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The new version of Szeged index

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In this paper, at first we introduce a new version of Szeged index and obtain some results about it. Then we compute this new index for some well-known graphs and zigzag nanotubes.

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1. Introduction

Let G be a simple molecular graph without directed and multiple edges and without loops. The graph G consists of the set of vertices $V(G)$ and the set of edges $E(G)$. In molecular graph, each vertex represented an atom of the molecule and bonds between atoms are represented by edges between corresponding vertices. The first topological index was Wiener index which is

$$W(G) = W_v(G) = \sum_{\{x,y\}\subseteq V(G)} d(x,y) \tag{1}$$

where $d(x,y)$ is the distance between to vertices x and y [1]. Numerous articles were published in the chemical and mathematical literature, devoted to the Wiener index and various methods for its calculation [2-5].

Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz [6]. The Szeged index is a modification of Wiener index to cyclic molecules. This was the vertex version of Sz index which had been defined as

$$Sz_v(G) = \sum_{e=uv\in E(G)} n_e(u).n_e(v) \tag{2}$$

where $n_e(u)$ is the number of vertices of G which are closer to u than to v and $n_e(v)$ is the number of vertices of G which are closer to v than to u. In [7-9], you can find computations of this index for some graphs.

The edge version of Szeged index introduced by Gutman and Ashrafi [10] that it is defined as

$$Sz_e(G) = \sum_{e=uv\in E(G)} m_e(u).m_e(v) \tag{3}$$

where $m_e(u)$ is the number of edges of G which are closer to u than to v and $m_e(v)$ is the number of edges of G which are closer to v than to u. In [11-13], you can find computations of this index for some graphs.

In the rest of this paper, we introduce the new version of Szeged index and name it total Szeged index. Next, by concluding some results about this version, we compute it for some graphs and zigzag nanotubes.

2. Discussion and results

Now, according to the definitions of edge and vertex versions of Szeged index, we are ready to introduce the new version of Szeged index.

Definition 2-1. The total version of Szeged index is

$$Sz_T(G) = \sum_{e=uv\in E(G)} t_e(u).t_e(v) \tag{4}$$

where $t_e(u)$ is the number of vertices and edges of G which are closer to u than to v and $t_e(v)$ is the number of vertices and edges of G which are closer to v than to u.

Due to the Definition (2-1), we can get the following results.

Result 2-2. We have

$$t_e(u) = n_e(u) + m_e(u)$$
$$t_e(v) = n_e(v) + m_e(v)$$

Proof. By using the definition of $t_e(u)$ and $t_e(v)$, the results can be concluded easily.

Result 2-3. The edge and vertex versions of Szeged index are the parts of summation of total Szeged index i.e.

$$Sz_T(G) = Sz_e(G) + Sz_v(G) + \sum_{e=uv\in E(G)} \left(m_e(u).n_e(v) + n_e(u).m_e(v)\right) \tag{5}$$

Proof. By using the Definition (2-1) and Result (2-2), the desire result can be concluded easily.

According to above definition and results we compute the total Szeged index for some familiar graphs.

In [6], there is a well-known relation about vertex Szeged index for a tree with n vertices which is

$$Sz_v(T) = W(T) \tag{6}$$

In [10], this relation was stated for edge version of Szeged index which is

$$Sz_e(T) = W(T) - W(S_n) \tag{7}$$

In the following theorem, we conclude the total version of relation (6). Before stating the theorem, we recall the vertex version of *PI* index which is

$$PI_v(G) = \sum_{e=uv\in E(G)} n_e(u) + n_e(v) \tag{8}$$

where $n_e(u)$ and $n_e(v)$ are mentioned in above.

Theroem 2-4. The relation (6) for total Szeged index of a tree with n vertices is

$$Sz_T(T) = 4W(T) - W(S_n) - PI_v(T) \tag{9}$$

Proof. According to the relation (4) and this fact that $t_e(u) = 2n_e(u) - 1$ and $t_e(v) = 2n_e(v) - 1$, we have:

$$\begin{aligned} Sz_T(T) &= 4W(T) - 2n(n-1) + (n-1) \\ &= 4W(T) - W(S_n) - n(n-1) \\ &= 4W(T) - W(S_n) - PI_v(T) \end{aligned}$$

In following example, we obtain the total Szeged index of some graphs.

Example 2-5. The total Szeged index of complete graph K_n, complete bipartite graph $K_{a,b}$ and cycle C_n are as follows:

1. $Sz_T(K_n) = \frac{1}{2}n(n-1)^3$
2. $Sz_T(K_{a,b}) = ab(2a-1)(2b-1)$
3. $Sz_T(C_n) = n(n-1)^2$

Now, we compute the total Szeged index of zigzag nanotubes. In Fig. 1, the zigzag nanotube is shown.

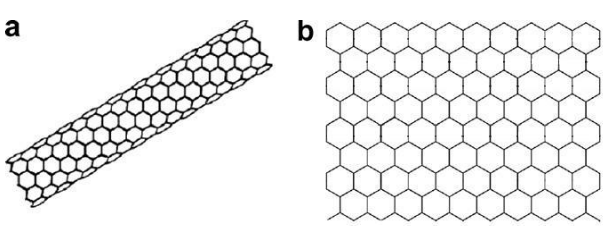

Fig. 1. (a) A zig-zag polyhex nanotube T, (b) 2-dimensional lattice of T, with p=10 and q=9.

We point the number of rows in two dimensional lattice of zigzag nanotube with q and the number of hexagons in each row with p, for example see the Fig. 1. We show the molecular graph of zigzag nanotube with G.

Lemma 2-6. Let $uv = e \in E(G)$ be the vertical edge of G between rows i and $i+1$. Then we have:

$$t_e(u) = 5pi - p$$

and

$$t_e(v) = 5pq - 5pi - p.$$

Proof. According to the Fig. 1, we have

$$\begin{aligned} t_e(u) &= n_e(u) + m_e(u) = 2pi + (2pi + p(i-1)) \\ &= 5pi - p \end{aligned}$$

and

$$\begin{aligned} t_e(v) &= n_e(v) + m_e(v) = 2p(q-i) + (2p(q-i) + p(q-i-1)) \\ &= 5pq - 5pi - p \end{aligned}.$$

Lemma 2-7. Let $uv = e \in E(G)$ be the oblique edge of G in row m. Then we have:

$$t_e(u) = \begin{cases} q(2m+2p-q-2) & , m \le p \ \& \ q-m \le p-1 \\ 3m-2p-3q+2mp+2pq- \\ (m-q)(m-q+1)-p^2 & , m > p \ \& \ q-m \le p-1 \\ (m+p-1)^2 & , m \le p \ \& \ q-m > p-1 \\ 4mp-4p+1 & , m > p \ \& \ q-m > p-1 \end{cases}$$

and

$$t_e(v) = \begin{cases} q(2p-2m+q) & , m \le p \ \& \ q-m \le p-1 \\ (p-m+q)^2 & , m > p \ \& \ q-m \le p-1 \\ 2mp-m^2-p^2+4pq+1 & , m \le p \ \& \ q-m > p-1 \\ 4pq+1 & , m > p \ \& \ q-m > p-1 \end{cases}$$

Proof. We compute only $t_e(u)$, because computation of $t_e(v)$ is similar ti computation of $t_e(u)$. By the Figure1, we have

$$n_e(u) = \begin{cases} mp+\frac{m(m-1)}{2}+(p-1)(q-m)- \\ \frac{(q-m)(q-m-1)}{2} & , m \le p \ \& \ q-m \le p-1 \\ 2p(m-p)+p^2+\frac{p(p-1)}{2}+ \\ (p-1)(q-m)-\frac{(q-m)(q-m-1)}{2} & , m > p \ \& \ q-m \le p-1 \\ mp+\frac{m(m-1)}{2}+(p-1)^2- \\ \frac{(p-1)(p-2)}{2} & , m \le p \ \& \ q-m > p-1 \\ 2p(m-p)+p^2+\frac{p(p-1)}{2}+ \\ (p-1)^2-\frac{(p-1)(p-2)}{2} & , m > p \ \& \ q-m > p-1 \end{cases}$$

and

$$m_e(u)=\begin{cases} m(p-1)+\dfrac{m(m-1)}{2}+(p-2)(q-m)-\dfrac{(q-m)(q-m-1)}{2} & ,m\le p\ \ \&\ \ q-m\le p-1 \\ 2p(m-p)+p(p-1)+\dfrac{p(p-1)}{2}+(p-2)(q-m)-\dfrac{(q-m)(q-m-1)}{2} & ,m>p\ \ \&\ \ q-m\le p-1 \\ m(p-1)+\dfrac{m(m-1)}{2}+(p-2)(p-1)-\dfrac{(p-1)(p-2)}{2} & ,m\le p\ \ \&\ \ q-m>p-1 \\ 2p(m-p)+p(p-1)+\dfrac{p(p-1)}{2}+(p-1)(p-2)-\dfrac{(p-1)(p-2)}{2} & ,m>p\ \ \&\ \ q-m>p-1 \end{cases}$$

According to the Result (2-2), $t_e(u)$ and $t_e(v)$ can be concluded.

For simplifying following computations, we use the following notations.

$$a_1=q(2m+2p-q-2)$$
$$a_2=3m-2p-3q+2mp+2pq-(m-q)(m-q+1)-p^2$$
$$a_3=(m+p-1)^2$$
$$a_4=4mp-4p+1$$
$$b_1=q(2p-2m+q)$$
$$b_2=(p-m+q)^2$$
$$b_3=2mp-m^2-p^2+4pq+1$$
$$b_4=4pq+1$$

Now, we are ready to state the total Szeged index of zigzag nanotube.

Theorem 2-8. The total Szeged index of zigzag nanotube is

$$Sz_T(G)=\begin{cases} \sum_{m=1}^{q}2pa_1b_1+\dfrac{p^3}{6}(q-1)(25q^2-5q+6) & ,q\le p \\ \sum_{m=1}^{p}2pa_3b_3+\sum_{m=p+1}^{q}2pa_2b_2+\dfrac{p^3}{6}(q-1)(25q^2-5q+6) & ,p<q\le 2p \\ \sum_{m=1}^{p}2pa_3b_3+\sum_{m=p+1}^{q-p}2pa_4b_4+\sum_{m=q-p+1}^{q}2pa_2b_2+\dfrac{p^3}{6}(q-1)(25q^2-5q+6) & ,q>2p \end{cases}$$

Proof. By the Lemma (2-6), we have

$$\sum_{\substack{e=uv\in E(G)\\ \text{and } e \text{ is vertical edge}}}\left[t_e(u)\times t_e(v)\right]=\frac{p^3}{6}(q-1)(25q^2-5q+6)$$

Also, by the Lemma (2-7) and notation a_i and b_i where $1\le i\le 4$, the desire result can be concluded.

3. Conclusion

In this paper, we have introduced the total Szeged index and compute it for some well-known graphs and in particular for zigzag nanotubes.

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