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The new version of PI index and its computation for zigzag nanotubes

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In this paper, at first we introduce a new version of PI 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 is 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 indices 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].

Khadikar and Co-authors [6-9] defined a new topological index and named it Padmakar-Ivan index. They abbreviated this new topological index as PI. If $e = uv$ is an edge of G, it is

$$PI_e(G) = \sum_{e=uv \in E(G)} \left[m_e(u) + m_e(v)\right] \tag{2}$$

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 [10-12], you can find computations of this index for some graphs.

The vertex version of PI index was also defined as [13],

$$PI_v(G) = \sum_{e=uv \in E(G)} \left[n_e(u) + n_e(v)\right] \tag{3}$$

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 [14-15], you can find computations of this index for some graphs.

In the rest of this paper, we introduce the total version of PI 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 PI index, we are ready to introduce the new version of PI index.

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

$$PI_T(G) = \sum_{e=uv \in E(G)} \left[t_e(u) + t_e(v)\right] \tag{4}$$

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 PI index are the parts of summation of total PI index i.e.

$$PI_T(G) = PI_e(G) + PI_v(G) \tag{5}$$

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 PI index for some familiar graphs.
At first we find the upper bound for total PI index.

Theorem 2-4. Let G be a connected graph. Then,

$$PI_T(G) \le |E(G)|\left(|V(G)|+|E(G)|-1\right) \tag{6}$$

with equality if and only if G is tree.

Proof. According to the definition of $PI_e(G)$ and $PI_v(G)$, we have $PI_e(G) \le |E(G)|\left(|E(G)|-1\right)$ and $PI_v(G) \le |E(G)||V(G)|$. Therefore,
$PI_T(G) \le |E(G)|\left(|V(G)|+|E(G)|-1\right)$.
Also, in [16] it is proved that $PI_v(G) = |E(G)||V(G)|$ if and only if G is bipartite. In addition, $PI_e(G) = |E(G)|\left(|E(G)|-1\right)$ if and only if G has not even cycle.
Therefore, the intersection of bipartite graphs and the graphs without even cycles are trees. Then, $PI_T(G) = |E(G)|\left(|V(G)|+|E(G)|-1\right)$ if and only if G is tree.

In following, we obtain the total PI index for some graphs.

Example 2-5. The total PI index of tree T, complete graph K_n, complete bipartite graph $K_{a,b}$ and cycle C_n are as follows:
1. $PI_T(T) = 2(n-1)^2$
2. $PI_T(K_n) = n(n-1)^2$
2. $PI_T(K_{a,b}) = 2ab(a+b-1)$
3. $PI_T(C_n) = 2n(n-1)$

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

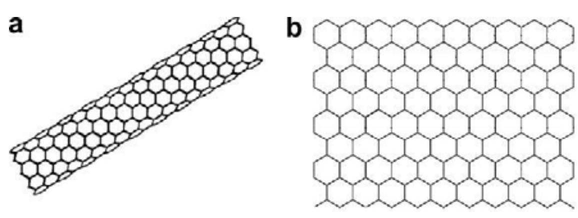

Fig. 1. (a) A zig-zag polyhex nanotube, (b) 2-dimensional lattice of zigzag nanotube, with p=10 and q=9.

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

$$t_e(u) = n_e(u) + m_e(u) = 2pi + (2pi + p(i-1))$$
$$= 5pi - p$$

and

$$t_e(v) = n_e(v) + m_e(v) = 2p(q-i) + (2p(q-i) + p(q-i-1))$$
$$= 5pq - 5pi - p$$

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 Result (2-2) and the Fig. 1, 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

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

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 PI index of zigzag nanotube.

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

$$PI_T(G)=\begin{cases} \sum_{m=1}^{q}2p(a_1+b_1)+(q-1)(2p^2q-2p^2) & ,q\le p \\ \sum_{m=1}^{p}2p(a_3+b_3)+\sum_{m=p+1}^{q}2p(a_2+b_2)+(q-1)(2p^2q-2p^2) & ,p<q\le 2p \\ \sum_{m=1}^{p}2p(a_3+b_3)+\sum_{m=p+1}^{q-p}2p(a_4+b_4)+\sum_{m=q-p+1}^{q}2p(a_2+b_2)+(q-1)(2p^2q-2p^2) & ,q>2p \end{cases}$$

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

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

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.

4. Conclusion

In this paper, we introduce the total PI index and compute it for some well-known graphs and in particular for zigzag nanotubes by concluding some results about this new topological index.

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