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Szeged and GA_2 indices of Suzuki's Bi-branched dendrimers

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Let G be a simple connected graph. If e = uv is an edge of G and $n_u(e)$ is the number of vertices closer to u than v and $n_v(e)$ is the number of vertices closer to v than u then the Szeged and second GA indices of G are defined as $Sz(G) = \Sigma_{e=uv} n_u(e)n_v(e)$ and $GA_2(G) = \Sigma_{e=uv} 2\sqrt{n_u(e)n_v(e)}/[n_u(e) + n_v(e)]$. In this paper, the Szeged and GA_2 indices of two types of dendrimers are computed for the first time.

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1. Introduction

Dendrimers are large and complex molecules with very well-defined chemical structures. They consist of three major architectural components: core, branches and end groups. Nanostar dendrimers are part of a new group of macromolecules. The topological study of these macromolecules is the subject of some recent papers [1,2].

Let G be a connected simple molecular graph with vertex and edge sets V(G) and E(G), respectively. As usual, the distance between the vertices u and v of G is denoted by $d_G(u,v)$ (or d(u,v) for short) and it is defined as the number of edges in a minimal path connecting vertices u and v [3].

The Szeged and second Geometric-Arithmetic indices of a graph G is defined as $Sz(G) = \Sigma_{e=uv}[n_u(e)n_v(e)]$ and $GA_2(G) = \sum_{e=uv} \frac{2\sqrt{n_u(e)n_v(e)}}{[n_u(e) + n_v(e)]}$, where $n_u(e)$ is the number of vertices lying closer to u than to v and $n_v(e)$ is defined analogously [4,5]. The mathematical properties of these topological indices can be found in some recent papers [6-13].

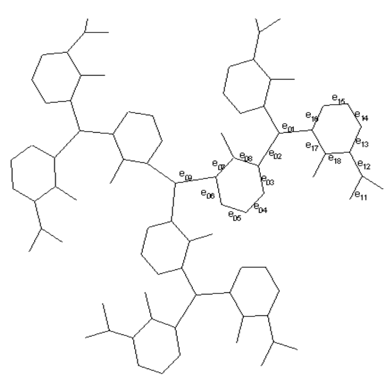

Fig. 1. The Suzuki's Bi-branched Dendrimer.

In this paper our notation is standard and taken mainly from the standard book of graph theory. The goal of this article is to compute the Szeged and GA_2 indices of two classes of dendrimeric nanostars.

2. The Szeged index of S[n]

In this section the Szeged and GA_2 indices of a class of nanostar dendrimers, S[n], are computed. If A and B are graphs such that $V(A) \subseteq V(B)$ and $E(A) \subseteq E(B)$ then A is called a subgraph of B, $A \leq B$. To compute these topological indices, we partition the edge set of S[n] into the classes with the same $n(e) = n_u(e)n_v(e)$, where e = uv is an edge of S[n]. We first notice that the graph S[n] can be constructed from subgraphs isomorphic to H and the core of S[n], see Figs. 2 and 3.

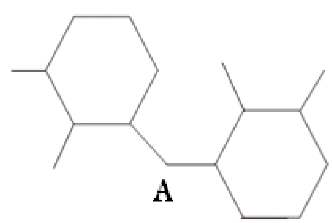

Fig. 2. The Peace H of S[n].

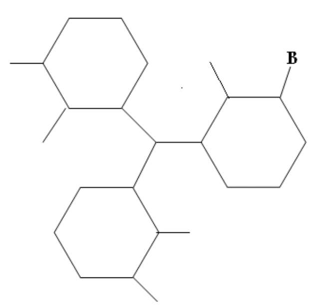

Fig. 3. The Core K of S[n].

We now explain our method for constructing S[n]. In the first step, we join a subgraph isomorphic to H from vertex A to a subgraph isomorphic to K in the vertex B. Since, K has exactly three branches, we can construct S[1] by K and three isomorphic subgraphs. In the second step, six subgraphs isomorphic to H join with S[1]. Finally, in the step r, 3×2^r subgraphs isomorphic to H are joined to S[r-1]. Begin by a simple calculation. Clearly, Sz(K) = 3564. For computing Sz(S[1]), it is enough to consider edges $e_{01}, e_{02}, e_{03}, e_{04}, e_{05}, e_{06}, e_{07}, e_{08}$ and e_{09} in the first step and edges $e_{11}, e_{12}, e_{13}, e_{14}, e_{15}, e_{16}, e_{17}, e_{18}$ in the second step of our algorithm. In what follows, our calculations are given in Table 1.

Table 1. The summation of $n_u(e)n_v(e)$ for the edges similar to e of S[1].

Types of Edges	Sum	Types of Edges	Sum
e_{01}	4500	e_{11}	1764
e_{02} e_{03}, e_{06}	12096	e_{12}, e_{13}, e_{16}	4428
e_{05}, e_{08}	8784	e_{15}, e_{18}	5688
e_{04}, e_{07}	9000	e_{14}, e_{17}	6552
e_{09}	4788		

By these calculations $Sz(S[1]) = 57600$. We now compute the Szeged index of S[2]. To do this, we compute.

Table 2. The summation of $n_u(e)n_v(e)$ for the edges similar to e of S[2].

Types of Edges	Sum	Types of Edges	Sum	Types of Edges	Sum
e_{21}	8649	e_{11}	21960	e_{01}	27720
e_{22}, e_{23}, e_{26}	20520	e_{12}, e_{13}, e_{16}	32508	e_{02} e_{03}, e_{06}	54054
e_{25}, e_{28}	26928	e_{15}, e_{18}	24336	e_{05}, e_{08}	38052
e_{24}, e_{27}	31248	e_{14}, e_{17}	25200	e_{04}, e_{07}	38700
				e_{09}	20286

By these calculations, Sz(S[2]) = 370152. We are now ready to calculate the step n of this nanostar. In Table 3, the values of $n_u(e)n_v(e)$ for types of edges are computed.

Set $A_1 = \{e_{n1}, e_{n2}, e_{n3}, e_{n4}, e_{n5}, e_{n6}, e_{n7}, e_{n8}, e_{(n-1)1}\}$, $A_2 = \{e_{(n-i)2}, e_{(n-i)3}, e_{(n-i)6} : 1 \le i \le n\}$, $A_3 = \{e_{(n-i)5}, e_{(n-i)8} : 1 \le i \le n\}$, $A_4 = \{e_{(n-i)4}, e_{(n-i)7} : 1 \le i \le n\}$ and $A_5 = \{e_{(n-i)1} : 2 \le i \le n\}$. Define S_i to be the summation of $n_u(e)n_u(v)$ over all edges $e = uv \in A_i$. By calculations given in Table 1, one can see that:

$S_1 = ((30 + 27n(n + 1)) \times 1)\times 3(2^{n+2} - 1) + (((30 + 27n(n + 1)) - 2) \times 3)(3^2 \times 2^n) + (((30 + 27n(n + 1)) - 5) \times 6)(3 \times 2^{n+1}) + (((30 + 27n(n + 1)) - 6) \times 7)(3 \times 2^{n+1}) + (((30 + 27n(n + 1)) - 9) \times 10)(3 \times 2^n) = 3654 \times 2^n + 3969n \times 2^n + 3969n^2 \times 2^n - 81n - 81n^2 - 90$,

$$S_2 = \sum_{i=1}^{n}(((30+27n(n+1)) - (20+(i-1)18)) \times (21+(i-1)18))(3\times 3)$$

$$= 2295 + 4131n^3 + 3483n^2 + 2187n^4$$

$$S_3 = \sum_{i=1}^{n}(((30+27n(n+1)) - (23+(i-1)18)) \times (24+(i-1)18))(3\times 2)$$

$$= 1602n + 3240n^3 + 2484n^2 + 1458n^4$$

$$S_4 = \sum_{i=1}^{n}(((30+27n(n+1)) - (24+(i-1)18)) \times (25+(i-1)18))(3\times 2)$$

$$= 1602n + 3402n^3 + 2538n^2 + 1458n^4$$

$$S_5 = \sum_{i=1}^{n-1}(((30+27n(n+1)) - (27+(i-1)18)) \times (28+(i-1)18))(3\times 2)$$

$$+ (((30+27n(n+1)) - (27+(n-1)18)) \times (28+(n-1)18))(3\times 1)$$

$$= -630 + 126n + 1404n^2 + 2430n^3 + 1458n^4$$

Table 1. The summation of $n_u(e)n_v(e)$ for the edges similar to e of S[n].

Types of Edges	Summation of $n_u(e)n_v(e)$
e_{n1}	$((30+27n(n+1))\times 1)3(2^{n+2}-1)$
e_{n2}, e_{n3}, e_{n6}	$(((30+27n(n+1))-2)\times 3)(3^2\times 2^n)$
e_{n5}, e_{n8}	$(((30+27n(n+1))-5)\times 6)(3\times 2^{n+1})$
e_{n4}, e_{n7}	$(((30+27n(n+1))-6)\times 7)(3\times 2^{n+1})$
$e_{(n-1)1}$	$(((30+27n(n+1))-9)\times 10)(3\times 2^n)$
$e_{(n-1)2}, e_{(n-1)6}, e_{(n-1)3}$	$(((30+27n(n+1))-20)\times 21)(3\times 3)$
$e_{(n-1)5}, e_{(n-1)8}$	$(((30+27n(n+1))-23)\times 24)(3\times 2)$
$e_{(n-1)4}, e_{(n-1)7}$	$(((30+27n(n+1))-24)\times 25)(3\times 2)$
$e_{(n-2)1}$	$(((30+27n(n+1))-27)\times 28)(3\times 2)$
$e_{(n-i)2}, e_{(n-i)6}, e_{(n-i)3}$	$(((30+27n(n+1))-(20+(i-1)18))\times(21+(i-1)18))(3\times 3)$
$e_{(n-i)5}, e_{(n-i)8}$	$(((30+27n(n+1))-(23+(i-1)18))\times(24+(i-1)18))(3\times 2)$
$e_{(n-i)4}, e_{(n-i)7}$	$(((30+27n(n+1))-(24+(i-1)18))\times(25+(i-1)18))(3\times 2)$
$e_{(n-(i+1))1}$	$(((30+27n(n+1))-(27+(i-1)18))\times(28+(i-1)18))(3\times 2)$
e_{12}, e_{16}, e_{13}	$(((30+27n(n+1))-(20+(n-2)18))\times(21+(n-2)18))(3\times 3)$
e_{15}, e_{18}	$(((30+27n(n+1))-(23+(n-2)18))\times(24+(n-2)18))(3\times 2)$
e_{14}, e_{17}	$(((30+27n(n+1))-(24+(n-2)18))\times(25+(n-2)18))(3\times 2)$
e_{11}	$(((30+27n(n+1))-(27+(n-2)18))\times(28+(n-2)18))(3\times 2)$
e_{02}, e_{06}, e_{03}	$((30+27n(n+1))-(20+(n-1)18)(21+(n-1)18)(3\times 3)$
e_{05}, e_{08}	$((30+27n(n+1))-(23+(n-1)18)(24+(n-1)18)(3\times 2)$
e_{04}, e_{07}	$((30+27n(n+1))-(24+(n-1)18)(25+(n-1)18)(3\times 2)$
e_{01}	$((30+27n(n+1))-(27+(n-1)18)(28+(n-1)18)(3\times 1)$

We are now ready to prove our first main result.

Theorem 1. The Szeged index of S[n] is computed as follows:

$$Sz(S[n]) = -720 + 5544n + 9828n^2 + 13203n^3 + 6561n^4 + 3969n^2 2^n + 3969n2^n + 36542^n.$$

Proof. By calculating S_1, S_2, S_3, S_4 and S_5, one can see that Sz(S[n]) $S_1 + S_2 + S_3 + S_4 + S_5$. So, by an straightforward calculation,

$$Sz(S[n]) = -720 + 5544n + 9828n^2 + 13203n^3 + 6561n^4 + 3969n^2 2^n + 3969n2^n + 36542^n.$$

3. The second geometric-arithmetic index of S[n] and S'[n]

The aim of this section is to compute the second GA index of the Suzuki's Bi-branched Dendrimer S[n] and another dendrimer S'[n] depicted in Figs. 4, 5. Define:

$A_1 = \{e_{n1}, e_{n2}, e_{n3}, e_{n4}, e_{n5}, e_{n6}, e_{n7}, e_{n8}, e_{(n-1)1}\}$,

$A_2 = \{e_{(n-i)2}, e_{(n-i)3}, e_{(n-i)6} \mid 1 \le i \le n\}$,

$A_3 = \{e_{(n-i)5}, e_{(n-i)8} \mid 1 \le i \le n\}$,

$A_4 = \{e_{(n-i)4}, e_{(n-i)7} \mid 1 \le i \le n\}$,

$A_5 = \{e_{(n-i)1} \mid 2 \le i \le n\}$.

We also define Si to be the summation of $n_u(e)n_u(v)$ over all edges $e = uv \in A_i$. By our calculations given in Table 3, one can see that:

$$S_1 = 3\sqrt{(30+27n^2+27n)}\times(2^{n+1}-1) + 9\sqrt{(84+81n^2+81n)}\times 2^n + 6\sqrt{(150+162n^2+162n)}\times 2^n + 6\sqrt{(168+189n^2+189n)}\times 2^n + 3\sqrt{(210+270n^2+270)}\times 2^n,$$

$$S_2 = \sum_{i=1}^{n}\left(9\sqrt{(28+27n(n+1)-18i)(3+18i)}\right),$$

$$S_3 = \sum_{i=1}^{n}\left(6\sqrt{(25+27n(n+1)-18i)(6+18i)}\right),$$

$$S_4 = \sum_{i=1}^{n}\left(6\sqrt{(24+27n(n+1)-18i)(7+18i)}\right),$$

$$S_5 = \sum_{i=1}^{n-1}\left(6\sqrt{(21+27n(n+1)-18i)(10+18i)}\right) + 3\sqrt{(21+27n^2+9n)(10+18n)}.$$

Theorem 2. The second GA index of S[n] is computed as follows:

$$GA_2(S[n]) = \frac{2}{|V(S[n])|}\Big[3\sqrt{(30+27n^2+27n)}\times(2^{n+1}-1) + 9\sqrt{(84+81n^2+81n)}\times 2^n + 6\sqrt{(150+162n^2+162n)}\times 2^n + 6\sqrt{(168+189n^2+189n)}\times 2^n + 3\sqrt{(210+270n^2+270)}\times 2^n + \sum_{i=1}^{n}\left(9\sqrt{(28+27n(n+1)-18i)(3+18i)}\right) + \sum_{i=1}^{n}\left(9\sqrt{(28+27n(n+1)-18i)(3+18i)}\right) + \sum_{i=1}^{n}\left(6\sqrt{(24+27n(n+1)-18i)(7+18i)}\right) + \sum_{i=1}^{n-1}\left(6\sqrt{(21+27n(n+1)-18i)(10+18i)}\right) + 3\sqrt{(21+27n^2+9n)(10+18n)}\Big].$$

Proof. From the partition of E(S[n]) given above, one can see that

$$GA_2(S[n]) = \frac{2}{(|V(S[n])|)(S_1+S_2+S_3+S_4+S_5)}.$$

We now apply MAPLE to simplify the equations.

In the end of this paper, we consider a new type of dendrimers denoted by S'[n], Figs. 4 and 5. By a similar argument as in Theorem 2, one can prove the following theorem:

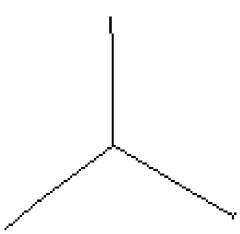

Fig. 4. The Core K of S'[n].

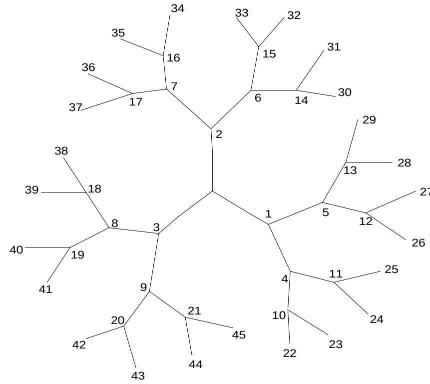

Fig. 5. The Molecular Graph of S'[n].

Theorem 3. The second GA index of S'[n] is computed as follows:

$$GA_2(S'[n]) = \frac{6}{|V(G)|}\sum_{0}^{n}\sqrt{((3\times(2^{n+1}-1)-2\times(2^i-1)\times(2^{i+1}-1))}\times 2^{n-i}.$$

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