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The Edge Szeged Polynomial of Graphs

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Abstract

The edge Szeged polynomial of a graph G is defined as $Sz_e(G,x) = \sum_{e=uv} x^{m_u(e)m_v(e)}$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u. In this paper the main properties of this newly proposed polynomial are investigated. We also compute this polynomial for some classes of well-known graphs. Finally, the edge Szeged polynomials of an infinite family of nanostar dendrimers are computed.

1. Introduction

Let G be a graph with vertex and edge sets V(G) and E(G), respectively. As usually, the distance between the vertices u and v of a connected graph G is denoted by d(u,v) and it is defined as the number of edges in a minimal path connecting the vertices u and v. Throughout the paper, a graph means an undirected, connected graph without loops and multiple edges.

In chemical graph theory, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of Graph Theory. A chemical graph is a graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

A topological index is a numeric quantity extracted from the structure of a graph which is invariant under automorphisms of G. Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most popular topological descriptor, the Wiener index, and used it to determine physical properties of alkanes [1]. Although this topological index is an easily calculable quantity, it does

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not uniquely correspond to the individual structure of a graph. John Platt was the only person who immediately realized the importance of the Wiener's pioneering work and wrote papers analyzing and interpreting the physical meaning of the Wiener index.

We recall some definitions that will be used in the paper. The Wiener index of a graph G is defined as the sum of all topological distances between the pair of vertices, where the topological distance is the number of edges on the shortest path between these vertices (see [2,3] for details). For two vertices u and v of G, the topological distance between them is denoted by d(u,v).

The PI index is a new topological index defined by Khadikar, [4-6]. It is defined as $PI(G) = \sum_{e=uv \in G}[m_u(e)+ m_v(e)]$, where $m_u(e)$ is the number of edges of G lying closer to u than to v and $m_v(e)$ is the number of edges of G lying closer to v than to u. Edges equidistant from both ends of the edge uv are not counted.

The Szeged index is another topological index which is introduced by Gutman, [7-9]. To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v. Suppose $n_u(e)$ is the number of vertices of G lying closer to u and $n_v(e)$ is the number of vertices of G lying closer to v. Then the Szeged index of the graph G is defined as $Sz(G) = \sum_{e=uv \in E(G)} n_u(e)n_v(e)$. Notice that vertices equidistant from u and v are not taken into account. In [10], the authors introduced an edge version of the Szeged index. It is defined as $Sz_e(G) = \sum_{e=uv \in E(G)} m_u(e)m_v(e)$, where $m_u(e)$ and $m_v(e)$ have the same meaning as above. Edges equidistant from both ends of an edge are not counted. In the mentioned paper, the main properties of this new index investigated and some open question addressed.

Diudea and Nagy in their recent book [11] wrote: “It is well-known that a graph can be described by: a connection table, a sequence of numbers, a matrix, a polynomial or a derived number called a topological index”. In this paper we apply a polynomial approach for studying the molecular graphs. Here, a finite sequence of some graph theoretical properties can be described by so-called counting polynomials $P(G,x) = \sum_k p(G,k) \cdot x^k$, where p(G,k) is the frequency of occurrence of the property partitions of G, of length k, and x is simply a parameter to hold k. The edge Szeged polynomial is a new counting polynomial for graphs defined by $Sz_e(G,x) = \sum_{e=uv} x^{m_u(e)m_v(e)}$, see [12,13].

The first attempt to study topological indices of nanostructures was done by Diudea and his co-authors, [14-20]. Next, the first author of this paper continued the

pioneering work of Diudea and his team to compute the PI and Szeged indices of some classes of nanostructures, [21-26]. We also encourage the reader to consult papers [27-31] for more information on this subject.

2. Examples

In this section the PI and edge Szeged polynomials of some well-known graphs are computed. In fact, the edge Szeged polynomials of K_n, C_n, W_n, P_n and $K_{n_1,n_2,\ldots,n_r}$ are computed. The PI polynomials of these graphs have been computed in [32].

Example 1. Consider the complete graph K_n and the cycle graph C_n. Then

$$Sz_e(K_n,x) = \binom{n}{2} x^{(n-2)^2} \; ; \; Sz_e(C_n,x) = \begin{cases} nx^{\left(\frac{n-2}{2}\right)^2} & 2 \mid n \\ nx^{\left(\frac{n-1}{2}\right)^2} & 2 \nmid n \end{cases}.$$

Example 2. Suppose P_n is the path with n vertices. Then $Sz_e(P_1,x) = Sz_e(P_2,x) = 1$, $Sz_e(P_3,x) = 2$ and for $n > 3$,

$$Sz_e(P_n,x) = \begin{cases} 2 + 2x^{n-3} + 2x^{2(n-4)} + \ldots + 2x^{n(n-4)/4} + x^{(n-2)^2/4} & 2 \mid n \\ 2 + 2x^{n-3} + 2x^{2(n-4)} + \ldots + 2x^{(n-1)(n-3)/4} & 2 \nmid n \end{cases}.$$

Example 3. Consider a complete r-partite graph $G = K_{n_1,n_2,\ldots,n_r}$ containing $n = |V(G)|$ vertices. By definition, the vertices V of this graph can be partitioned into subsets V_1, V_2, ..., V_r such that for every i, $1 \le i \le r$, there is no edge between the vertices of V_i (Figure 1). Then $Sz_e(K_{n_1,n_2,\ldots,n_r},x) = \sum_{1 \le i \le j \le r} n_i n_j x^{(n-n_i-1)(n-n_j-1)}$. In particular, if S_n denotes the star graph on n+1 vertices then $Sz_e(S_n,x) = n$.

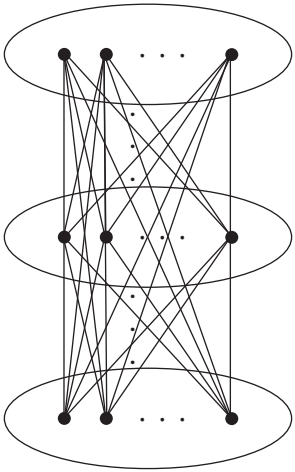

Figure 1. An r-partite Graphs.

Example 4. A wheel W_n is a graph of order n which contains a cycle of order n, and for which every vertex in the cycle is connected to the central vertex, Figure 2. Then $Sz_e(W_3,x) = 6x^4$, $Sz_e(W_4,x) = 4x^4 + 4x^6$ and for $n > 4$, $Sz_e(W_n,x) = nx^9 + nx^{2(2n-5)}$.

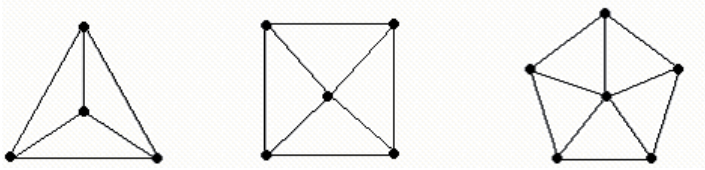

Figure 2. The Wheel Graph W_3, W_4 and W_5.

3. Main Results and Discussion

In this section, some basic properties of edge Szeged polynomial are investigated. Then the edge Szeged polynomial of a particular type of nanostar dendrimer is computed.

Lemma 1. Let G be a connected graph with n vertices and m edges. Then

a) $Sz_e(G,1) = m$,

b) $Sz_e'(G,1) = Sz_e(G)$,

c) $\deg Sz_e(G,x) \le \begin{cases} \frac{m(m-2)}{4} & 2|m \\ \frac{(m-1)^2}{4} & 2\nmid m \end{cases}$ and $Sz_e(G,x) \le \begin{cases} \frac{m^2(m-2)}{4} & 2|m \\ \frac{m(m-1)^2}{4} & 2\nmid m \end{cases}$,

d) If T is a tree then $Sz_e(T,x) = x^{1-n}Sz(T,x)$, with $Sz(T,x)$ being the Szeged polynomial defined on vertices: $Sz(G,x) = \sum_{e=uv\in E(G)} x^{n_u(e)n_v(e)}$.

Proof. (a) and (b) are trivial. To prove c), notice that $m_u(e) + m_v(e) \le m - 1$. So the maximum value of $m_u(e)m_v(e)$ is $\frac{m(m-2)}{4}$ or $\frac{(m-1)^2}{4}$, when m is even or odd, respectively. We now assume that T is tree. Then

$$\begin{aligned} Sz_e(T,x) &= \sum_{e=uv} x^{m_u(e)m_v(e)} \\ &= \sum_{e=uv} x^{(n_u(e)-1)(n_v(e)-1)} \\ &= \sum_{e=uv} x^{n_u(e)n_v(e)-[n_u(e)+n_v(e)-1]} \\ &= \sum_{e=uv} x^{n_u(e)n_v(e)-n+1} \\ &= x^{1-n}\sum_{e=uv} x^{n_u(e)n_v(e)} \\ &= x^{1-n}Sz(T,x). \end{aligned}$$ ♦

By part (b) of the previous Lemma and also Example 3, one can see that $Sz_e(K_{n_1,n_2,\ldots,n_r}) = \sum_{1\le i\le j\le r} n_i n_j (n-n_i-1)(n-n_j-1)$. In what follows, we first define the concepts of weighted edge Szeged polynomial and hyper-edge Szeged index of a graph G. Then the main properties of this polynomial is proved, [37,38].

Question 1: Under which condition(s) the equality holds in part (c)?

Definition. A vertex weighted graph is a graph which associates a label (weight) with every vertex in the graph. Weights are usually real numbers. They may be restricted to rational numbers or integers. Let G be a connected vertex weighted graph with weight function w: $V(G) \to R$. The weighted edge Szeged polynomial of G is defined as $Sz_{ew}(G,x) = \sum_{e=uv} w(u)w(v)x^{m_u(e)m_v(e)}$. We also define the hyper-edge Szeged index of G as $Sz^{(2)}_{ew}(G) = \sum_{e=uv} w(u)w(v)[(m_u(e))^2(m_v(e))^2 + m_u(e)m_v(e)]$.

Lemma 2. $Sz^{(2)}_{ew}(G) = 2Sz'_{ew}(G,1) + Sz''_{ew}(G,1)$.

Proof. By definition

$$\begin{aligned} 2Sz'_{ew}(G,1)+Sz''_{ew}(G,1) &= 2\sum_{e=uv} w(u)w(v)m_u(e)m_v(e) \\ &+ \sum_{e=uv} w(u)w(v)m_u(e)m_v(e)[m_u(e)m_v(e)-1] \\ &= \sum_{e=uv} w(u)w(v)[2m_u(e)m_v(e)+m_u(e)^2 m_v(e)^2 - m_u(e)m_v(e)] \\ &= \sum_{e=uv} w(u)w(v)[m_u(e)m_v(e)+m_u(e)^2 m_v(e)^2] \\ &= Sz^{(2)}_{ew}(G). \end{aligned}$$ ♦

The nanostar dendrimer is part of a new group of macromolecules that seem photon funnels just like artificial antennas and also, it is a great resistant of photo bleaching. The nanostar dendrimer promises to have great applications but first the structure must be understood. In what follows, the edge Szeged polynomial of a particular class of nanostar dendrimer, NS[n], is computed, Figure [3].

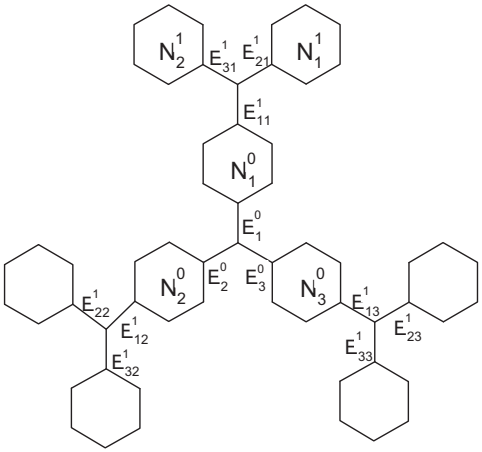

Figure.3. The Nanostar Dendrimer NS[1].

Using a simple calculation, one can show that $|V(NS[n])| = 39\times2^n - 20$ and $|E(NS[n])| = 45\times2^n - 24$. For the edges $e = E_1^0 = a_1b_1$, $E_2^0 = a_2b_2$, $E_3^0 = a_3b_3$, $m_{a_r}(E_r^0) = \frac{|E(NS[n])|}{3} - 1 = 15\times2^n - 9$, $1 \le r \le 3$. Consider edges of E_{rk}^i, $r = 1, 2, 3$, $1 \le i \le n$ and $1 \le k \le 3\times2^{i-1}$. If $e = uv = E_{2k}^i$ then $m_u(e) = 12(2^{n-i}-1) + 3(2^{n-i}-1) + 6 = 15\times2^{n-i} - 9$ and for $f = xy = E_{1k}^i$, $m_x(f) = 30\times2^{n-i}-16$.

Finally, if h = ab = E_{3k}^{i}, $m_a(h) = 12(2^{n-i}-1) + 3(2^{n-i}-1) + 6 = 15\times2^{n-i} - 9$. On the other hand, for edge e = uv of hexagons N_j^i, $0\le i\le n$, $1\le j\le 3\times2^i$, Figure 3, $m_u(e) = 12(2^{n-i}-1) + 3(2^{n-i}-1) + 2 = 15\times2^{n-i} - 13$. Therefore,

$$
\begin{aligned}
Sz_e(NS[n],x) &= \sum_{e=uv} x^{m_u(e)m_v(e)} \\
&= 3x^{(15\times2^n-9)(30\times2^n-16)} \\
&+ 6\sum_{i=1}^{n} 2^{i-1}x^{(15\times2^{n-i}-9)(45\times2^n-15\times2^{n-i}-16)} \\
&+ 3\sum_{i=1}^{n} 2^{i-1}x^{(30\times2^{n-i}-16)(45\times2^n-30\times2^{n-i}-9)} \\
&+ 18\sum_{i=0}^{n} 2^{i}x^{(15\times2^{n-i}-13)(45\times2^n-15\times2^{n-i}-13)} \\
&= 3\sum_{i=1}^{n} 2^{i}(x^{675\times2^{2n-i}-225\times2^{2n-2i}-105\times2^{n-i}-405\times2^n+144} + \frac{1}{2}x^{1350\times2^{2n-i}-900\times2^{2n-2i}+210\times2^{n-i}-720\times2^n+144} \\
&+ 6x^{675\times2^{2n-i}-225\times2^{2n-2i}-585\times2^n+169}) + 3(x^{450\times4^n-510\times2^n+144} + 6x^{450\times4^n-585\times2^n+169})
\end{aligned}
$$

This completes our calculations.

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