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ON OMEGA AND RELATED POLYNOMIALS OF DENDRIMERS

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ABSTRACT. Omega polynomial was introduced by Diudea. Following Omega polynomial, the Sadhana polynomial was defined by Ashrafi et al. In this paper we compute Omega and Sadhana polynomials of three classes of dendrimers.

Key Words: *Omega, Theta and Sadhana Polynomials, Chain graph, Dendrimer*

INTRODUCTION

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They have been studied from the topological point of view, including vertex and fragment enumeration and calculation of some topological descriptors, such as topological indices, sequences of numbers or polynomials. In the present work we compute Omega, Theta and Sadhana polynomials of three classes of dendrimers by using the definition of chain graphs [1, 2]. Let G be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge-sets of which being denoted by $V(G)$ and $E(G)$, respectively. Suppose G is a connected molecular graph and $x, y \in V(G)$. The distance $d(x,y)$ between x and y is defined as the length of a minimum path between x and y. Two edges $e = ab$ and $f = xy$ of G are called codistant, "e co f", if and only if $d(a,x) = d(b,y) = k$ and $d(a,y) = d(b,x) = k+1$ or vice versa, for a non-negative integer k. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary transitive. Set $C(e) := \{f \in E(G) \mid f \text{ co } e\}$. If the relation "co" is transitive on $C(e)$ then $C(e)$ is called an orthogonal cut "oc" of the graph G. The graph G is called co-graph if and only if the edge set $E(G)$ is the union of disjoint orthogonal cuts. Observe *co* is a Θ relation, (*Djoković-Winkler*) [3, 4]:

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$$d(x,u)+d(y,v)\neq d(x,v)+d(y,u)$$

and Θ is a *co*-relation if and only if *G* is a partial cube, as Klavžar [5] correctly stated in a recent paper. Relation Θ is reflexive and symmetric but need not be transitive. Klavžar noted by Θ* the Θ transitive closure, then Θ* is an equivalence (see also the co relation). In this respect, recall some other definitions.

Let *m*(*G*,*c*) be the number of *qoc* strips of length *c* in the graph *G*; for the sake of simplicity, *m*(*G*,*c*) will hereafter be written as *m*. Two counting polynomials have been defined [6–9] on the ground of *qoc* strips, $\Omega(G,x)=\sum_c m\cdot x^c$ and $\Theta(G,x)=\sum_c m\cdot c\cdot x^c$. In a counting polynomial, the first derivative (in *x*=1) defines the type of property which is counted; for the two polynomials they are $\Omega'(G,1)=\sum_c m\cdot c=e=|E(G)|$ and $\Theta'(G,1)=\sum_c m\cdot c^2$.

The Sadhana index Sd(G) was defined by Khadikar et al [10,11] as $Sd(G)=\sum_c m(G,c)(|E(G)|-c)$, where *m*(*G,c*) is the number of strips of length *c*. The Sadhana polynomial *Sd*(*G,x*) was defined by Ashrafi et al. [12] as $Sd(G,x)=\sum_c m(G,c)\times x^{|E|-c}$. From the definition of Omega polynomial, one can obtain the Sadhana polynomial by replacing x^c with $x^{|E|-c}$. Then the Sadhana index will be the first derivative of *Sd*(*G, x*) evaluated at *x* = 1. The aim of this study is to compute the Omega and two related polynomials for some special cases of chain graphs. Throughout this paper, our notations are standard and all of graphs are simple and connected. We encourage the reader to consult papers [13 − 21].

RESULTS AND DISCUSSION

In this section we present explicit formulas for the Omega and Sadhana polynomials of some chain graphs. We also encourage the reader to consult [18] for background material, as well as for basic computational techniques. Let G_i's ($1\leq I\leq k$) be some graphs. A chain graph can be obtained from union of G_i's by joining each v_i to v_{i+1} where $v_i\in G_i$. We denote a chain graph by $G = G(G_1, \ldots, G_k, v_1, \ldots, v_k)$, Figure 1. It is easy to see that $|V(G)|=\sum_{i=1}^{k}|V(G_i)|$, $|E(G)|=(k-1)+\sum_{i=1}^{k}|E(G_i)|$ and the following Lemmas for a chain graph holds:

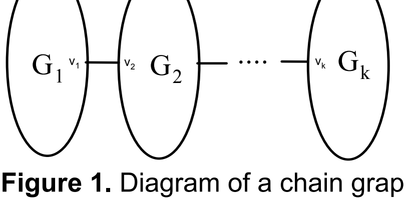

Figure 1. Diagram of a chain graph

Lemma 1. Let $G = G(G_1,...,G_k,v_1,...,v_k)$ be a simple connected chain graph and e$\in$ E(G_1) and f $\in$E(G_2). Then the edges *e* and *f* don't satisfy the "co" relation, in other words, $e \not\Theta f$.

Proof. Let *e* = *ab* $\in$ G_1 and *f* = *xy* $\in$ G_2 be arbitrary edges. We consider the following cases:

(*i*) $d(a,v_1) = d(b,v_1) = k_1$ and $d(x,v_2) = d(y,v_2) = k_2$. Then

$$d(a,y) = d(a,v_1) + d(v_1,v_2) + d(v_2,y) = k_1 + k_2 + 1$$

and

$d(a,x) = d(a,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1$. This implies that $e \not\Theta f$.

(*ii*) $d(a,v_1) = d(b,v_1) = k_1$ and $d(x,v_2) = k_2, d(y,v_2) = k_2 + 1$. So,

$$d(a,x) = d(a,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1$$

and

$$d(b,x) = d(b,v_1) + d(v_1,v_2) + d(v_2,x) = k_1 + k_2 + 1.$$

This implies that. $e \not\Theta f$.

(*iii*) $d(a,v_1) = k_1, d(b,v_1) = k_1 + 1$ and so,

$$d(x,a) = d(x,v_2) + d(v_2,v_1) + d(v_1,a) = k_2 + k_1 + 1$$

and

$$d(y,a) = d(y,v_2) + d(v_2,v_1) + d(v_1,a) = k_2 + k_1 + 1.$$

This implies that $e \not\Theta f$.

Lemma 2. Let $G = G(G_1,...,G_k,v_1,...,v_k)$ be a chain graph, $u \in V(G_i)$ and $v \in V(G_j)$ ($1 \le i, j \le k, i \ne j$). Then

$$d(u,v) = d(u,v_i) + d(v_i,v_j) + d(v_j,v) = d(u,v_i) + d(v_j,v) + |i - j|.$$

Proof. For every $1 \le i, j \le k, i \ne j$, $d(u_i,u_j)= |I - j|$ and this completes the proof.

Theorem 3. Let *G* be a graph with two blocks G_1, G_2 and a cut-edge $uv \in E(G)$ (Figure 2). Then: $\Omega(G,x) = x + \Omega(G_1,x) + \Omega(G_2,x)$.

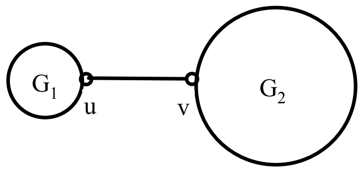

Figure 2. Diagram of a chain graph with two blocks

Proof. By using definition of Omega polynomial and Lemma 1 one can see that

$$\Omega(G,x) = x + \sum_{c_1} m(G_1,c_1)x^{c_1} + \sum_{c_2} m(G_2,c_2)x^{c_2} = x + \Omega(G_1,x) + \Omega(G_2,x).$$

Corollary 4. If $G = G(G_1,...,G_k,v_1,...,v_k)$ is a simple connected chain graph then we have:

$$\Omega(G,x) = (k-1)x + \sum_{i=1}^{k}\Omega(G_i,x).$$

Corollary 5. Let $G = G(G_1,...,G_k,v_1,...,v_k)$ be a chain graph. Then,

$$Sd(G,x) = (k-1)x^{|E(G)|-1} + \sum_{i=1}^{k}\sum_{c_i} m(G_i,c_i)x^{|E(G)|-c_i}.$$

Further, if *G* is a bipartite graph then

$$\theta(G,x) = (k-1)x + \sum_{i=1}^{k}\theta(G_i,x).$$

Theorem **6**. Let *T* be a tree with *n* vertices and

$T = T_n = T(T_{n-1},T_1,v_{n-1},v_1)$. Then $\Omega(T_n,x) = (n-1)x$.

Proof. Let T_{n-1} be a tree with *n*-1 vertices constructed by cutting a pendant vertex *v* of T_n. It is easy to see that T is a chain graph and we can suppose

$T = T_n = G(T_{n-1}, T_1, u, v)$, Figure 3. By cutting a pendant vertex of T_{n-1}, then $T_{n-1} = G(T_{n-2}, T_1, u', v')$ and so on. We have the following equations:

$$\Omega(T_n,x) - \Omega(T_{n-1},x) = x$$
$$\Omega(T_{n-1},x) - \Omega(T_{n-2},x) = x$$
$$\vdots$$
$$\Omega(T_2,x) - \Omega(T_1,x) = x.$$

By summation of these relations one can see that $(T, x) = (n - 1)x$.

Example 7. Consider the graph of dendrimer *D* with *n* vertices in Figure 3. Since this graph is a tree with *n* vertices, according to Theorem 6, $\Omega(D,x) = (n-1)x$ and $\mathrm{Sd}(D, x) = (n-1)x^{n-2}$. Because a tree is bipartite (and a partial cube) then $\Theta(D, x) = (n-1)x$.

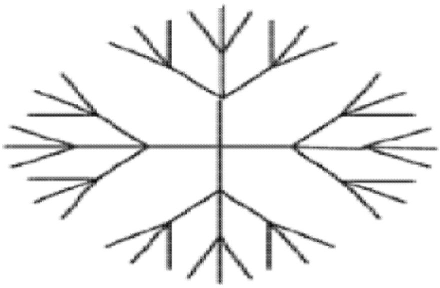

Figure 3. Graph of the dendrimer *D* of n = 52

Example 8. Consider the graph of the dendrimer S_1 with n vertices, Figure 4. It is easy to see that $\Omega(S_1, x) = 3x + 9x^2$. Now let S be a nanostar dendrimer shown in Figure 5. By computing the number of vertices and the number of edges we have $||V(S)| = 19n$ and $|E(S)| = 22n - 1$. Furthermore we can suppose $S = G(N_{n-1}, N_1, v_{n-1}, v_1)$ So we have the following relations:

$$\begin{aligned} \Omega(G_n, x) - \Omega(G_{n-1}, x) &= x + \Omega(G_1, x) \\ \Omega(G_{n-1}, x) - \Omega(G_{n-2}, x) &= x + \Omega(G_1, x) \\ &\vdots \\ \Omega(G_2, x) - \Omega(G_1, x) &= x + \Omega(G_1, x) \end{aligned},$$

By Summation of these relations one can easily deduce that $\Omega(S_n, x) - \Omega(S_1, x) = (n-1)x + (n-1)\Omega(S_1, x)$. This implies Omega polynomial of S_n is $\Omega(S_n, x) = (n-1)x + n\Omega(S_1, x)$. Because $\Omega(S_1, x) = 3x + 9x^2$ then, $\Omega(S_n, x) = 9nx^2 + (4n-1)x$ and so Sadhana polynomial is $Sd(S_n, x) = (4n-1)x^{22n-2} + 9nx^{22n-3}$. On the other hand S_n is bipartite and then $\Theta(S_n, x) = 18nx^2 + (4n-1)x$.

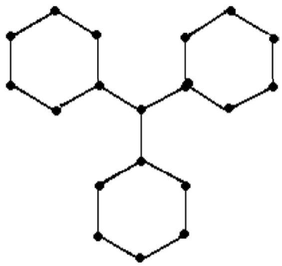

Figure 4. Graph of the dendrimer S_1

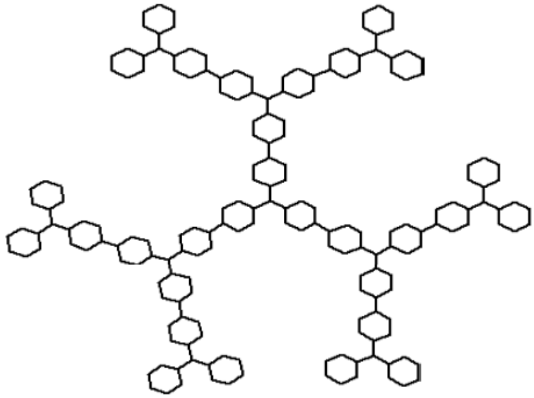

Figure 5. Graph of the nanostar dendrimer S for $n = 3$

Example 9. Now consider the graph H_1 shown in Figure 6. It is easy to see that $\Omega(H\text{-}1, x) = 4x+15x^2$. By using definition of chain graph the graph H_n (Figure 7), it is easy to see that

$$H_n = (H_{n-1}, H_1; u, v):$$

So, we have the following equations:

$$\begin{aligned}
\Omega(H_n, x) - \Omega(H_{n-1}, x) &= x + \Omega(H_1, x)\\
\Omega(H_{n-1}, x) - \Omega(H_{n-2}, x) &= x + \Omega(H_1, x)\\
&\vdots\\
\Omega(H_2, x) - \Omega(H_1, x) &= x + \Omega(H_1, x)
\end{aligned}$$

By summation of these equations one can see that $\Omega(H_n, x) = (n + 3)x + 15nx^2$. Finally let D be the nanostar dendrimer in Figure 8. Clearly D is a chain graph and $\Omega(D, x) = (4n + 17)x + 4(30n + 3)x^2$. Because $|V(D)| = 120n + 12$ and $|E(D)| = 140n + 13$, then $Sd(D, x) = 4(30n + 3)x^{140n+11} + (4n + 17)x^{140n+12}$ and $\Theta(D, x) = 4(30n + 3)\, x^2 + (4n + 17)x$.

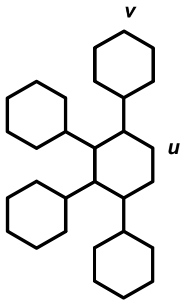

Figure 6. Graph of the nanostar dendrimer H_1

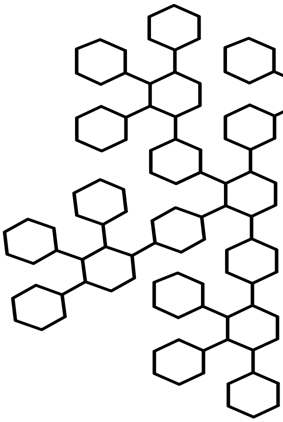

Figure 7. Graph of the nanostar dendrimer H_n

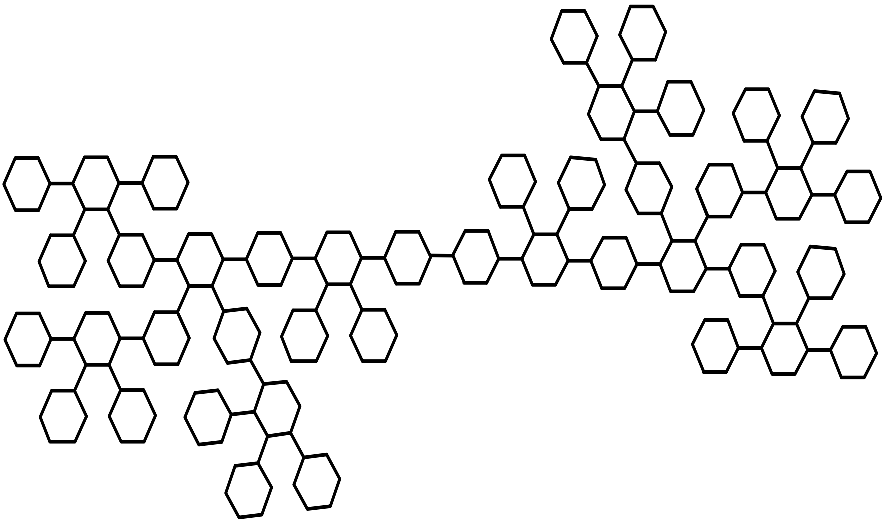

Figure 8. Graph of the nanostar dendrimer D

CONCLUSIONS

Nanostar dendrimers can be designed by using the concept of the chain graph. Because of their size, it is difficult to calculate these polynomials in higher generation dendrimers. Formulas for some families of nanostar dendrimers were derived. By this formula we can compute Omega and related polynomials of any nanostructures whose molecular graph is isomorphic to a chain graph.

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