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Computing the First and Third Zagreb Polynomials of Cartesian Product of Graphs

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ABSTRACT

Let G be a graph. The first Zagreb polynomial $M_1(G, x)$ and the third Zagreb polynomial $M_3(G, x)$ of the graph G are defined as: $M_1(G,x) = \sum_{e=uv\in E(G)} x^{[d(u)+d(v)]}$, $M_3(G,x) = \sum_{e=uv\in E(G)} x^{|d(u)-d(v)|}$. In this paper, we compute the first and third Zagreb polynomials of Cartesian product of two graphs and a type of dendrimers.

Keywords: Zagreb polynomial, Zagreb index, graph.

1. INTRODUCTION

Molecules and molecular compounds are often modeled by molecular graph. A molecular graph is a representation of the structural formula of a chemical compound in terms of graph theory, whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds.

A topological index is a graph invariant applicable in chemistry. The Wiener index is the first topological index introduced by chemist Harold Wiener.[1,2] There are some topological indices based on degrees such as the first and third Zagreb indices of molecular graphs. The first Zagreb index $M_1 = M_1(G)$ and the third Zagreb index $M_3 = M_3(G)$ of a graph G are defined as:

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$$M_1(G) = \sum_{e=uv\in E(G)}[d(u) + d(v)], \qquad M_3(G) = \sum_{e=uv\in E(G)}|d(u) - d(v)|$$

where d(u) denotes the degree of a vertex u in G. [3–8]

The first Zagreb polynomial $M_1(G,x)$ and the second Zagreb polynomial $M_3(G,x)$of a graph G are defined as:

$$M_1(G,x) = \sum_{e=uv\in E(G)} x^{[d(u)+d(v)]}, \qquad M_3(G,x) = \sum_{e=uv\in E(G)} x^{|d(u)-d(v)|}.$$

For more study about polynomial in graph theory you can see [9–14].

The path P_n is the shortest walk between two vertices. We denote Star, wheel, cycle and complete graph by S_n, W_n, C_n and K_n, respectively. The union of $G\cup H$ of graphs G and H is a graph such that $V(G\cup H) = V(G) \cup V(H)$, and $E(G \cup H) = E(G) \cup E(H)$. The Cartesian product $G \times H$ of graphs G and H is a graph such that $V(G \times H) = V(G) \times V(H)$, and any two vertices (a,b) and (u,v) are adjacent in $G \times H$ if and only if either a = u and b is adjacent with v, or b = v and a is adjacent with u. [12]

2. THE FIRST AND THIRD ZAGREB POLYNOMIALS OF A GRAPH.

The considerations in the subsequent sections are based on the applications of the following definitions. In this section, we present some new bounds for the first and third Zagreb indices of graphs and compare them with each other.

Example. Let K_n, S_n and W_n are complete, star and wheel graphs, then

$$M_1(K_n,x) = n(n-1)/2x^{2(n-1)},$$
$$M_3(K_n,x) = n(n-1),$$
$$M_1(S_n,x) = (n-1)x^n,$$
$$M_3(G,x) = (n-1)x^{n-2},$$
$$M_1(W_n,x) = (n-1)x^{n+2} + (n-1)x^6,$$
$$M_3(W_n,x) = (n-1)x^{(n-4)} + n - 1.$$

Lemma 1. Let G and H be two graphs, then

$$M_1(G\cup H,x) = M_1(G,x) + M_1(H,x)$$

and

$$M_3(G\cup H,x) = M_3(G,x) + M_3(H,x).$$

Proof. The proof is straightforward. □

Theorem 2. Let G and H be two graphs, then

$$M_1(G\times H,\ x) = d(G,x^2)M_1(H,\ x) + d(H,x^2)M_1(G,\ x),$$

where d(G, x)= $\sum_{i=1}^{n} x^{d_i}$.

Proof. By definition of G × H, we have $d_{G\times H}(a,b) = d_G(a) + d_H(b)$ then

$$\begin{aligned}
M_1(G\times H,x) &= \sum_{e=(a,b)(c,d)\in E(G\times H)} x^{d(a,b)+d(c,d)} \\
&= \sum_{e=(a,b)(a,d)\in E(G\times H)} x^{d(a,b)+d(a,d)} + \sum_{e=(a,b)(c,b)\in E(G\times H)} x^{d(a,b)+d(c,b)} \\
&= \sum_{e=(a,b)(a,d)\in E(G\times H)} x^{2d(a)+d(b)+d(d)} + \sum_{e=(a,b)(c,b)\in E(G\times H)} x^{2d(b)+d(a)+d(c)} \\
&= \sum_{e=(a,b)(a,d)\in E(G\times H)} x^{2d(a)} x^{d(b)+d(d)} + \sum_{e=(a,b)(c,b)\in E(G\times H)} x^{2d(b)} x^{d(a)+d(c)} \\
&= \sum_{e=bd\in E(H),a\in V(G)} x^{2d(a)} x^{d(b)+d(d)} + \sum_{e=ac\in E(G),b\in V(H)} x^{2d(b)} x^{d(a)+d(c)} \\
&= \sum_{e=bd\in E(H),a\in V(G)} (x^2)^{d(a)} x^{d(b)+d(d)} + \sum_{e=ac\in E(G),b\in V(H)} (x^2)^{d(b)} x^{d(a)+d(c)} \\
&= \sum_{a\in V(G)} (x^2)^{d(a)} \sum_{e=bd\in E(H)} x^{d(b)+d(d)} + \sum_{b\in V(H)} (x^2)^{d(b)} \sum_{e=ac\in E(G)} x^{d(a)+d(c)} \\
&= d(G,x^2)M_1(H,x) + d(H,x^2)M_1(G,x).
\end{aligned}$$

This completes our argument. □

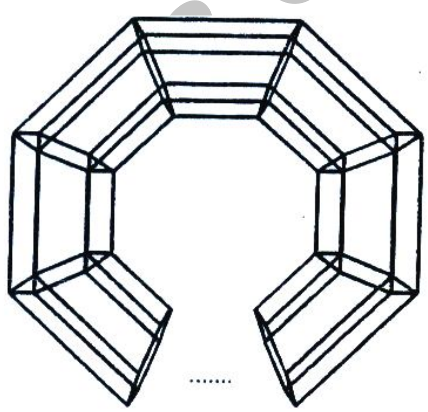

Figure 1. $C_m \times C_n$.

Corollary 3. $M_1(C_m \times C_n,\ x) = 2mnx$ and $M_2(C_m \times C_n,\ x) = 2mnx$.

Proof. The graph $C_m \times C_n$ is 4–regular, so by Theorem 2 we have $M_1(C_m \times C_n,\ x) = 2mnx$. The second equation is obtained by definition of the second Zagreb index. □

Theorem 4. Let G and H be two graphs then

$$\frac{M_3(\prod_{i=1}^{k} G_i,\ x)}{|\prod_{i=1}^{k} G_i|} = \sum_{i=1}^{k} \frac{M_3(G_i,\ x)}{|G_i|}.$$

Proof. At first we prove for G×H. We have $d_{G\times H}(a,b) = d_G(a) + d_H(b)$ then

$$\begin{aligned} M_3(G\times H, x) &= \sum_{e=(a,b)(c,d)\in E(G\times H)} x^{|d(a,b)-d(c,d)|} \\ &= \sum_{e=(a,b)(a,d)\in E(G\times H)} x^{|d(a,b)-d(a,d)|} + \sum_{e=(a,b)(c,b)\in E(G\times H)} x^{|d(a,b)-d(c,b)|} \\ &= \sum_{e=(a,b)(a,d)\in E(G\times H)} x^{|d(b)-d(d)|} + \sum_{e=(a,b)(c,b)\in E(G\times H)} x^{|d(a)-d(c)|} \\ &= \sum_{e=bd\in E(H), a\in V(G)} x^{|d(b)-d(d)|} + \sum_{e=ac\in E(G), b\in V(H)} x^{|d(a)-d(c)|} \\ &= |G| \sum_{e=bd\in E(H)} x^{|d(b)-d(d)|} + |H| \sum_{e=ac\in E(G)} x^{|d(a)-d(c)|} \\ &= |G|\, M_3(H,x) + |H|\, M_3(G,x). \end{aligned}$$

Now we proceed by induction on k to complete the proof. □

Corollary 5. $M_3(C_m \times C_n,\ x) = 2mn.$

3. THE FIRST AND THIRD ZAGREB POLYNOMIALS OF A NANOSTAR DENDRIMER

In this section, we compute the first and third Zagreb polynomials of a type of nanostar dendrimers, Figure 1.

Theorem 6. Let Ns[n] be above nanostar dendrimer, then

$$M_1(NS(n), x) = (2^{n+1}-2)x^6 + (6\times 2^{n+1}-3)x^5 + (6\times 2^{n+1}-3)x^4,$$

and

$$M_3(NS(n), x) = (6\times 2^{n+1}-4) + (7\times 2^{n+1}-4)x^1.$$

Proof. The graph NS[n] has three type of edge, with degrees 2 and 2, degrees 2 and 3, degrees 1 and 3. Thus by definition of Zagreb polynomials we can compute

$$M_1(NS(n), x) = (2^{n+1}-2)x^6 + (6\times 2^{n+1}-3)x^5 + (6\times 2^{n+1}-3)x^4,$$

and

$$M_3(NS(n), x) = (6\times 2^{n+1}-4) + (7\times 2^{n+1}-4)x^1.$$

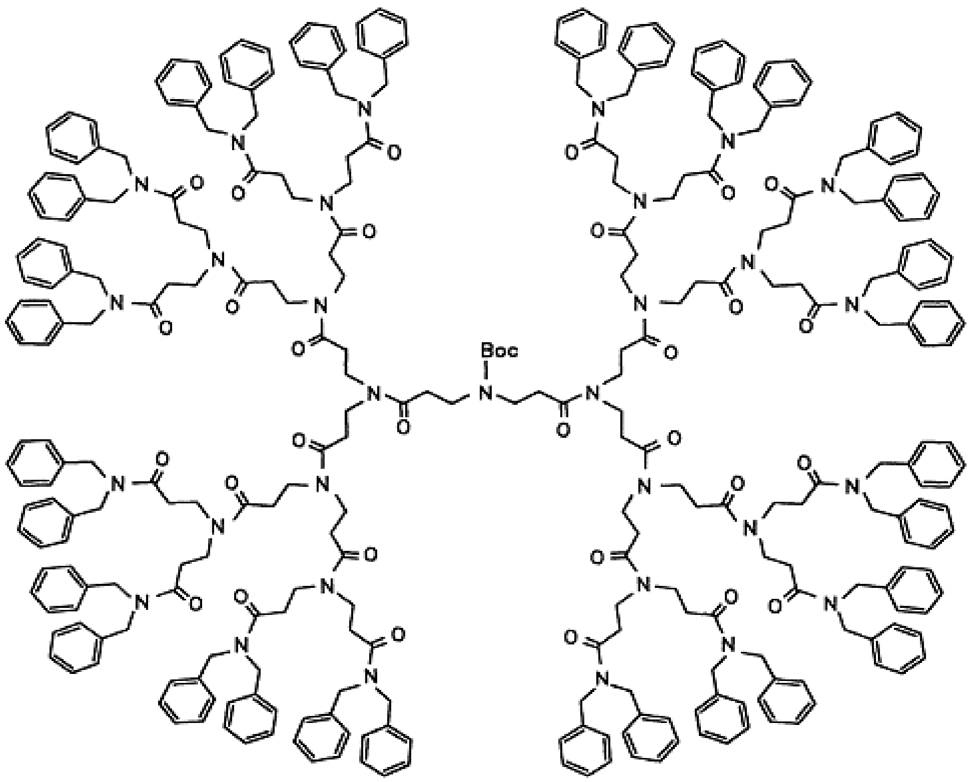

Figure 2. Nanostar Dendrimer Ns[4].

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