Digest Journal of Nanomaterials and Biostructures Vol. 5, No 4, October-December 2010, p. 843-849

COMPUTING OMEGA AND PI POLYNOMIALS OF GRAPHS

M. GHORBANI, M. GHAZI
Department of Mathematics, Faculty of Science, Shahid Rajaee Teacher Training University, Tehran, 16785 – 136, I. R. Iran;

A new counting polynomial, called Omega $\Omega(G,x)$, was recently proposed by Diudea. It is defined on the ground of "opposite edge strips" *ops*. The Sadhana polynomial $Sd(G,x)$ can also be calculated by ops counting. In this paper we compute these polynomials for some classes of 8 – cycle graphs.

(Received September 29, 2010; accept4ed October 15, 20010)

Keywords: Omega polynomial, Sadhana Polynomial, 8 -Cycles Graph.

1. Introduction

Nano-era is a suitable name for the period started with the discovery of C_{60} fullerene and carbon nanotubes.[1-3] It opened a new gate for the science and technology at nanometer scale with wide implications in the human activities. After the discovery of carbon nanotubes, the question about the possible existence of nanotubular forms of other elements was addressed by scientists and they tried to obtain inorganic nanostructures.[4-6] Mathematical calculations are absolutely necessary to explore important concepts in chemistry. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics. Chemical graph theory is an important tool for studying molecular structures. This theory had an important effect on the development of the chemical sciences.

Let $G(V,E)$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of G are called *codistant e co f* if they obey the following relation:[7,8]

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

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e*. In general, relation *co* is not transitive, an example showing this fact is the complete bipartite graph $K_{2,n}$. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges $C(e) := \{f \in E(G);\ f\ co\ e\}$ is called an *orthogonal cut oc* of G, $E(G)$ being the union of disjoint orthogonal cuts: $E(G) = C_1 \cup C_2 \cup ... \cup C_k,\ C_i \cap C_j = \emptyset, i \neq j$. Klavžar[9] has shown that relation *co* is a theta Djoković-Winkler relation.[10,11]

*Corresponding author: mghorbani@srttu.edu

Let $e = uv$ and $f = xy$ be two edges of G which are *opposite* or topologically parallel and denote this relation by *e op f*. A set of opposite edges, within the same face/ring, eventually forming a strip of adjacent faces/rings, is called an *opposite* edge *strip ops*, which is a quasi-ortogonal 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. The length of *ops* is maximal irrespective of the starting edge. Let $m(G,s)$ be the number of *ops* strips of length s. The Omega polynomial is defined as[12,13]

$$\Omega(x) = \sum_s m(G,s) \cdot x^s$$

The first derivative (in x=1) equals the number of edges in the graph

$$\Omega'(1) = \sum_s m(G,s) \cdot s = e = |E(G)|$$

An example is given in Figure 2, which illustrates just the pattern of TiO_2 lattice.

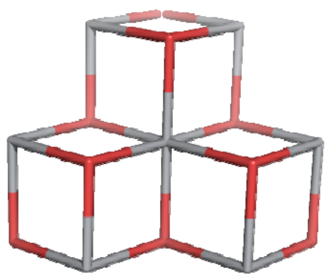

Fig. 1. TiO_2 pattern; counting polynomial examples:

$$\Omega(G,x) = 3x^3 + 3x^5\ ;\ \Omega'(G,1) = 24 = e(G)\ ;$$

$$Sd(G,x) = 3x^{19} + 3x^{21}\ ;\ Sd'(G,1) = 120 = Sd(G)\ ;$$

The Sadhana index $Sd(G)$ was defined by Khadikar *et al.*[14,15] as

$$Sd(G) = \sum_s m(G,s)(|E(G)| - s),$$

where $m(G,s)$ is the number of strips of length s. The Sadhana polynomial $Sd(G,x)$ was defined by Ashrafi *et al.*[16] as

$$Sd(x) = \sum_s m(G,s) \cdot x^{|E(G)|-s}\ .$$

Clearly, the Sadhana polynomial can be derived from the definition of Omega polynomial by replacing the exponent s by $|E(G)-s|$. Then the Sadhana index will be the first derivative of $Sd(x)$ evaluated at x=1.

The aim of this study is to compute the Omega and Sadhana polynomials of 8 – cycles graphs. Here our notations are standard and mainly taken from [17 - 22].

2. Main results

In this section by using Omega and Sadhana polynomials we compute these polynomials for three classes of bipartite graphs. Finally, by using a relation between Omega and PI polynomials we compute the PI polynomial of them. To do this we need definition of some graphs mentioned above.

3. Polyomino chains of 8– Cycles

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, see Klarner [23].

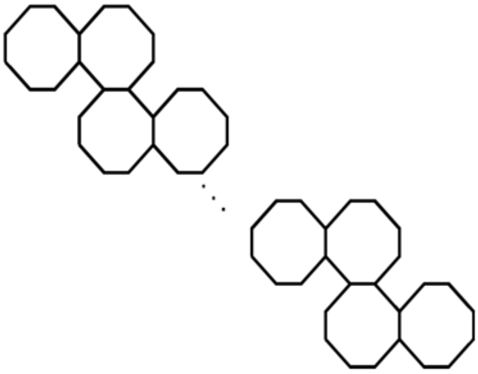

Fig. 2. The zig-zag chain of 8-cycles.

Example 1. Consider the graph G shown in Figure 3. One can see this graph has exactly 2 strips C_1 and C_2. On the other hand $|C_1| = 3$ and $|C_2| = 2$. Hence,

$$\Omega(x) = 3x^3 + 10x^2 \text{ and } Sd(x) = 3x^{26} + 10x^{27}.$$

Example 2. For the graph H depicted in Figure 4, there exist two distinct strips C_1 and C_2. Similarly, $|C_1| = 3$ and $|C_2| = 2$. Hence,

$$\Omega(x) = 7x^3 + 18x^2 \text{ and } Sd(x) = 7x^{28n-2} + 18x^{28n-1}.$$

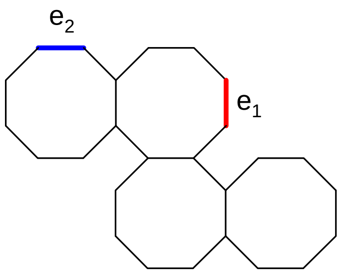

Fig. 3. The zig-zag chain of 8-cycles, n = 1.

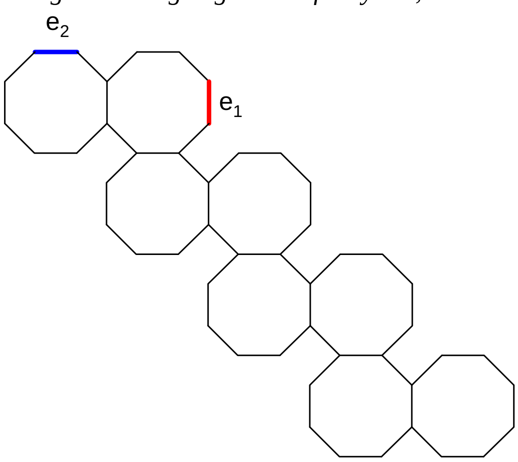

Fig. 4. The zig-zag chain of 8-cycles, n =2.

In generally, this graph has two distinct strips of lengths 2 and 3, respectively. In other words we have the following Theorem:

Theorem 1. Consider the graph of 2-polyomino system depicted in Figure 2. Then:

$$\Omega(x) = (4n-1)x^3 + (8n+2)x^2 \text{ and } Sd(x) = (4n-1)x^{28n-2} + (8n+2)x^{28n-1}.$$

Consider now, another version of 2-polyomino system H_n. when n = 1(Figure 5), there exist three strips of length 2, 3 and 4, respectively. In other words,

$$\Omega(x) = x^4 + 2x^3 + 13x^2 \text{ and } Sd(x) = x^{32} + 2x^{33} + 13x^{34}.$$

Similarly for n = 2 (Figure 6), there exist three strips of length 2, 3 and 4, respectively. This implies $\Omega(x) = 2x^4 + 5x^3 + 24x^2$ and $Sd(x) = 2x^{67} + 5x^{68} + 24x^{69}$.

By continuing this method it is easy to check that this graph has only three strips of length 2, 3 and 4, respectively. Thus by computing number of strips of equal size and substitute in the Omega polynomial the following Theorem can be deduced:

Theorem 2. Let H_n be the graph of 2-polyomino system shown in Figure 6. Then:

$$\Omega(x) = nx^4 + (3n-1)x^3 + (11n+2)x^2 \textit{ and}$$

$$Sd(x) = nx^{35n-3} + (3n-1)x^{35n-2} + (11n+2)x^{35n-1}.$$

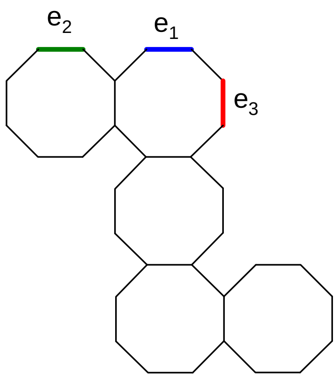

Fig. 5. The graph of 2-polyomino system H_n, n = 1.

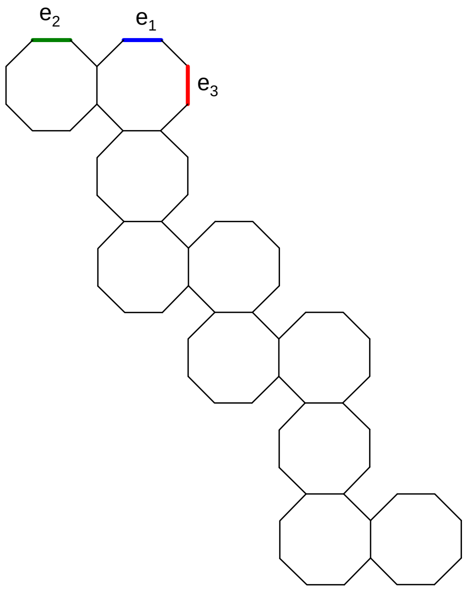

Fig. 6. The graph of 2-polyomino system H_n, n = 2.

4. Triangular Benzenoid

In this section we compute counting polynomials mentioned in the text of triangular benzenoid graphs (see Figure 7). At first consider the graph of triangular benzenoid $G[n]$ for n = 1. The Omega and Sadhana polynomials are $\Omega(x) = 3x^2$ and $\Omega(x) = 3x^4$, respectively. By continuing this method, there exist n strips of length 2, 3, …, n + 1, respectively. In other words, if

$C_1, C_2, \ldots, C_n$ be all strips of $G[n]$, then there are 3 strips equivalent with $|C_i|$, $i = 1, 2, \ldots$ Hence we proved the following Theorem:

Theorem 3.
$\Omega(G[n],x) = 3(x^2 + x^3 + \cdots + x^{n+1})$ and $Sd(G[n],x) = 3(x^{|E|-2} + x^{|E|-3} + \cdots + x^{|E|-n-1})$, where $|E| = 28n + 1$.

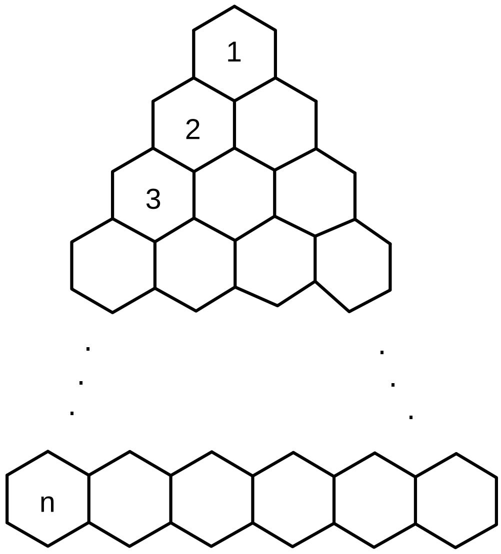

Fig. 7. The graph of triangular benzenoid graphs.

5. PI Index

Let $\sum$ be the class of finite graphs. A topological index is a function Top from $\sum$ into real numbers with this property that $Top(G) = Top(H)$, if G and H are isomorphic. Obviously, the number of vertices and the number of edges are topological index. The Wiener[24] index is the first reported distance based topological index and is defined as half sum of the distances between all the pairs of vertices in a molecular graph. If $x, y \in V(G)$ then the distance $d_G(x, y)$ between x and y is defined as the length of any shortest path in G connecting x and y.

Khadikar introduced another index called Padmakar-Ivan (*PI*) index [25,26]. The PI index of a graph G is defined as:

$$PI = PI(G) = \Sigma\, [m_{eu}(e|G) + m_{ev}(e|G)]$$

where for edge $e = uv$, $m_{eu}(e|G)$ is the number of edges of G lying closer to u than v, $m_{ev}(e|G)$ is the number of edges of G lying closer to v than u and summation goes over all edges of G. Similar to Sadhana polynomial we can define the PI polynomial. Then the PI index will be the first derivative of PI(x) evaluated at x=1.

Let C_e be a strips containing all parallel edges with e. If G be a bipartite graph it is well – known fact that $PI(x) = \sum_S s \times m(G,s) \cdot x^{|E|-s}$. In other words, by using Omega polynomial in bipartite graph we can compute the PI polynomial and then PI index. Hence the following Theorems are resulted from Theorems 1, 2 and 3, respectively:

Theorem 4. Consider the graph of 2-polyomino system depicted in Figure 2. Then:

$$PI(x) = 3(4n-1)x^{28n-2} + 2(8n+2)x^{28n-1}.$$

Theorem 5. Let H_n be the graph of 2-polyomino system shown in Figure 6. Then:

$$PI(x) = 4nx^{35n-3} + 3(3n-1)x^{35n-2} + 2(11n+2)x^{35n-1}.$$

Theorem 6. For the graph of triangular benzenoid graphs depicted in Figure 7 we have:

$$PI(G[n],x) = 3(2x^{|E|-2} + 3x^{|E|-3} + \cdots + (n+1)x^{|E|-n-1}) .$$

where $|E| = 28n + 1$.

References

[1] E. Osawa, Kagaku (Kyoto), **25**, 854 (1970).
[2] H. Kroto, J. R. Heath, S. C. O'Brian, R. F. Curl, and R. E. Smalley, Nature (London), **318** 162 (1985).
[3] W. Kraetschmer, L. D. Lamb, K. Fostiropoulos, and D. R. Huffman, Nature (London), **347** 354 (1990).
[4] R. Tenne, Chem. Eur. J., **8**, 5296 (2002).
[5] C. N. R. Rao, M. Nath, Dalton Trans., **1**, 1 (2003).
[6] G. R. Patzke, F. Krumeich and R. Nesper, Angew. Chem., Int. Ed., **41**, 2447 (2002).
[7] M. V. Diudea, A. Ilić, Carpath. J. Math., 2009 (submitted).
[8] A. R. Ashrafi, M. Jalali, M. Ghorbani, M. V. Diudea, MATCH, Commun. Math. Comput. Chem., **60**, 905 (2008).
[9] S. Klavžar, MATCH Commun. Math. Comput. Chem., **59**, 217 (2008).
[10] D. Ž. Djoković, J. Combin. Theory Ser. B, **14**, 263 (1973).
[11] P. M. Winkler, Discrete Appl. Math., **8**, 209 (1984).
[12] M. V. Diudea, Carpath. J. Math., **22**, 43 (2006).
[13] P. E. John, A. E. Vizitiu, S. Cigher, and M. V. Diudea, MATCH Commun. Math. Comput. Chem., **57**, 479 (2007).
[14] P. V. Khadikar, V. K. Agrawal and S. Karmarkar, Bioorg. Med. Chem., **10**, 3499 (2002).
[15] P. V. Khadikar, S. Joshi, A. V. Bajaj and D. Mandloi, Bioorg. Med.Chem. Lett., **14**, 1187 (2004).
[16] A. R. Ashrafi, M. Ghorbani and M. Jalali, Ind. J. Chem., **47**A, 535 (2008).
[17] A. R. Ashrafi, M. Jalali, M. Ghorbani and M. V. Diudea, MATCH Commun. Math. Comput. Chem., **60**(3), 905 (2008).
[18] M. Jalali and M. Ghorbani, Studia Universitatis Babe –Bolyai, Chemia, **4**, 25 (2009).
[19] M. Ghorbani and M. Jalali, MATCH Commun. Math. Comput. Chem., **62**, 353 (2009).
[20] A. R. Ashrafi and M. Ghorbani, Fullerenes, Nanotubes, and Carbon Nanostructures, **18**, 198 (2010).
[21] M. Ghorbani, Iranian Journal of Mathematical Chemistry, **1**, 105 (2010).
[22] A. R. Ashrafi, M. Ghorbani and M. Jalali, Fullerenes, Nanotubes, and Carbon Nanostructures, **18**, 107 (2010).
[23] D. A. Klarner, Polyominoes, In: J. E. Goodman and J. O'Rourke, (eds.) Handbook of Discrete and Computational Geometry, pp. 225–242. CRC Press, Boca Raton (1997) Chapter 12.
[24] H. Wiener, J. Am. Chem. Soc., **69**, 17 (1947).
[25] P. V. Khadikar, Nat. Acad. Sci. letters 23, 113 (2000).
[26] P. V. Khadikar, S. Karmarkar and V.K. Agrawal, J. Chem. Inf. Comput. Sci. **41**, 934 (2001).
[27] A. R. Ashrafi, H. Saati and M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **3**(4), 227 (2008).
[28] A. R. Ashrafi, M. Ghorbani and M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 245 (2008).
[29] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2008).
[30] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 313 (2009).
[31] A. R. Ashrafi, M. Ghorbani, M. Hemmasi, Digest Journal of Nanomaterials and Biostructures, **4**(3), 483 (2009).
[32] A. R. Ashrafi, M. Ghorbani, Digest Journal of Nanomaterials and Biostructures, **4**(2), 389 (2009).

[33] M. Ghorbani, M. B. Ahmadi and M. Hemmasi, Digest Journal of Nanomaterials and Biostructures, **3**(4), 269 (2009).
[34] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(1), 177 (2009).
[35] M. Ghorban, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**(3), 403 (2009).
[36] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4(**4), 681 (2009).