^k with $k \geq 3$, $n \geq 1$. We prove it by using Table 1. We know that

$$Sd(G, x) = \sum_c m(G, c) \times x^{e-c}$$

$$Sd(P_n^k, x) = (kn - 2n + 1)x^{3kn-1} + nx^{3kn-2} + x^{3kn-k+1} + (n-1)x^{3kn-k}$$

□

Next we compute PI polynomial of this polyomino chain system. Following theorem explains the PI polynomial of this family of polyomino chains.

Theorem 2.2.3 Consider the graph of P_n^k with $k \geq 3$, $n \geq 1$. Then its PI polynomial is as follows:

$$PI(P_n^k, x) = 2(kn - 2n + 1)x^{3kn-1} + 3nx^{3kn-2} + x^{kn-k+n-1} + (n-1)x^{3kn-k}$$

Proof. Let G be the graph of P_n^k with $k \geq 3$, $n \geq 1$. We prove it by using data given in Table 1. We know that

$$PI(G, x) = \sum_c m(G, c) \times c \times x^{e-c}$$

$$PI(P_n^k, x) = 2(kn - 2n + 1)x^{3kn-1} + 3nx^{3kn-2} + x^{kn-k+n-1} + (n-1)x^{3kn-k}$$

□

Open Problem

Investigate $C(G, x)$ for 3-parametric 4-polyomino system $P_r^k(n)$, where $k = k' + m + t$, and r is the number of squares between kinks inclusively in a unit and n is the dimension.

CONCLUSION AND GENERAL REMARKS

In this paper, three important counting polynomials called omega, Sadhana and PI are studied. These polynomials are useful in determining omega, Sadhana and PI topological indices which play an important role in QSAR/QSPR study. These counting polynomials play an important role in topological description of bipartite structures as well as counts equidistance and non-equidistance edges in graphs. In this paper, we studied these polynomials for polyomino chains or conducted the counting of qoc strips in these bipartite chemical graphs alternatively. An open problem is proposed for study of polyomino chains and k-polyomino system.

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REFERENCES

1. M. V. Diudea, *Carpath. J. Math.*, **22**, 43 (2006).
2. A.R. Ashrafi, M. Ghorbani, M. Jalali, *Indian J. Chem.*, **47A**, 535 (2008).
3. A.Bahrami, J. Yazdani, *Dig. J. Nanomater. Biostruc.*, **3**, 265 (2008).
4. K. C. Das, F. M. Bhatti, S. G. Lee, I. Gutman, *MATCH Commun. Math. Comput. Chem.*,**65**, 753 (2011).
5. M. V. Diudea, I. Gutman, J. Lorentz, Molecular Topology, Nova, Huntington, 2001.
6. M. V. Diudea, S. Cigher, P. E. John, *MATCH Commun. Math. Comput. Chem.*, **60**, 237 (2008).
7. M. Ghorbani, M. Ghazi, *Dig. J. Nanomater. Biostruc.*, **5** (4), 843 (2010).
8. M. Imran, S. Hayat, M. K. Shafiq, *Optoelectron. Adv. Mater. Rapid Commun.*, **8**, 948 (2014).
9. M. Imran, S. Hayat, M.K. Shafiq, *Optoelectron. Adv. Mater. Rapid Commun.*, **8**, 1218 (2014).
10. P. V. Khadikar, *Nat. Acad. Sci. letters*, **23**, 113 (2000).

11. P. V. Khadikar, S. Karmarkar, V. K. Agrawal, *J. Chem. Inf. Comput. Sci.*, **41**, 931 (2001).
12. D. A. Klarner, Polyominoes, In: J. E. Goodman, J. O'Rourke, (eds.), Handbook of Discrete and Computational Geometry, CRC Press, Boca Raton, 1997, p.225.
13. A. Rajan, A. William, C. Grigorious, S. Stephen, *J. Comp. Math. Sci.*, **5**, 30 (2012).
14. S. Hayat, M. Imran, *J. Comput. Theor. Nanosci.*, **12**, 7 (2015).
15. I. Tomescu, S. Kanwal, *MATCH Commun. Math. Comput. Chem.*, **69**, 535 (2013).
16. Z. Yarahmadi, A. R. Ashrafi, S. Moradi, *App. Math. Lett.*, **25**, 166 (2012).
17. I. Yazdani, A. Bahrami, *Dig. J. Nanomater. Biostruc.*, **4**, 507 (2009).
18. M. Alaeiyan, A. Gilani, R. Mojarad, *Kuwait J. Sci.*, **41** (1), 85 (2014).

ВЪРХУ БРОЙНИ ПОЛИНОМИ НА НЯКОИ ПОЛИМИНО ВЕРИГИ

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Бройният полином $C(G,x)$ е поредица, описваща топологично свойство, така че степенните показатели изразяват размерите на неговите дялове, докато коефициентите са свързани с честотата на тези дялове. Полиномите Ω, на Sadhana и Padmakar-Ivan са разширени примери на бройни полиноми, които играят важна роля в топологичното писание на двуделни структури, както и в преброяването на еквидистантни и не еквидистантни ребра на графи. Тези полиноми преброяват квазиортогоналните отрезни (КОО) ленти в графи, генерирани от двуделни химически структури. КОО лента, дефинирана по отношение на кое и да е ребро на графа $G(V,E)$, представлява най-малката подгрупа от ребра, затворени при вземане на противоположни ребра върху лицата.

В тази статия, ние се фокусираме върху бройните полиноми на полимино вериги от различни възможни форми. Ние извеждаме точните формули на полиномите omega, на Sadhana и PI за 2-параметрична 4-полимино система P_n^k за $k \geq 3, n \geq 1$. Предложена е отворена задача за по-нататъшни изследвания в тази посока.