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Szeged and Balaban indices of zigzag polyhex nanotubes

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Abstract
The Sezegd index of a graph G is defined as Sz(G)= $\sum_{e\in E(G)} n_u(e)n_v(e)$, where $n_u(e)$ is the number of vertices of G lying closer to u than to v, $n_v(e)$ is the number of vertices of G lying closer to v than to u and the summation goes over all edges $e = uv$ of G. Also Balaban index of G is defined by $J(G) = \frac{m}{(\mu+1)} \sum_{uv\in E(G)} [d(u)d(v)]^{-0.5}$, where $d(v) = \sum_{x\in V(G)} d(v,x)$, is the summation of distances between v and all vertices of G, m is the number of edges in G and μ is the cyclomatic number of G. In this paper we find an exact expression for Szeged and Balaban indices of $TUHC_6[2p,q]$, the zigzag polyhex nanotubes, using a theorem of Dobrynin and Gutman on connected bipartite graphs (see Ref [11]).

1. Introduction

Let G be an undirected connected graph without loops or multiple edges. The set of vertices and edges of G are denoted by $V(G)$ and $E(G)$ respectively. For vertices x and y in $V(G)$, we denote by $d(x,y)$ (or $d_G(x,y)$ when we deal with more than one graph) the topological distance i.e., the number of edges on the shortest path, joining the two vertices of G. Since G is connected, $d(x,y)$ exists for all $x,y \in V(G)$. The distance of a vertex u of G is defined as

$$d(u) = \sum_{x\in V(G)} d(u,x),$$

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the summation of distances between u and all vertices of G.

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling or pictorial representation of a graph. Wiener index is one of the most studied topological indices and is connected to the problem of distances in graph. In 1947, Harold Wiener published a paper entitled "Structural Determination of Paraffin Boiling Points". In this work the quantity W(G), eventually named Wiener index or Wiener number, was introduced for the first time. In 1947 and 1948, Wiener published a whole series of papers [1]-[5] showing that there are excellent correlations between W(G) and a variety of physicochemical properties of organic compounds. The Wiener index of the graph G is the half sum of distances over all its vertex pairs (u, v):

$$W(G) = \frac{1}{2}\sum_{u,v\in V(G)} d(u,v) = \frac{1}{2}\sum_{u\in V(G)} d(u).$$

Gutman proposed a new index which was named the Szeged index. Many properties of Szeged index are discussed (see for example [6]-[10]). Let u and v be two adjacent vertices of the graph G and $e = uv$ be the edge between them. Let $B_u(e)$ be the set of all vertices of G lying closer to u than to v and $B_v(e)$ be the set of all vertices of G lying closer to v than to u, that is

$$B_u(e) = \{x \mid x \in V(G), d_G(x,u) < d_G(x,v)\}$$
$$B_v(e) = \{x \mid x \in V(G), d_G(x,v) < d_G(x,u)\}.$$

Let $n_u(e) = |B_u(e)|$ and $n_v(e) = |B_v(e)|$. The Szeged index of G is defined as

$$Sz(G) = \sum_{e\in E(G)} n_u(e)n_v(e).$$

The Balaban J index of G is defined by

$$J(G) = \frac{m}{(\mu+1)}\sum_{uv\in E(G)} [d(u)d(v)]^{-0.5},$$

where m is the number of edges in G and μ is the cyclomatic number of G (see [12]-[13]). The cyclomatic number μ of a connected graph G is defined as $\mu(G) = |E(G)| - |V(G)| + 1$ (see [14]).

In a series of papers, Diudea and coauthors [22]-[29] computed the Wiener index of some nanotubes. In this paper we find exact expressions for Szeged and Balaban indices of the zigzag polyhex nanotubes, $G := TUHC_6[2p, q]$. For this purpose we choose a coordinate label for vertices of G as shown in Figure 1. In Appendix we include a MATHEMATICA [30] program to produce the graph of $TUHC_6[2p, q]$ and compute the Szeged and Balaban indices of the graph, using the definitions. First we note that G is a bipartite graph. Recall that a graph G is bipartite if the vertices can be colored with white and black so that adjacent vertices have different color, or equivalently, every cycle has even length. So we can use a theorem of Dobrynin and Gutman [11] on connected bipartite graphs. We state the theorem for convenience of the reader.

Theorem 1 *([11, Theorem 3]) If G is a connected bipartite graph with n vertices and m edges, then*

$$Sz(G) = \frac{1}{4}\left(n^2 m - \sum_{uv\in E(G)} (d(u) - d(v))^2\right). \tag{1}$$

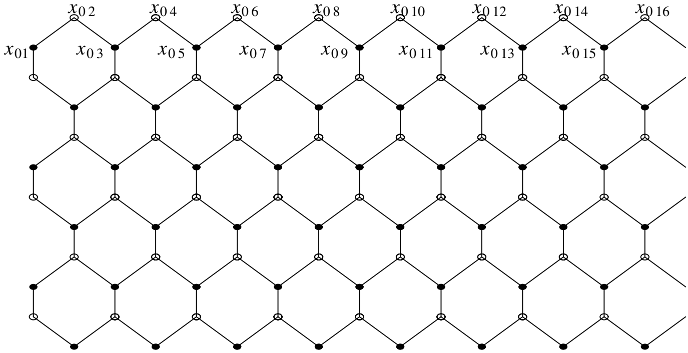

Figure 1: A $TUHC_6[2p, q]$ Lattice with $p = 8$ and $q = 6$.

Obviously the number of vertices and the number of edges of $G = TUHC_6[2p, q]$ is $n = |V(G)| = 2pq$ and $m = |E(G)| = 3pq - p$, respectively. Thus we need to compute $d(u) - d(v)$, for all edges $e = uv$. Throughout this paper $G := TUHC_6[2p, q]$, denotes an arbitrary zigzag polyhex nanotube in terms of their circumference $2p$ and their length q, see Figure 1.

2. Szeged index of zigzag polyhex nanotubes

In this section we derive an exact formula for the Szeged index of $G := TUHC_6[2p, q]$. John and Diudea in [22] mentioned a formula for the distances of one white (black) vertex of level 0 to all vertices on level k (see Figure 1). In Lemma below we give a proof for this formula.

Lemma 1. The distances of one white vertex of level 0 to all vertices is given by

$$\begin{aligned} w_k := \sum_{x \in \ level \ k} d(x_{02}, x) &= \sum_{x \in \ level \ k} d(x_{04}, x) \\ &\ \ \vdots \\ &= \begin{cases} (p+k)^2 + k & \text{if} \quad 0 \le k < p \\ \\ p(4k+1) & \text{if} \quad p \le k \end{cases} \end{aligned}$$

and the distances of one black vertex of level 0 to all vertices of level k is given by

$$\begin{aligned} b_k := \sum_{x \in \ level \ k} d(x_{01}, x) &= \sum_{x \in \ level \ k} d(x_{03}, x) \\ &\ \ \vdots \\ &= \begin{cases} (p+k)^2 - k & \text{if} \quad 0 \le k < p \\ \\ p(4k-1) & \text{if} \quad p \le k. \end{cases} \end{aligned}$$

Proof: We compute b_k. It is suffices for considering x_{01}. For other black vertices, the argument is similar. At first note that the lattice is symmetric (with respect to the line joining x_{01} to x_{11}). We distinguish three cases:

Case 1: $k \geq p$ and k is even. In this case

$$x_{01} \rightarrow x_{11} \rightarrow x_{12} \rightarrow x_{13} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k-1,p+1} \rightarrow x_{k,p+1}$$

is a shortest path between x_{01} and $x_{k,p+1}$ and its length is $2k$, and

$$x_{01} \rightarrow x_{11} \rightarrow x_{12} \rightarrow x_{13} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k,p}$$

is a shortest path between x_{01} and $x_{k,p}$, and its length is $2k-1$. Also

$$x_{01} \rightarrow x_{11} \rightarrow x_{1,2p} \rightarrow x_{2,2p} \rightarrow x_{2,1} \rightarrow x_{3,1} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k-1,p-1} \rightarrow x_{k,p-1}$$

is a shortest path between x_{01} and $x_{k,p-1}$ and its length is $2k$ and

$$x_{01} \rightarrow x_{11} \rightarrow x_{1,2p} \rightarrow x_{2,2p} \rightarrow x_{2,1} \rightarrow x_{3,1} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k-1,p-1}$$

is a shortest path between x_{01} and $x_{k,p}$, and its length is $2k-1$.
By this algorithm, for all $1 \leq j \leq p+1$, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k-1 & \text{if } \ j \ \text{ is even} \\ \\ 2k & \text{if } \ j \ \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain p vertices having distance $2k-1$ from x_{01}, and p vertices having $2k$ distance from with x_{01}. So

$$\sum_{u \in \ level \ k} d(x_{01}, u) = \sum_{j \ is \ even} d(x_{01}, x_{kj}) + \sum_{j \ is \ odd} d(x_{01}, x_{kj}) = p(2k-1) + p(2k) = p(4k-1).$$

Case 2: $k \geq p$ and k is odd. In this case

$$x_{01} \rightarrow x_{11} \rightarrow x_{12} \rightarrow x_{13} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k-1,p+1} \rightarrow x_{k,p+1}$$

is a shortest path between x_{01} and $x_{k,p+1}$ and its length is $2k-1$, and

$$x_{01} \rightarrow x_{11} \rightarrow x_{1,2p} \rightarrow x_{2,2p} \rightarrow x_{21} \rightarrow x_{31} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k-1,p} \rightarrow x_{k,p}$$

is a shortest path between x_{01} and $x_{k,p}$, and its length is $2k$. Also

$$x_{01} \rightarrow x_{11} \rightarrow x_{1,2p} \rightarrow x_{2,2p} \rightarrow x_{21} \rightarrow x_{31} \rightarrow \cdots \rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots x_{k-1,p-1} \rightarrow x_{k,p-1}$$

is a shortest path between x_{01} and $x_{k,p-1}$, and its length is $2k-1$, and

$$x_{01} \rightarrow x_{11} \rightarrow x_{1,2p} \rightarrow x_{2,2p} \rightarrow x_{2,2p-1} \rightarrow x_{3,2p-1} \rightarrow x_{3,2p} \rightarrow x_{4,2p} \rightarrow x_{41} \rightarrow \cdots$$
$$\rightarrow x_{r,s} \rightarrow x_{r,s+1} \rightarrow \cdots \rightarrow x_{k,p-3} \rightarrow x_{k,p-2}$$

is a shortest path between x_{01} and $x_{k,p-2}$ and its length is $2k$. By this algorithm, for all $1 \leq j \leq p+1$, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } j \text{ is even} \\ \\ 2k-1 & \text{if } j \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain p vertices having distance $2k-1$ from x_{01}, and p vertices having $2k$ distance from with x_{01}. So

$$\sum_{u \in \ level\ k} d(x_{0,1}, u) = \sum_{j\ is\ even} d(x_{0,1}, x_{kj}) + \sum_{j\ is\ odd} d(x_{0,1}, x_{kj}) = p(2k) + p(2k-1) = p(4k-1).$$

Case 3: $k \leq p-1$. For all $p+1 \leq j$ and $j > k+1$, the path

$$x_{01} \to x_{11} \to x_{12} \to x_{13} \to \cdots \to x_{r,s} \to x_{r,s+1} \to \cdots \to x_{k,k+1} \to x_{k,k+1} \to \cdots \to x_{k,j}$$

is a shortest path between x_{01} and $x_{k,j}$ and its length is $k+j-1$. Thus the summation of the distances between x_{01} and x_{kj} (for all j such that $p+1 \leq j$ and $j > k+1$) and their symmetric vertices is

$$S_1 = 2\sum_{j=k+2}^{p}(k+j-1) + k + p + 1 - 1 = 2kp - 2k + p^2 - 3k^2.$$

Also if $1 \leq j \leq k+1$, then the path

$$x_{01} \to x_{11} \to x_{12} \to x_{13} \to \cdots \to x_{r,s} \to x_{r,s+1} \to \cdots \to x_{k,k} \to x_{k,k+1}$$

is a shortest path between x_{01} and $x_{k,k+1}$ and its length is $2k$. The above path shows that the distance between x_{01} and $x_{k,k}$ is $2k-1$. Now the path

$$x_{01} \to x_{11} \to x_{1,2p} \to x_{2,2p} \to x_{21} \to x_{31} \to \cdots \to x_{r,s} \to x_{r,s+1} \to \cdots \to x_{k,k-1}$$

is a shortest path from x_{01} to $x_{k,k-1}$ and its length is $2k$. The above path also shows that the distance between x_{01} and $x_{k,k-2}$ is $2k-1$. By repeating this process and considering the symmetry of these vertices we obtain $k+1$ vertices having distance $2k$, and k vertices having distance $2k-1$ from x_{01}, respectively. Therefore the summation of the distances between x_{01} and x_{kj} (for all j such that $1 \leq j \leq k+1$) and their symmetric vertices is

$$S_2 = (k+1)2k + k(2k-1) = 4k^2 + k.$$

Hence

$$b_k = S_1 + S_2 = 2kp - 2k + p^2 - 3k^2 + 4k^2 + k = (p+k)^2 - k.$$

In a similar manner we can compute w_k. □

Corollary 2. (a) $d_G(x_{02}) = d_G(x_{04}) = \cdots = d_G(x_{0,2p}) = w_0 + w_1 + \cdots + w_{q-1}$.
(b) $d_G(x_{01}) = d_G(x_{03}) = \cdots = d_G(x_{0,2p-1}) = b_0 + b_1 + \cdots + b_{q-1}$.

Proof: By Lemma 1, we have

$$\begin{aligned} d_G(x_{02}) &= \sum_{x\in level\ 0} d_G(x_{02},x) + \sum_{x\in level\ 1} d_G(x_{02},x) + \cdots + \sum_{x\in level\ q-1} d_G(x_{02},x) \\ &= w_0 + w_1 + \cdots + w_{q-1} \end{aligned}$$

and so $d_G(x_{02}) = d_G(x_{04}) = \cdots = d_G(x_{0,2p}) = w_0 + w_1 + \cdots + w_{q-1}$.
The proof of (b) is similar. □

Lemma 3. If $0 \le j \le q-1$ is an odd number, then
(a) $d_G(x_{j1}) = d_G(x_{j3}) = \cdots = d_G(x_{j,2p-1}) = w_0 + w_1 + \cdots + w_{q-(j+1)} + b_1 + \cdots + b_j$.
(b) $d_G(x_{j2}) = d_G(x_{j4}) = \cdots = d_G(x_{j,2p)}) = b_0 + b_1 + \cdots + b_{q-(j+1)} + w_1 + \cdots + w_j$.

Proof: First suppose $j = 1$. We consider the tube that can be built up from two halves collapsing at level 1. The bottom part is the graph $G_1 = TUHC_6[2p, q-1]$ and we can consider x_{11} as one of the white edges in the first row of the graph G_1. According to Corollary 2, we have

$$d_{G_1}(x_{11}) = d_{G_1}(x_{13}) = \cdots = d_{G_1}(x_{1,2p-1}) = w_0 + w_1 + \cdots + w_{q-2}.$$

The top part is the graph $TUHC_6[2p, 2] = \widehat{G_1}$ and level 1 of graph G is the first its row and x_{11} is such a black vertex of $\widehat{G_1}$. Therefore by Lemma 2, $d_{\widehat{G_1}}(x_{11}) = b_0 + b_1$ and

$$d_{\widehat{G_1}}(x_{11}) = d_{\widehat{G_1}}(x_{13}) \cdots = d_{\widehat{G_1}}(x_{1(2p-1)}) = b_0 + b_1.$$

Since $w_0 = b_0$ and $d_G(x_{11}) = d_{G_1}(x_{11}) + d_{\widehat{G_1}}(x_{11}) - b_0$, we have $d_G(x_{11}) = w_0 + \cdots + w_{q-2} + b_1$ and similarly

$$d_G(x_{11}) = d_G(x_{13}) = \cdots = d_G(x_{1,2p-1}) = w_0 + \cdots + w_{q-2} + b_1.$$

Similarly for x_{12} we can see that

$$d_G(x_{12}) = d_G(x_{14}) = \cdots = d_G(x_{1,2p}) = b_0 + \cdots + b_{q-2} + w_1.$$

By repetition of this argument we obtain the result. □

Lemma 4. If $0 \le j \le q-1$ is an even number, then
(a) $d_G(x_{j1}) = d_G(x_{j3}) = \cdots = d_G(x_{j,2p-1}) = b_0 + b_1 + \cdots + b_{q-(j+1)} + w_1 + \cdots + w_j$.
(b) $d_G(x_{j2}) = d_G(x_{j4}) = \cdots = d_G(x_{j,2p}) = w_0 + w_1 + \cdots + w_{q-(j+1)} + b_1 + \cdots + b_j$.

Proof: First Suppose that $j = 2$. We consider the tube can be built up from two halves collapsing at level 2. The bottom part is the graph $G_2 = TUHC_6[2p, q-2]$ and the level 2 of G is the first level of G_2 and we can consider x_{21} one of the black edges in the first row of graph G_2. According to Corollary 2, we have

$$d_{G_2}(x_{21}) = d_{G_2}(x_{23}) = \cdots = d_{G_2}(x_{2,2p-1}) = b_0 + b_1 + \cdots + b_{q-3}.$$

The top part is the graph $TUHC_6[2p, 3] = \widehat{G_2}$ and level 2 of graph G is the first level of $\widehat{G_2}$ and x_{21} is such a white vertex of $\widehat{G_2}$. Therefore by Corollary 2, $d_{\widehat{G_2}}(x_{21}) = w_0 + w_1 + w_2$ and

$d_{\widehat{G_2}}(x_{21}) = d_{\widehat{G_2}}(x_{23}) = \cdots = d_{\widehat{G_2}}(x_{2,2p-1}) = w_0 + w_1 + w_2$. Since $w_0 = b_0$ and $d_G(x_{21}) = d_{G_2}(x_{21}) + d_{\widehat{G_2}}(x_{21}) - w_0$, we have

$$d_G(x_{21}) = b_0 + \cdots + b_{q-3} + w_1 + w_2$$

and similarly

$$d_G(x_{21}) = d_G(x_{23}) = \cdots = d_G(x_{2,2p-1}) = b_0 + \cdots + b_{q-3} + w_1 + w_2.$$

We can similarly repeat this process for x_{22} and see that

$$d_G(x_{22}) = d_G(x_{24}) = \cdots = d_G(x_{2,2p}) = w_0 + \cdots + w_{q-3} + b_1 + b_2.$$

By repetition of this argument we obtain the result. □

Now we want to determine the sum $\sum_{uv\in E(G)} (d_G(v) - d_G(u))^2$, in Theorem 1, that we need to compute $Sz(G)$. For all $0 \le j \le q-1$, put

$$f(j) = w_0 + w_1 + \cdots + w_{q-(j+1)} + b_1 + \cdots + b_j$$

and

$$g(j) = b_0 + b_1 + \cdots + b_{q-(j+1)} + w_1 + \cdots + w_j.$$

Note that $g(j) = f(q-(j+1))$.
There are two types of edges in the graph G, horizontal and vertical. At level 1 we have

$$\begin{aligned} (d(x_{01}) - d(x_{02}))^2 &= (g(0) - f(0))^2 \\ &\vdots \\ &\vdots \\ (d(x_{01}) - d(x_{0(2p)}))^2 &= (g(0) - f(0))^2. \end{aligned}$$

Therefore, by adding both sides of the above identities, we have

$$\sum_{uv\in \text{ level } 0} (d_G(v) - d_G(u))^2 = 2p(f(0) - g(0))^2.$$

Similarly for each $1 \le j \le q-1$ we have

$$\sum_{uv\in \text{ level } j} (d_G(v) - d_G(u))^2 = 2p(f(j) - g(j))^2.$$

Thus, summing up on levels j, for $1 \le j \le q-1$, we obtain that

$$\sum_{uv \text{ is horizontal}} (d_G(v) - d_G(u))^2 = 2p\sum_{j=0}^{q-1}(f(j) - g(j))^2. \tag{2}$$

Similarly we can obtain

$$\sum_{uv\ is\ vertical}(d_G(v)-d_G(u))^2 = p\sum_{j=0}^{q-2}(f(j+1)-g(j))^2. \tag{3}$$

Finally, by adding both sides of (2) and (3) we have

$$\begin{aligned}\sum_{uv\in E(G)}(d_G(v)-d_G(u))^2 &= p\sum_{j=0}^{q-2}(f(j+1)-g(j))^2+2p\sum_{j=0}^{q-1}(f(j)-g(j))^2\\ &= p\sum_{j=0}^{q-2}(f(j+1)-f(q-(j+1)))^2+\\ &\qquad 2p\sum_{j=0}^{q-1}(f(j)-f(q-(j+1)))^2 \end{aligned}\tag{4}$$

Now we are in the position to prove the main result of this section.

Theorem 2. The Szeged index of $G := TUHC_6[2p,q]$ nanotubes is given by

$$Sz(G)=\begin{cases}\frac{pq}{6}(16p^2q^2-4p^2-q^4+q^2) & \text{if} \quad p\geq q\\ \frac{p}{30}(20q^3p^2+4p-4q-10p^3+6p^5-q^5-30pq^2+\\ \qquad 10pq^4+80q^2p^3+20p^2q-40p^4q+5q^3) & \text{if} \quad 2p>q\\ \frac{p^2}{15}(30q^3p-2-13p^4-20pq+15p^2+20p^3q) & \text{if} \quad 2p<q\\ \frac{p^2}{15}(267p^4-25p^2-2) & \text{if} \quad 2p=q\end{cases}$$

Proof: The number of vertices and edges of the graph G are $m=p(3q-1)$ and $n=2pq$, respectively. Thus we need to compute $\sum_{uv\in E(G)}(d_G(v)-d_G(u))^2$ and use Theorem 1. To compute this summation we may use equation (4).

First suppose that $p\geq q$. Then, by Lemma 1, for each $0\leq k\leq q-1$ we have $w_k=(p+k)^2+k$ and $b_k=(p+k)^2-k$. So, by definition of $f(j)$ and performing some computations we have

$$p\sum_{j=0}^{q-2}(f(j+1)-f(q-(j+1)))^2+2p\sum_{0}^{q-1}(f(j)-f(q-(j+1)))^2=\frac{2pq}{3}(q-1)(q^3+q^2+2p^2q-4p^2).$$

Therefore by (4) and Theorem 1, we have

$$\begin{aligned}Sz(G) &= \frac{1}{4}n^2m-\frac{1}{4}\sum_{uv\in E(G)}(d(u)-d(v))^2\\ &= \frac{pq}{6}(p^2q^2-4p^2-q^4+q^2).\end{aligned}$$

Now suppose that $q > p$. Let

$$\begin{aligned} A_1 &:= \{j \mid 0 \le j \le p-1, \quad 0 \le q-j-1 \le p-1\} \\ A_2 &:= \{j \mid 0 \le j \le p-1, \quad p \le q-j-1 \le q-1\} \\ A_3 &:= \{j \mid p \le j \le q-1, \quad 0 \le q-j-1 \le p-1\} \\ A_4 &:= \{j \mid p \le j \le q-1, \quad p \le q-j-1 \le q-1\}. \end{aligned}$$

Note that if $A_1 \neq \varnothing$, then $2p > q$. Also if $A_4 \neq \varnothing$, then $2p < q$. Therefore first suppose that $A_1 \neq \varnothing$. Thus $A_4 = \varnothing$ and $2p > q$. So, by Lemma 1

$$j \in A_1 \implies f(j) = \sum_{k=0}^{q-j-1} ((p+k)^2 + k) + \sum_{k=1}^{j}((p+k)^2 - k).$$

$$j \in A_2 \implies f(j) = \sum_{k=0}^{p-1}((p+k)^2 + k) + \sum_{k=p}^{q-j-1} p(4k+1) + \sum_{k=1}^{j}((p+k)^2 - k).$$

$$j \in A_3 \implies f(j) = \sum_{k=0}^{q-j-1} ((p+k)^2 + k) + \sum_{k=1}^{p-1}((p+k)^2 - k) + \sum_{k=p}^{j} p(4k-1).$$

Also, by Lemma 1, we have

$$j \in A_1 \implies f(q-(j+1)) = \sum_{k=0}^{j-1}((p+k)^2 + k) + \sum_{k=1}^{q-j-1} ((p+k)^2 - k).$$

$$j \in A_2 \implies f(q-(j+1)) = \sum_{k=0}^{j}((p+k)^2 + k) + \sum_{k=1}^{p-1}((p+k)^2 - k) + \sum_{k=p}^{q-j-1} p(4k-1).$$

$$j \in A_3 \implies f(q-(j+1)) = \sum_{k=0}^{p}((p+k)^2 + k) + \sum_{k=p}^{j} p(4k+1) + \sum_{k=1}^{q-j-1} ((p+k)^2 - k).$$

Therefore straightforward computations show that

$$\begin{aligned} \sum_{j=0}^{q-1}(f(j) - f(q-(j+1)))^2 &= \sum_{j\in A_1} (f(j) - f(q-(j+1)))^2 + \\ &\quad \sum_{j\in A_2} (f(j) - f(q-(j+1)))^2 + \sum_{j\in A_3} (f(j) - f(q-(j+1)))^2 \\ &= \sum_{j=q-p}^{p-1} (1 + 2j - q - (j+1)^2 + (q-j)^2)^2 + \\ &\quad \sum_{j=0}^{q-p-1} (1 - p + j - p^2 - (j+1)^2 + 2p(q-j))^2 + \\ &\quad \sum_{j=p}^{q-1}(p + j - q + p^2 - 2p(j+1) + (q-j)^2)^2 \\ &= -\frac{4}{15}p + \frac{4}{15}q + \frac{2}{3}p^3 - \frac{2}{5}p^5 + \frac{1}{1}5q^5 + 2pq^2 - \\ &\quad \frac{2}{3}pq^4 + 4q^3p^2 - \frac{16}{3}q^2p^3 - \frac{8}{3}p^2q + \frac{8}{3}p^4q - \frac{1}{3}q^3 \qquad (5) \end{aligned}$$

Now let $OA_1 = A_1 - \{p-1\}$, $OA_2 = A_2 - \{p-1\}$ and $OA_3 = A_3 - \{q-1\}$. Since $f(j+1) = f(j) + b_{j+1} - w_{q-j-1}$, we have

$$\begin{aligned}
j \in OA_1 &\implies f(j+1) = \sum_{k=0}^{q-j-2}((p+k)^2+k) + \sum_{k=1}^{j+1}((p+k)^2-k).\\
j \in OA_2 &\implies f(j+1) = \sum_{k=0}^{p-1}((p+k)^2+k) + \sum_{k=p}^{q-j-2} p(4k+1) + \sum_{k=1}^{j+1}((p+k)^2-k).\\
j \in OA_3 &\implies f(j+1) = \sum_{k=0}^{q-j-2}((p+k)^2+k) + \sum_{k=1}^{p-1}((p+k)^2-k) + \sum_{k=p}^{j+1} p(4k-1).\\
j = p-1 &\implies f(p-1+1) = \sum_{k=0}^{q-p-2}((p+k)^2+k) + \sum_{k=1}^{p-1}((p+k)^2-k) + p(4p-1).
\end{aligned}$$

Hence, by straightforward computations we have

$$\begin{aligned}
\sum_{j=0}^{q-2}(f(j+1)-f(q-(j+1)))^2 &= \sum_{j\in\ OA_1}(f(j+1)-f(q-(j+1)))^2 + \\
&\quad \sum_{j\in\ OA_2}(f(j+1)-f(q-(j+1)))^2 + \\
&\quad \sum_{j\in\ OA_3}(f(j+1)-f(q-(j+1)))^2 + \\
&\quad f(p-1+1) - f(q-(p+1)) \\
&= \sum_{j=q-p}^{p-2}(1+2j-q-(j+1)^2+(q-j)^2)^2 + \\
&\quad \sum_{j=0}^{q-p-1}(1-p+j-p^2-(j+1)^2+2p(q-j))^2 + \\
&\quad \sum_{j=p}^{q-2}(p+j-q+p^2-2p(j+1)+(q-j)^2)^2 + (2p(2p-q))^2 \\
&= \frac{4}{3}p^2 q(q-1)(q-2) \qquad (6)
\end{aligned}$$

Therefore by (4), (5), (6) and Theorem 1, we have

$$\begin{aligned}
Sz(G) &= \frac{1}{4}n^2 m - \frac{1}{4}\sum_{uv\in E(G)}(d(u)-d(v))^2 \\
&= p\sum_{j=0}^{q-2}(f(j+1)-f(q-(j+1)))^2 + 2p\sum_{j=0}^{q-1}(f(j)-f(q-(j+1)))^2 \\
&= \frac{1}{30}p(20q^3p^2+4p-4q-10p^3+6p^5-q^5-30pq^2+10pq^4+ \\
&\qquad 80q^2p^3+20p^2q-40p^4q+5q^3).
\end{aligned}$$

Similarly we can handle the cases $q > 2p$ and $q = 2p$. □

p	q	$Sz(G)$	p	q	$Sz(G)$
4	1	128	5	2	2480
4	2	1264	5	3	8570
4	3	4336	5	4	20200
4	4	10112	5	5	38750
5	1	250	6	5	68280
10	10	2495000	15	15	28451250
10	9	1840800	15	9	6394950
10	8	1306240	15	8	4509360
10	7	882560	15	7	3030090
10	6	559400	15	6	1911600

Table 1: Szeged index of short $TUHC_6[2p, q]$ tubes, $q \leq p$

p	q	$Sz(G)$	p	q	$Sz(G)$
2	5	2120	3	9	41406
2	6	3608	4	9	101536
2	7	5672	4	10	137504
3	7	19986	4	11	181152
3	8	29400	1	6	432
10	21	20437320	15	31	222515970
10	22	23343320	15	32	243618720
10	23	26513320	15	33	266017470
10	24	29959320	15	34	289752720
10	25	33693320	15	35	314864970

Table 2: Szeged index of long $TUHC_6[2p, q]$ tubes, $q > 2p$

If $T(p, q) = TUHC_6[2p, q]$, then by Theorem 2, $Sz(T(p, 1)) = 2p^3$ and so $\lim_{p \longrightarrow \infty} \frac{Sz(T(p,p))}{p^6} = \frac{5}{2}$. If p is fix, then $\lim_{q \longrightarrow \infty} \frac{Sz(T(p,q))}{q^3} = 2p^3$ and $\lim_{p \longrightarrow \infty} \frac{Sz(T(p,2p))}{p^6} = \frac{89}{5}$.

In Tables (1) and (2) the numerical data for Szeged index in tubes $TUHC_6[2p, q]$ of various dimensions are given.

3. Balaban index of zigzag polyhex nanotubes

In this section we use the method given in Theorem 2 and write an algorithm and implement a computer program in MAPLE [37] to computing a formula for the Balaban index of zigzag polyhex nanotubes. The number of vertices and edges of the graph $G := TUHC_6[2p, q]$ are $m = p(3q - 1)$ and $n = 2pq$, respectively. Now we compute $J(TUHC_6[2p, q])$. There are two types of edges in the graph G, horizontal and vertical. At level 1 we have

$$
\begin{aligned}
(d(x_{01})(d(x_{02}))^{-0.5} = (g(0)f(0))^{-0.5} &= (g(0)f(0))^{-0.5} \\
&\vdots \\
(d(x_{01})d(x_{0,2p}))^{-0.5} = (g(0)f(0))^{-0.5} &= (f(0)g(0))^{-0.5}.
\end{aligned}
$$

Therefore, by adding both sides of the above identities, we have

$$\sum_{uv \in level\ 0} (d_G(v)d_G(u))^{-0.5} = 2p(f(0)g(0))^{-0.5}.$$

Similarly for each $1 \leq j \leq q-1$ we have

$$\sum_{uv \in level\ j} (d_G(v)d_G(u))^{-0.5} = 2p(f(j)g(j))^{-0.5}.$$

Thus, summing up on levels j, for $1 \leq j \leq q-1$ we obtain that

$$\sum_{uv\ is\ horizontal} (d_G(v)d_G(u))^{-0.5} = 2p\sum_{j=0}^{q-1}(f(j)g(j))^{-0.5}. \tag{7}$$

Similarly we can obtain

$$\sum_{uv\ is\ vertical} (d_G(v)d_G(u))^{-0.5} = p\sum_{j=0}^{q-2}(f(j+1)g(j))^{-0.5}. \tag{8}$$

Finally, by adding (7) and (8) we have

$$
\begin{aligned}
\sum_{uv \in E(G)} (d_G(v)d_G(u))^{-0.5} &= p\sum_{j=0}^{q-2}(f(j+1)g(j))^{-0.5} + 2p\sum_{j=0}^{q-1}(f(j)g(j))^{-0.5} \\
&= p\sum_{j=0}^{q-2}(f(j+1)f(q-(j+1)))^{-0.5} + 2p\sum_{j=0}^{q-1}(f(j)f(q-(j+1)))^{-0.5}.
\end{aligned}
$$

Now by this algorithm and the proof of Theorem 1, we write a MAPLE program to derive the exact expression for the Balaban index of $TUHC_6[2p, q]$.

```
when  p\geq q
J1:=proc(p,q)
  restart;
  f:=j->sum((p+k)^2+k,k=0..(q-(j+1)))+sum((p+k)^2-k,k=0..j):
  l:=factor(p*sum((f(j+1)*f(q-(j+1)))^(-1/2),j=0..q-2)+
  2*p*sum((f(j)*f(q-(j+1)))^(-1/2),j=0..q-1)):
  d:=unapply(l,p,q):
  s:=factor(d(p,q)):
  balaban2:=unapply(s,p,q):
  J:=(p*(3*q-1))/(p*(3*q-1)-2*p*q+2)*balaban2(p,q):
 return(J):
end proc;
```

$$
\begin{aligned}
J &= (p(3q-1))/(p(3q-1)-2pq+2) \\
&\quad p(\sum_{j=0}^{q-2}(3/((-3q^2j+3qj^2+3p^2q-3q^2+6qj+q^3+12p+2q+3pq^2-9qp+6pj^2+18pj-6pqj) \\
&\quad (-3q^2j+3qj^2+3p^2q-3q^2+6qj+q^3+2q+3pq^2-3qp+6pj^2+6pj-6pqj))^{(\frac{1}{2})})+ \\
&\quad 2\sum_{j=0}^{q-1}(3/((-3q^2j+3qj^2+3p^2q+q^3-q+3pq^2-3qp+6pj^2+6pj-6pqj) \\
&\quad (-3q^2j+3qj^2+3p^2q-3q^2+6qj+q^3+2q+3pq^2-3qp+6pj^2+6pj-6pqj))^{(\frac{1}{2})}))
\end{aligned}
$$

```
when 2p>q>p
J2:=proc(p,q)
 restart;
 a_1:=(sum((p+k)^2+k,k=0..j)+
      sum((p+k)^2-k,k=1..(q-(j+1))))*(sum((p+k)^2+k,k=0..(q-(j+1)))+
      sum((p+k)^2-k,k=1..j)):
 a_2:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))+
      sum((p+k)^2-k,k=1..j))*(sum((p+k)^2+k,k=0..j)+
     sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-(j+1)))):
 a_3:=(sum((p+k)^2+k,k=0..(q-(j+1)))+sum((p+k)^2-k,k=1..(p-1))+
      sum(p*(4*k-1),k=p..j))*(sum((p+k)^2+k,k=0..(p-1))+
      sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(q-(j+1)))):
 sa_1:=sum((a_1)^(-1/2),j=(q-p)..(p-1)):
 sa_2:=sum((a_2)^(-1/2),j=0..(q-p-1)):
 sa_3:=sum((a_3)^(-1/2),j=p..(q-1)):
 oo:=factor(sa_1+sa_2+sa_3):
 sig1:=2*p*oo: oa_1:=(sum((p+k)^2+k,k=0..j)+
       sum((p+k)^2-k,k=1..(q-(j+1))))*(sum((p+k)^2+k,k=0..(q-(j+2)))+
       sum((p+k)^2-k,k=1..(j+1))):
 oa_2:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+2)))+
       sum((p+k)^2-k,k=1..(j+1)))*(sum((p+k)^2+k,k=0..j)+
       sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-(j+1)))):
 oa_3:=(sum((p+k)^2+k,k=0..(q-(j+2)))+sum((p+k)^2-k,k=1..(p-1))+
       sum(p*(4*k-1),k=p..(j+1)))*(sum((p+k)^2+k,k=0..(p-1))+
       sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(q-(j+1)))):
 oa_5:=(sum((p+k)^2+k,k=0..(q-(p+1)))+
       sum((p+k)^2-k,k=1..(p-1))+p*(4*p-1))*(sum((p+k)^2+k,k=0..(p-1))+
       sum((p+k)^2-k,k=1..(q-p))):
 osa_1:=sum((oa_1)^(-1/2),j=(q-p)..(p-2)):
 osa_3:=sum((oa_3)^(-1/2),j=p..(q-2)):
 osa_2:=sum((oa_2)^(-1/2),j=0..(q-p-1)):
 oooo:=factor(osa_1+osa_2+osa_3+(oa_5)^(-1/2)):
 sig2:=p*oooo:
 dd:=sig1+sig2:
 balaban1:=unapply(dd,p,q):
 J:=(p*(3*q-1))/(p*(3*q-1)-2*p*q+2)*balaban1(p,q):
 return(J):
end proc:
```

$$
\begin{aligned}
J &= (p(3q-1))/(p(3q-1)-2pq+2) \\
& 2p(\sum_{j=q-p}^{p-1}(3/((6pj^2+6pj+3p^2q-3q^2+6qj+3pq^2-3qp-3q^2j+3qj^2+q^3-6pqj+2q) \\
& \quad (6pj^2+6pj+3p^2q+3pq^2-3qp-3q^2j+3qj^2+q^3-6pqj-q))^{(\frac{1}{2})}) \\
&+ \sum_{j=0}^{-p+q-1}(3/((p^3-p-3qp+6pj+6pq^2-12pqj+9pj^2+3p^2j-j+j^3) \\
& \quad (3p^2j+3p^2+9pj^2+12pj+2p+2j+j^3+3j^2+p^3-9qp+6pq^2-12pqj))^{(\frac{1}{2})}) \\
&+ \sum_{j=p}^{q-1}(3/((3p^2q-3p^2j+3pq^2-6pqj+9pj^2-3qp+6pj-q+j+q^3-3q^2j+3qj^2-j^3+p^3-p) \\
& \quad (p^3-3p^2+2p+12pj+9pj^2+3p^2q-3p^2j+3pq^2-6pqj-3qp-3q^2+6qj- \\
& \quad 3j^2+2q-2j+q^3-3q^2j+3qj^2-j^3))^{(\frac{1}{2})})) \\
&+ p(\sum_{j=q-p}^{p-2}(3/((6pj^2+6pj+3p^2q-3q^2+6qj+3pq^2-3qp-3q^2j+3qj^2+q^3-6pqj+2q) \\
& \quad (6pj^2+18pj+3p^2q-3q^2+6qj+3pq^2-9qp-3q^2j+3qj^2+q^3-6pqj+12p+2q))^{(\frac{1}{2})}) \\
& \quad ((6p^3-3qp+6p^2-q+q^3)(3qp+q^3+6p^3-q-6p^2))^{(\frac{1}{2})} \\
&+ \sum_{j=0}^{-p+q-1}(3/((3p^2j+3j^2+9pj^2+24pj+6pq^2-15qp+j^3+p^3-12pqj+14p+2j+3p^2) \\
& \quad (3p^2j+3p^2+9pj^2+12pj+2p+2j+j^3+3j^2+p^3-9qp+6pq^2-12pqj))^{(\frac{1}{2})}) \\
& \quad ((6p^3-3qp+6p^2-q+q^3)(3qp+q^3+6p^3-q-6p^2))^{(\frac{1}{2})} \\
&+ \sum_{j=p}^{q-1}(3/((-3p^2j-3j^2+9pj^2+24pj+3p^2q-3q^2+6qj+3pq^2-9qp-3q^2j+3qj^2- \\
& \quad j^3+q^3+p^3-6pqj+14p-2j+2q-3p^2)(p^3-3p^2+2p+12pj+9pj^2+3p^2q-3p^2j+3pq^2 \\
& \quad -6pqj-3qp-3q^2+6qj-3j^2+2q-2j+q^3-3q^2j+3qj^2-j^3))^{(\frac{1}{2})}) \\
& \quad ((6p^3-3qp+6p^2-q+q^3)(3qp+q^3+6p^3-q-6p^2))^{(\frac{1}{2})}+3)/((6p^3-3qp+6p^2-q+q^3) \\
& \quad (3qp+q^3+6p^3-q-6p^2))^{(\frac{1}{2})}
\end{aligned}
$$

```
when q=2p
J3:=proc(p,q)
 restart;
 a_2:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))+
       sum((p+k)^2-k,k=1..j))*(sum((p+k)^2+k,k=0..j)+
       sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-(j+1)))):
a_3:=(sum((p+k)^2+k,k=0..(q-(j+1)))+sum((p+k)^2-k,k=1..(p-1))+
      sum(p*(4*k-1),k=p..j))*(sum((p+k)^2+k,k=0..(p-1))+
      sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(q-(j+1)))):
 oo:=factor(sum((a_2)^(-1/2),j=0..(p-1))+sum((a_3)^(-1/2),j=p..(q-1))):
 q:=2*p:sig1:=2*p*oo:
 aa:=((sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(2*p-(j+2)))+
      sum((p+k)^2-k,k=1..(j+1)))*(sum((p+k)^2+k,k=0..j)+
      sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(2*p-(j+1)))))^(-1/2):
 bb:=((sum((p+k)^2+k,k=0..(2*p-(j+2)))+sum((p+k)^2-k,k=1..(p-1))+
      sum(p*(4*k-1),k=p..(j+1)))*(sum((p+k)^2+k,k=0..(p-1))+
      sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(2*p-(j+1)))))^(-1/2):
 oooo:=factor(sum(aa,j=0..(p-1))+sum(bb,j=p..(2*p-1))):
```

```
 sig2:=p*oooo:
 t:=sig1+sig2:
 balaban3:=unapply(t,p):
 J:=(p*(3*q-1))/(p*(3*q-1)-2*p*q+2)*balaban3(p):
 return(J):
end proc:
```

$$
\begin{aligned}
J \quad = \quad & p(6p-1)/(2p^2-p+2) \\
& 2p(\sum_{j=0}^{p-1}(3/((25p^3-p-6p^2+6pj-21p^2j+9pj^2-j+j^3) \\
& (-21p^2j-15p^2+9pj^2+12pj+2p+2j+j^3+3j^2+25p^3))^{(\frac{1}{2})})+ \\
& \sum_{j=p}^{2p-1}(3/((27p^3-27p^2j+15pj^2-6p^2+6pj-3p+j-j^3) \\
& (27p^3-21p^2+6p+24pj+15pj^2-27p^2j-3j^2-2j-j^3))^{(\frac{1}{2})}))+ \\
& p(\sum_{j=0} p-1(3/((25p^3+14p-27p^2+24pj-21p^2j+9pj^2+2j+j^3+3j^2) \\
& (-21p^2j-15p^2+9pj^2+12pj+2p+2j+j^3+3j^2+25p^3))^{(\frac{1}{2})}+ \\
& \sum_{j=p}^{2p-2}(3/((-j^3+27p^3+18p-2j-33p^2+36pj-3j^2+15pj^2-27p^2j) \\
& (27p^3-21p^2+6p+24pj+15pj^2-27p^2j-3j^2-2j-j^3))^{(\frac{1}{2})}))
\end{aligned}
$$

```
when q>2p
J4:=proc(p,q)
 a_2:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))+
       sum((p+k)^2-k,k=1..j))*(sum((p+k)^2+k,k=0..j)+sum((p+k)^2-k,k=1..(p-1))+
       sum(p*(4*k-1),k=p..(q-(j+1)))):
 a_3:=(sum((p+k)^2+k,k=0..(q-(j+1)))+sum((p+k)^2-k,k=1..(p-1))+
       sum(p*(4*k-1),k=p..j))*(sum((p+k)^2+k,k=0..(p-1))+
       sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(q-(j+1)))):
 a_4:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))+
       sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..j))*(sum((p+k)^2+k,k=0..(p-1))+
       sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-(j+1)))):
 bs_4:=sum((a_4)^(-1/2),j=p..(q-p-1)):
 bs_3:=sum((a_3)^(-1/2),j=(q-p)..(q-1)):
 bs_2:=sum((a_2)^(-1/2),j=0..(p-1)):
 oo:=factor((bs_3+bs_2+bs_4)):
 oa_2:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))-(p*(4*(q-j-1)+1))+
        sum((p+k)^2-k,k=1..(j+1)))*(sum((p+k)^2+k,k=0..j)+sum((p+k)^2-k,k=1..(p-1))+
        sum(p*(4*k-1),k=p..(q-(j+1)))):
 oa_3:=(sum((p+k)^2+k,k=0..(q-(j+1)))-((p+q-j-1)^2+q-j-1)+sum((p+k)^2-k,k=1..(p-1))+
        sum(p*(4*k-1),k=p..(j+1)))*(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..j)+
        sum((p+k)^2-k,k=1..(q-(j+1)))):
 oa_4:=(sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-(j+1)))-(p*(4*(q-j-1)+1))+
        sum((p+k)^2-k,k=1..(p-1))+
        sum(p*(4*k-1),k=p..(j+1)))*(sum((p+k)^2+k,k=0..(p-1))+
        sum(p*(4*k+1),k=p..j)+sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-(j+1)))):
 obs_4:=sum((oa_4)^(-1/2),j=p..(q-p-1)):
 obs_3:=sum((oa_3)^(-1/2),j=(q-p)..(q-2)):
```

```
 obs_2:=sum((oa_2)^(-1/2),j=0..(p-2)):
 ob_5:=((sum((p+k)^2+k,k=0..(p-1))+sum(p*(4*k+1),k=p..(q-p-1))+
        sum((p-k)^2+k,k=1..(p-1))+p*(4*p-1))*(sum((p+k)^2+k,k=0..(p-1))+
        sum((p+k)^2-k,k=1..(p-1))+sum(p*(4*k-1),k=p..(q-p))))^(-1/2):
 oooo:=factor(obs_3+obs_2+obs_4+ob_5):
 sig1:=2*p*oo:     sig2:=p*oooo:
 t:=sig1+sig2:
 balaban1:=unapply(t,p,q):
 J:=(p*(3*q-1))/(p*(3*q-1)-2*p*q+2)*balaban1(p,q):
 return(J):
end proc:
```

$$
\begin{aligned}
J \;=\; & (p(3q-1))/(p(3q-1)-2pq+2)p(2(p^2(14p^2+6p-2-3q+6q^2-12pq) \\
& \quad (14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})} \\
& \sum_{j=q-p}^{q-1}(3/((3p^2q-3p^2j+3pq^2-6pqj+9pj^2-3pq+6pj-q+j+q^3-3q^2j+3qj^2-j^3+p^3-p) \\
& \quad (p^3-3p^2+2p+12pj+9pj^2+3p^2q-3p^2j+3pq^2-6pqj-3pq-3q^2+6qj-3j^2+ \\
& \quad 2q-2j+q^3-3q^2j+3qj^2-j^3))^{(\frac{1}{2})})+ \\
& 2(p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})} \\
& \sum_{j=0}^{p-1}(3/((p^3-p-3pq+6pj+6pq^2-12pqj+9pj^2+3p^2j-j+j^3) \\
& (3p^2j+3p^2+9pj^2+12pj+2p+2j+j^3+3j^2+p^3-9pq+6pq^2-12pqj))^{(\frac{1}{2})})+ \\
& 2(p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})} \\
& \sum_{j=p}^{-p+q-1}(3/(p^2(2p^2-2-3q+6j+6q^2-12qj+12j^2)(2p^2+4+18j+12j^2-9q+6q^2-12qj))^{(\frac{1}{2})})+ \\
& \sum_{j=q-p}^{q-1}(3/((-3p^2+3p^2q+q^3-j^3+3qj^2-3q^2j-3q^2+6qj-3j^2+14p+2q-2j-6pqj+ \\
& \quad 24pj+9pj^2-9pq+3pq^2-3p^2j+p^3)(p^3-3p^2+2p+12pj+9pj^2+3p^2q-3p^2j+3pq^2-6pqj- \\
& \quad 3pq-3q^2+6qj-3j^2+2q-2j+q^3-3q^2j+3qj^2-j^3))^{(\frac{1}{2})}) \\
& \quad (p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})}+ \\
& \sum_{j=0}^{p-2}(3/((3p^2+j^3+3j^2+14p+2j-12pqj+24pj+9pj^2-15pq+6pq^2+3p^2j+p^3) \\
& \quad (3p^2j+3p^2+9pj^2+12pj+2p+2j+j^3+3j^2+p^3-9pq+6pq^2-12pqj))^{(\frac{1}{2})}) \\
& \quad (p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})} \\
+ \; & \sum_{j=p}^{-p+q-1}(3/(p^2(2p^2+16-15q+30j+6q^2-12qj+12j^2)(2p^2+4+18j+12j^2-9q+6q^2-12qj))^{(\frac{1}{2})}) \\
& \quad (p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})}+3) \\
& \quad (p^2(14p^2+6p-2-3q+6q^2-12pq)(14p^2-6p-2+3q+6q^2-12pq))^{(\frac{1}{2})}
\end{aligned}
$$

```
balaban:=proc(p,q)
     if p>q or p= q then return(J1(p,q));
        elif q>2p then then return(J4(p,q));
         elif 2p>q and q>p then return(J2(p,q));
          elif 2p=q then return(J3(p,q));
      end if;
 end proc:
```

p	q	$J(G)$	p	q	$J(G)$
3	2	1.816153384	3	3	1.570369020
4	2	1.634533430	4	3	1.419631938
4	4	1.243417185	5	1	2.000000000
5	2	1.468736612	5	3	1.277119467
10000	10000	0.0004978663204	100000	553	0.00008972330154
10000	9999	0.0004978924006	100000000	1000	0.00000009002944001
10000	9998	0.0004979184861	10000000000	55300	0.0000000009000020881
10000	9997	0.0004979445685	15	7	0.4671996224
10000	9996	0.0004979706549	15	6	0.4671996224

Table 3: Balaban index of short $TUHC_6[2p, q]$ tubes, $q \leq p$

p	q	$J(G)$	p	q	$J(G)$
1	5	1.055419721	5	11	0.5868560594
2	5	1.190105784	2	6	1.028989158
3	7	0.9032034971	3	8	0.8076749363
4	9	0.7140624259	4	10	0.653287625
10000	21000	0.0003021584021	15	31	0.2062347925
10000	22000	0.0002909149996	15	32	0.2009448960
10000	23000	0.0002804011873	15	33	0.1958934458
10000	24000	0.0002705559202	15	34	0.1910664974
10000	25000	0.0002613237687	15	35	0.1864510072

Table 4: Balaban index of long $TUHC_6[2p, q]$ tubes, $q > 2p$

In Tables (1) and (2) the numerical data for Balaban index in tubes $T(p, q) = TUHC_6[2p, q]$ of various dimensions are given. Note that $J(T(p, 1)) = 2$ and $\lim_{p \longrightarrow \infty} pJ(T(p, 2)) = 12.5$. We conclude this section by the following conjecture

Conjecture: For all positive integer q we have $\lim_{p \longrightarrow \infty} pJ(T(p, q)) < \infty$.

Appendix

In this appendix we include a MATHEMATICA [30] program to produce the graph of $T(p, q)$ and compute the Szeged and Balaban indices of the graph.

```
<<Graphics`Arrow`
<<DiscreteMath`Combinatorica`
verlin[x_,y_]:={{x,y},{x,y+1/2}};
oddlin[x_,y_]:={{{x,y},{x+1/2,y+1/2}},{{x+1/2,y+1/2},{x+1,y}}};
evelin[x_,y_]:={{{x,y},{x+1/2,y-1/2}},{{x+1/2,y-1/2},{x+1,y}}};
positiveslop[x_,y_]:={{x,y},{x+1/2,y+1/2}};
negativeslop[x_,y_]:={{x,y},{x+1/2,y-1/2}};
```

```
pts[x_,y_]:={{x,y},{x+1,y}};
(*generating the coordinates*)
zigzag[p_,q_]:=Join[Flatten[Table[oddlin[x,y],{y,q,1,-2},{x,0,p-2,1}],2],
                    Table[positiveslop[p-1,y],{y,q,1,-2}],
                    Flatten[Table[evelin[x,y],{y,q-1/2,1,-2},{x,0,p-2,1}],2],
                    Table[negativeslop[p-1,y],{y,q-1/2,1,-2}],
                    Flatten[Table[verlin[x,y],{y,q-1/2,1,-2},{x,0,p-1,1}],1],
                    Flatten[Table[verlin[x,y],{y,q-3/2,1,-2},{x,1/2,p,1}],1],
                    Table[{{0,y},{p-1/2,y+1/2}},{y,q,1,-2}],
                    Table[{{0,y-1/2},{p-1/2,y-1}},{y,q,2,-2}]
                     ]
p=5; q=3; (* for example*)
pic=zigzag[p,q];(*show picture *)
(*generating the graph *)
Show[Graphics[Map[Line,pic]],AspectRatio->Automatic];
drawgraph[edgs_]:=Module[{vert,G,n,t,e,vv},
   vert=Union[Flatten[edgs,1]];
   n=Length[vert];
   t=Length[edgs];
   e={};  vv=Table[{vert[[t]],VertexLabel->t},{t,1,n}];
   For[i=1,i<=t,
       z=edgs[[i]];
       AppendTo[e,{{Position[vert,z[[1]]][[1,1]],Position[vert,z[[2]]][[1,1]]}}];
       i++];
G=Graph[e,vv]; ShowGraph[G]; Return[G]; ]
K=drawgraph[pic];(* Show graph*)
(* computing the Szeged index  *)
sz[G_]:=Module[{vert,findninj,edgs},
   edgs=Edges[G];
   vert=Union[Flatten[edgs,1]];
   findninj[ed_]:=Module[{i,j,ni,nj,L1,L2,t},
      ni=0;nj=0;i=ed[[1]];j=ed[[2]];
      For[t=1,t<=Length[vert],
          L1=Length[ShortestPath[G,i,vert[[t]]]]-1;
          L2=Length[ShortestPath[G,j,vert[[t]]]]-1;
          If[L1<L2,ni=ni+1];
          If[L1>L2,nj=nj+1];
      t++ ];
      Return[ni*nj];
               ];
  Return[Sum[findninj[edgs[[i]]],{i,1,Length[edgs]}]];
                  ]
sz[K] (* The Szeged index of the graph *)
(* computing the Balaban index  *)
bal[G_]:=Module[{vert,finddudv,edgs,n,m},
     edgs=Edges[G];  m=Length[edgs];
     vert=Union[Flatten[edgs,1]];  n=Length[vert];
     finddudv[ed_]:=Module[{u,v,du,dv,t},
```

```
        u=ed[[1]]; v=ed[[2]];
        du=Sum[Length[ShortestPath[G,u,vert[[t]]]]-1,{t,1,n}];
        dv=Sum[Length[ShortestPath[G,v,vert[[t]]]]-1,{t,1,n}];
        Return[1/Sqrt[du*dv]]
                         ];
 Return[N[m*Sum[finddudv[edgs[[i]]],{i,1,Length[edgs]}]/(m-n+2),10]];
                ]
bal[K]   (* The Balaban index of the graph *)
```

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