MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **59** (2008) 437-450

ISSN 0340 - 6253

Szeged index of armchair polyhex nanotubes

Mehdi Eliasi* and **Bijan Taeri†**

Department of Mathematical Sciences, Isfahan University of Technology,
Isfahan 84156-83111, Iran

(Received January 10, 2007)

Abstract

Topological indices of nanotubes are numerical descriptors that are derived from graph of chemical compounds. Such indices based on the distances in graph are widely used for establishing relationships between the structure of nanotubes and their physico-chemical properties. The Szeged index is obtained as a bond additive quantity where bond contributions are given as the product of the number of atoms closer to each of the two end points of each bond. In this paper we find an exact expression for Szeged index of $TUVC6[2p, q]$, the armchair polyhex nanotubes, using a theorem of A. Dobrynin and I. Gutman on connected bipartite graphs (see Ref [1]).

1. Introduction

One of the most important problems in chemistry is to convert chemical structure into mathematical molecular descriptors that are relevant to the physical, chemical or biological properties. Molecular structure is one of the basic concepts of chemistry, since properties and chemical and biological behaviors of molecules are determined by it.Topological indices are a convenient method of translating chemical constitution into numerical values that can be used for correlations with physical properties studies. This method has been introduced by Harold Wiener as a descriptor for explaining the boiling points of paraffins (see [2]-[6]). Harold Wiener [2] in 1947 introduced the notion of path number of a graph as the sum of the distances between

*E-mail: eliasi@math.iut.ac.ir
†E-mail: b.taeri@cc.iut.ac.ir (Corresponding Author)

two carbon atoms in the molecules, in terms of carbo-carbon bound. Since then, the spectrum of physico-chemical and biological properties enlarged continuously and several analogues have been defined.

In 1991 Iijima [7] discovered carbon nanotubes as multi walled structures. Carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials. These mechanical characteristics clearly predestinate nanotubes for advanced composites. Carbon nanotubes are one of the most promising materials for use as an electron emission source owing to their substantial emission current at relatively low applied voltage in addition to their excellent mechanical and chemical stability [8], [9],[10]. Field emission tests have been performed on individual carbon nanotubes and carbon nanotube films, and the characteristic values of threshold field, saturation current, and current stability have been measured. These tests have shown that a single tube can emit a current of $0.1mA$ [11] while a current density exceeding $1A/cm^2$ has been observed for carbon nanotube films [12]. Operation for more than 5000 hours has also been established [13].

Let us recall some algebraic definitions that will be used in the paper. 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

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

the summation of distances between u and all vertices of G. The Wiener index of the graph G is the half sum of distances over all its vertex pairs (u, v):

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

A Wiener index analogue, referred to as the Szeged index, Sz, was recently proposed by Gutman et al. (see for example [14]-[18]). The main advantage of the Szeged index is that it is a modification of Wiener index for cyclic graphs; otherwise, it coincides with Wiener index (see, for example [1])).

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

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

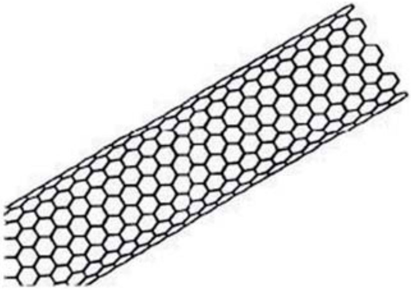

Figure 1: An armchair polyhex nanotube

Diudea was the first chemist which considered the problem of computing topological indices of nanostructures (see for example [19]-[24]). Recently computing topological indices of nanostructures has been the object of many papers. We encourage the reader to consult papers [25]-[36] on computing topological indices of some nanotubes. In [31], [32] we computed the Szeged index of some nanotubes. In this paper we continue this program to find an exact expression for Szeged index of the armchair polyhex nanotubes, $G = TUVC_6[2p, q]$ (see Figure 1). For this purpose we choose a coordinate label for vertices of G as shown in Figure 2.
Firstly we note that G is a bipartite graph. Recall that a graph G is bipartite if the vertices can be colored with withe and black so that adjacent vertices have different color, or equivalently, every cycle has even length (see [37, Theorem 2.4]). So we can use the following theorem of Dobrynin and Gutman [1] on connected bipartite graphs.

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

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

Obviously the number of vertices and the number of edges of $G = TUVC_6[2p, q]$ is $n = |V(G)| = 2pq$ and $m = |E(G)| = 3pq - 2p$, respectively. Thus we need to compute $d(u) - d(v)$, for all edges $e = uv$.

3. Computing the Szeged index of armchair polyhex nanotubes

Throughout this section $G := TUVC_6[2p, q]$, denotes an arbitrary armchair polyhex nanotube in terms of their circumference $2p$ and their length q, see Figure 1. In this section we derive an exact formula for the Szeged index of G. At first we consider an armchair lattice and choose a coordinate label for it, as illustrated in Figure 2. In Figure 3 the distances from x_{10} to all vertices are given. In [36] a MATHEMATICA [38] program that producing the graph of $TUVC_6[2p, q]$ is given.

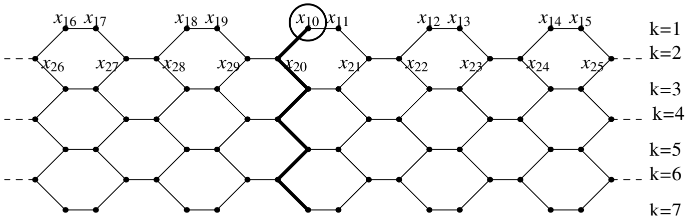

Figure 2: A $TUVC_6[2p, q]$ Lattice with $p = 5$ and $q = 7$.

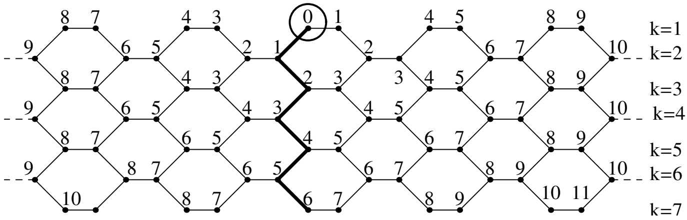

Figure 3: Distances from x_{10} to all vertices of $TUVC_6[2p, q]$ with $p = 5$ and $q = 7$.

Now we prove a key lemma on G.

Lemma 4. The sum of distances of one vertex of level 1 ($k = 1$) to all vertices of level k is given by

$$w_k := \sum_{x \in \ level \ k} d(x_{10}, x) = \sum_{x \in \ level \ k} d(x_{11}, x)$$

$$\vdots$$

$$= \begin{cases} 2p^2 + k^2 - 2k - 2p + 1 + H(p,k) & \text{if} \quad 1 \le k < p \\ \\ p(p + 2k - 2) & \text{if} \quad k \ge p, \end{cases}$$

where

$$H(p,k) = \begin{cases} 2p - 1 & \text{if} \quad k + p \quad \text{is even} \\ \\ 2p & \text{if} \quad k + p \quad \text{is odd.} \end{cases}$$

Proof: We calculate the value of w_k. We consider the tube can be built up from two halves collapsing at the polygon line joining x_{10} to $x_{q,0}$ (as high lighted in Figure 3). The right part is the graph G_1 consists of polygon lines on oblique levels $0, 1, \ldots, p$ (joining x_{1j} to x_{qj}, $j = 0, 1, \ldots, p$) and x_{10} is one of the vertices in the first row of the graph G_1. The left part is the graph G_2 consists of polygon lines on oblique levels $(p+1), (p+2), \ldots, 2p-1$ (joining x_{1j} to x_{qj}, $j = p+1, p+2, , \ldots, 2p-1$). We change the indices of the vertices of G_2 in the following way:

$$V(G_2) = \{\widehat{x}_{ji} \mid \widehat{x}_{j,i} = x_{j,2p-i} \in V(G)\} \quad \text{(See Figure 4)}$$

We must consider two cases:

Case 1: $k \geq p$. In the graphs G_1 and for $0 \leq i \leq p$ we have

$$d(x_{10}, x_{k,i}) = k + i - 1.$$

Also in the graph G_2 and for $1 \leq i < p$, we have

$$d(x_{10}, \widehat{x}_{k,i}) = k + i - 1.$$

Therefore

$$\begin{aligned}\sum_{x \in \; level \; k} d(x_{10}, x) &= \sum_{i=0}^{p} d(x_{10}, x_{k,i}) + \sum_{i=1}^{p-1} d(x_{10}, \widehat{x}_{k,i}) \\ &= 2\sum_{i=1}^{p-1}(k + i - 1) + (0 + k - 1) + (p + k - 1) \\ &= p(p + 2k - 2),\end{aligned}$$

as desired.

Case 2: $k < p$. First suppose that $1 \leq i < k$. In the graphs G_1 and G_2 we have

$$d(x_{10}, x_{k,i}) = k + i - 1 = d(x_{10}, \widehat{x}_{k,i}) = k + i - 1.$$

We put

$$SS_1 = \sum_{i=0}^{k-1} d(x_{10}, x_{k,i}) + \sum_{i=1}^{k-1} d(x_{10}, \widehat{x}_{k,i}) = (3k - 1)(k - 1).$$

Now suppose that $k \leq i < p$. Then in the graph G_1 we can see that if k is odd, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i & \text{if } i \text{ is even} \\ 2i - 1 & \text{if } i \text{ is odd} \end{cases}$$

and if k is even, then

$$d(x_{10}, x_{k,i}) = \begin{cases} 2i - 1 & \text{if } i \text{ is even} \\ 2i & \text{if } i \text{ is odd.} \end{cases}$$

Also in G_2 we have

$$d(x_{10}, \widehat{x}_{k,i}) = \begin{cases} 2i & \text{if } i \text{ is even} \\ 2i + 1 & \text{if } i \text{ is odd} \end{cases}$$

if k is odd and

$$d(x_{10}, \widehat{x}_{k,i}) = \begin{cases} 2i+1 & \text{if} \quad i \quad \text{is even} \\ \\ 2i & \text{if} \quad i \quad \text{is odd} \end{cases}$$

if k is even.

Finally (if $k = p$) in the graph G_1 we have

$$d(x_{10}, x_{k,p}) = H(p, k).$$

We must compute $\sum_{i=k}^{p-1} d(x_{10}, x_{ki})$ and $\sum_{i=k}^{p-1} d(x_{10}, \widehat{x}_{ki})$. We break down these summations into odd and even indices. Let $A = \{k, k+1, k+2, \ldots, (p-1)\}$, $A_1 = \{i \in A \mid i \text{ is even}\}$ and $A_2 = \{i \in A \mid i \text{ is odd}\}$. Put $S_1 = \sum_{i \in A_1} d(x_{10}, x_{ki})$, $S_2 = \sum_{i \in A_2} d(x_{10}, x_{ki})$, $\widehat{S}_1 = \sum_{i \in A_1} d(x_{10}, \widehat{x}_{ki})$ and $\widehat{S}_2 = \sum_{i \in A_2} d(x_{10}, \widehat{x}_{ki})$.

Case 2.1. Suppose that k is odd. It is easy to see that, if p is odd, then

$$A_1 = \left\{k + 2t + 1 \mid t = 0, \ldots, \frac{(p-1) - k - 1}{2}\right\}, A_2 = \left\{k + 2t \mid t = 0, \ldots, \frac{(p-1) - k - 1}{2}\right\},$$

and if p is even, then

$$A_1 = \left\{k + 2t + 1 \mid t = 0, \ldots, \frac{(p-1) - k}{2} - 1\right\}, A_2 = \left\{k + 2t \mid t = 0, \ldots, \frac{(p-1) - k}{2}\right\}.$$

Therefore we have

$$S_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} 2(k + 2t + 1) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} 2(k + 2t + 1) & \text{if } p \text{ is even} \end{cases}$$

and

$$S_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} [2(k + 2t) - 1] & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} [2(k + 2t) - 1] & \text{if } p \text{ is even.} \end{cases}$$

Also we have

$$\widehat{S}_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} 2(k + 2t + 1) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} 2(k + 2t + 1) & \text{if } p \text{ is even} \end{cases}$$

and

$$\widehat{S}_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} [2(k+2t)+1] & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} [2(k+2t)+1] & \text{if } p \text{ is even.} \end{cases}$$

Therefore the summation of distances from x_{10} to all vertices on level k, in the graph G, is

$$\begin{aligned}\sum_{x\in level\ k} d(x_{10},x) &= \left[\sum_{i=0}^{k-1} d(x_{10},x_{ki}) + \sum_{i=1}^{k-1} d(x_{10},\widehat{x}_{ki})\right] + \sum_{i=k}^{p-1} d(x_{10},x_{ki}) + \sum_{i=k}^{p-1} d(x_{10},\widehat{x}_{ki}) + d(x_{10},x_{kp}) \\ &= SS_1 + [S_1+S_2] + [\widehat{S}_1+\widehat{S}_2] + H(p,k) \\ &= 2p^2+k^2-2k-2p+1+H(p,k) \qquad \text{(in both cases } p \text{ is odd or even)}\end{aligned}$$

Case 2.2. Suppose that k is even. It is easy to see that, if p is odd, then

$$A_1 = \left\{k+2t \mid t=0,\ldots,\frac{(p-1)-k}{2}\right\}, A_2 = \left\{k+2t+1 \mid t=0,\ldots,\frac{(p-1)-k}{2}-1\right\},$$

and if p is even, then

$$A_1 = \left\{k+2t \mid t=0,\ldots,\frac{(p-1)-k-1}{2}\right\}, A_2 = \left\{k+2t+1 \mid t=0,\ldots,\frac{(p-1)-k-1}{2}\right\}.$$

Therefore

$$S_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} [2(k+2t)-1] & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} [2(k+2t)-1] & \text{if } p \text{ is even} \end{cases}$$

and

$$S_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} 2(k+2t+1) & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} 2(k+2t+1) & \text{if } p \text{ is even.} \end{cases}$$

Also

$$\widehat{S}_1 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}} [2(k+2t)+1] & \text{if } p \text{ is odd} \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} [2(k+2t)+1] & \text{if } p \text{ is even} \end{cases}$$

and

$$\widehat{S}_2 = \begin{cases} \displaystyle\sum_{t=0}^{\frac{(p-1)-k}{2}-1} 2(k+2t+1) & \text{if } p \text{ is odd} \\ \\ \displaystyle\sum_{t=0}^{\frac{(p-1)-k-1}{2}} [2(k+2t)+1] & \text{if } p \text{ is even.} \end{cases}$$

Therefore the summation of distances from x_{10} to all vertices on level k, in the graph G, is

$$\begin{aligned} \sum_{x \in level\ k} d(x_{10}, x) &= \left[\sum_{i=0}^{k-1} d(x_{10}, x_{ki}) + \sum_{i=1}^{k-1} d(x_{10}, \widehat{x}_{ki}) \right] + \sum_{i=k}^{p-1} d(x_{10}, x_{ki}) + \sum_{i=k}^{p-1} d(x_{10}, \widehat{x}_{ki}) + d(x_{10}, x_{kp}) \\ &= SS_1 + [S_1 + S_2] + [\widehat{S}_1 + \widehat{S}_2] + H(p,k) \\ &= 2p^2 + k^2 - 2k - 2p + 1 + H(p,k) \qquad \text{(in both cases } p \text{ is odd or even)} \end{aligned}$$

which is the same as case 2.1.

As a summary of case 2 we have

$$\sum_{x \in \ level\ k} d(x_{10}, x) = 2p^2 + k^2 - 2k - 2p + 1 + H(p,k),$$

which completes the proof for x_{10}. For other vertices we can apply a similar argument by choosing suitable G_1 and G_2. □

By a straightforward computation we can see

$$\begin{aligned} H(p,k) &= 2p - 1 + \mathrm{irem(k+p,2)} \\ &= 2p - 1 + \frac{1}{2} + \frac{1}{2}(-1)^{k-\mathrm{irem}(p,2)+1}, \end{aligned}$$

where

$$\mathrm{irem(p,2)} = \begin{cases} 0 & \text{if} \quad p \quad \text{is even} \\ \\ 1 & \text{if} \quad p \quad \text{is odd.} \end{cases}$$

So, by Lemma 1, when $1 \le k \le p$, we have

$$w_k = 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\mathrm{irem}(p,2)+1}.$$

Also in the graph G,

$$\begin{aligned} d(x_{10}) &= \sum_{x \in level\ 1} d(x_{10}, x) + \sum_{x \in level\ 2} d(x_{10}, x) + \cdots + \sum_{x \in level\ q} d(x_{10}, x) \\ &= w_1 + w_2 + \cdots + w_q. \end{aligned}$$

So

$$d(x_{10}) = d(x_{11}) = \cdots = d(x_{2p-1,1}) = w_1 + w_2 + \cdots + w_q. \tag{2}$$

Corollary 3. For each $x_{j,i} \in V(G)$, where $j \geq 2$, we have

$$d(x_{j,i}) = w_1 + w_2 + \cdots + w_{q-j+1} + w_2 + \cdots + w_j.$$

Proof: We consider the tube that can be built up from two halves collapsing at level j. The bottom part is the graph $G_1 = TUVC_6[2p, q-j+1]$ and we can consider $x_{j,i}$ as one of the vertices in the first row of the graph G_1. According to (2) we have

$$d_{G_1}(x_{j,i}) = w_1 + w_2 + \cdots + w_{q-j+1}.$$

The top part is the graph $TUVC_6[2p, j] = \widehat{G}_1$ and level j of graph G is the first its row and $x_{j,i}$ is such a vertex of $\widehat{G_1}$. Therefore by (2), $d_{\widehat{G}_1}(x_{j,i}) = w_1 + w_2 + \cdots + w_j$. So

$$d_G(x_{j,i}) = d_{G_1}(x_{j,1}) + d_{\widehat{G}_1}(x_{j,1}) - w_1 = w_1 + w_2 + \cdots + w_{q-j+1} + w_2 + \cdots + w_j,$$

which completes the proof. □

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

Theorem 4. The Szeged index of $G := TUVC_6[2p, q]$ nanotubes is given by

Case 1: If p is even, then

$$Sz(G) = \begin{cases} \frac{-1}{12}p\Big(-36p^2q^3 + 24p^2q^2 - 3q + 6q^2 + 2q^5 - 6(-1)^q q^2 + \\ \quad 4q^3 - 3 + 3(-1)^q q + 3(-1)^q - 6q^4\Big) & \text{if} \quad q \leq p \\ \frac{1}{60}p\Big(12p^5 + 30p^4 - 80qp^4 - 120qp^3 + 160q^2p^3 + 60q^3p^2 + \\ \quad 80p^2q - 120q^2p + 30p(-1)^q + 18p + 20q^4p - 33q - 2q^5 + \\ \quad 15(-1)^{(q+1)}q + 20q^3\Big) & \text{if} \quad p < q < 2p-2 \\ \frac{-1}{30}p^2\Big(-70pq^3 + 24 + 26p^4 - 80p^2 - 15p^3 + 60p^2q - 40p^3q + 80pq\Big) & \text{if} \quad q \geq 2p-2. \end{cases}$$

Case 2: If p is odd, then

$$Sz(G) = \begin{cases} \frac{-1}{12}p\Big(-36p^2q^3 + 24p^2q^2 + 9q - 6q^2 - 9(-1)^q q + 2q^5 + \\ \quad 6(-1)^q q^2 + 4q^3 - 3 + 3(-1)^q - 6q^4\Big) & \text{if} \quad q \leq p \\ \frac{1}{60}p\Big(30 - 80qp^4 - 120qp^3 + 160q^2p^3 + 60q^3p^2 + 80p^2q - \\ \quad 120q^2p + 30p(-1)^q + 20q^4p + 12p^5 + 30p^4 + 20q^3 - 60p^2 - \\ \quad 2q^5 + 15(-1)^{(q+1)}q + 120pq - 33q - 42p\Big) & \text{if} \quad p < q < 2p-2 \\ \frac{-1}{30}p\Big(-60pq + 54p + 30p^2 - 15 - 80p^3 - 15p^4 - 70p^2q^3 - \\ \quad 40p^4q + 60p^3q + 80p^2q + 26p^5\Big) & \text{if} \quad q \geq 2p-2. \end{cases}$$

Proof: The number of vertices and edges of the graph G are $m = 3pq - 2p$ and $n = 2pq$, respectively. 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 $1 \le j \le q$, put $f(j) = d(x_{j,i})$, then by Corollary 3,

$$f(j) = \sum_{k=1}^{q-j+1} w_k + \sum_{k=2}^{j} w_k$$

where $\sum_{k=2}^{1} w_k := 0$. There are two types of edges in the graph G, the edges on horizontal and oblique levels. For each edge on horizontal levels, for example the edge $x_{j,i}x_{j,i+1}$, we have

$$(d(x_{j,i}) - d(x_{j,i+1}))^2 = (f(j) - f(j))^2 = 0.$$

Therefore, we should only consider the edges on oblique levels. For these edges it is sufficient to do computations on the edges $x_{j,0}x_{j+1,0}$, with $1 \le j \le q-1$. We have

$$d(x_{j,i}) - d(x_{j+1,i}) = d(x_{j,0}) - d(x_{j+1,0}) = f(j) - f(j+1).$$

Thus we need to compute $\sum_{j=1}^{q-1}(f(j) - f(j+1))^2$ and use Theorem 1.

First suppose that $q \le p$ and p is even. Then for each k, where $1 \le k \le q$, we have

$$\begin{aligned} w_k &= 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k-\mathrm{irem}(p,2)+1} \\ &= 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k+1}. \end{aligned}$$

So, by definition of $f(j)$ we have

$$\sum_{j=1}^{q-1}(f(j) - f(j+1))^2 = \frac{1}{6}(q-1)\Big(2q^4 - 4q^3 + 6q - 6(-1)^q q + 3 - 3(-1)^q\Big).$$

The above sum is for the polygon line consisting of oblique edges joining $x_{1,0}$ to $x_{q,0}$. Note that we have $2p$ polygon lines consisting of oblique edges joining $x_{1,i}$ to $x_{q,i}$, $i = 0, 2, \ldots, 2p-1$. Therefore by Theorem 1, we have

$$\begin{aligned} Sz(G) &= \frac{1}{4}n^2m - \frac{1}{4}\sum_{uv\in E(G)} (d(u) - d(v))^2 \\ &= \frac{1}{4}n^2m - \frac{1}{4}\left[2p\sum_{j=1}^{q-1}(f(j) - f(j+1))^2\right] \\ &= \frac{1}{4}(2pq)^2(3pq - 2p) - \frac{1}{4}\left[2p\frac{1}{6}(q-1)(2q^4 - 4q^3 + 6q - 6(-1)^q q + 3 - 3(-1)^q)\right] \\ &= \frac{-1}{12}p\Big(- 36p^2q^3 + 24p^2q^2 - 3q + 6q^2 + 2q^5 - 6(-1)^q q^2 + 4q^3 - \\ &\qquad 3 + 3(-1)^q q + 3(-1)^q - 6q^4\Big). \end{aligned}$$

Now suppose that $q > p$ and p is even. Let

$$\begin{aligned} A_1 : &= \{j \mid 1 \leq q-j+1 \leq p-1, 1 \leq j \leq p-1\} \\ A_2 : &= \{j \mid 1 \leq q-j+1 \leq p-1, p \leq j \leq q\} \\ A_3 : &= \{j \mid p \leq q-j+1 \leq q, 1 \leq j \leq p-1\} \\ A_4 : &= \{j \mid p \leq q-j+1 \leq q, p \leq j \leq q\}, \end{aligned}$$

and

$$\begin{aligned} w_k : &= 2p^2 + k^2 - 2k + \frac{1}{2} + \frac{1}{2}(-1)^{k+1} \\ ww_k : &= p(p+2k-2). \end{aligned}$$

Note that if $A_1 \neq \varnothing$, then $q < 2p-2$. Also if $A_4 \neq \varnothing$, then $2p-2 \leq q$. Therefore first suppose that $A_1 \neq \varnothing$. Thus $A_4 = \varnothing$ and $2p-3 \geq q$. So, by Lemma 1 we obtain that

$$\begin{aligned} &\text{if } j \in A_1 \quad \text{then} \quad f(j) = \sum_{k=1}^{q-j+1} w_k + \sum_{k=2}^{j} w_k. \\ &\text{if } j \in A_2 \quad \text{then} \quad f(j) = \sum_{k=1}^{q-j+1} w_k + \sum_{k=2}^{p-1} w_k + \sum_{k=p}^{j} ww_k. \\ &\text{if } j \in A_3 \quad \text{then} \quad f(j) = \sum_{k=1}^{p-1} w_k + \sum_{k=p}^{q-j+1} ww_k + \sum_{k=2}^{j} w_k. \end{aligned}$$

Therefore straightforward computations show that

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

Hence, we have

$$\begin{aligned} Sz(G) &= \frac{1}{4}n^2m - \frac{1}{4}\sum_{uv\in E(G)}(d(u)-d(v))^2 \\ &= \frac{1}{4}n^2m - \frac{1}{4}\left[2p\sum_{j=1}^{q-1}(f(j)-f(j+1))^2\right] \end{aligned}$$

$$= \frac{1}{60}p\Big(12p^5 + 30p^4 - 80qp^4 - 120qp^3 + 160q^2p^3 + 60q^3p^2 + 80p^2q - 120q^2p$$
$$+30p(-1)^q + 18p + 20q^4p - 33q - 2q^5 + 15(-1)^{(q+1)}q + 20q^3\Big).$$

Similarly we can handle the other cases. □

Acknowledgement: The second author was partially supported by Center of Excellence of Mathematics of Isfahan University of Technology (CEAMA).

References

[1] I. Gutman and A. Dobrynin, On a graph invariant related to the sum of all distances in a graph, Publ. Inst. Math. (Beograd) **56** (1994) 18-22.

[2] H. Wiener, Structural determination of paraffin boiling points, J. Am. Chem. Soc. **69** (1947) 17-20.

[3] H. Wiener, Correlation of heats of isomerization and differences in heats of vaporization of isomers, among the paraffin hydrocarbons, J. Am. Chem. Soc.**69**(1947) 2636-2638.

[4] H. Wiener, Influence of interatomic forces on paraffin properties, J. Chem. Phys. **15** (1947) 766-766.

[5] H. Wiener, Vapor pressure - temperature relationships among the branched paraffin hydrocarbons, J. Phys. Chem. **52** (1948) 425-430.

[6] H. Wiener, Relation of the physical properties of the isomeric alkanes to molecular structure. Surface tension, specific dispersion, and critical solution temperature in aniline, J. Phys. Chem. **52** (1948) 1082-1089.

[7] S. Iijima, Helical microtubules of graphitic carbon, Nature **354** (1991) 56-58.

[8] L. Nilsson, O. Groening, C. Emmenegger, O. Kuettel, E. Schaller, L. Schlapbach, H. Kind, J. M. Bonard and K. Kern, Scanning field emission from patterned carbon nanotube films, Appl. Phys. Lett. **76** (2000) 2071-2073.

[9] W. A. de Heer, A. Chatelain and D. Ugarte, A carbon nanotube field-emission electron source, Science **270** (1995) 1179-1180.

[10] S. C. Kung, K. C. Hwang and I. N. Lin, Oxygen and ozone oxidation-enhanced field emission of carbon nanotubes, Appl. Phys. Lett. **80** (2002) 4819-4821.

[11] J. M. Bonard, J. P. Salvetat, T. Stöckli, L. Forró, and A. Châtelain, Field emission from carbon nanotubes: perspectives for applications and clues to the emission mechanism, Appl. Phys. **69** (1999) 245-254.

[12] W. Zhu, C. Bower, G. P. Kochanski and S. Jin, Electron field emission from nanostructured diamond and carbon nanotubes, Solid-State Electronics **45** (2001) 921-928.

[13] S. Uemura, T. Nagasako, J. Yotani, T. Shimojo and Y. Saito, Carbon Nanotube FED Elements, SID98 Digest, (1998) 1052-1055.

[14] I. Gutman, A Formula for the Wiener Number of Trees and Its Extension to Graphs Containing Cycles, Graph Theory Notes New York **27** (1994) 9-15.

[15] I. Gutman, P. Khadikar, N. Deshpande, P. Kale, A. Dobrynin and G. Dömötör, The Szeged Index and an Analogy with the Wiener Index, J. Chem. Inf. Comput. Sci. **35** (1995) 547-550.

[16] I. Gutman, L. Popovic, P. Khadikar, S. Karmarkar, S. Joshi and M. Mandloi, Relations between Wiener and Szeged indices of monocyclic molecules, MATCH Commun. Math. Comput. Chem. **35** (1997) 91-103.

[17] I. Gutman, P. Khadikar and T. Khaddar, Wiener and Szeged indices of benzenoid hydrocarbons containing a linear polyacene fragment, MATCH Commun. Math. Comput. Chem. **35** (1997) 105-116.

[18] I. Gutman, P. Khadikar, P. Rajput and S. Karmarkar, The Szeged index of polyacenes, J. Serb. Chem. Soc. **60** (1995) 759-764.

[19] M. V. Diudea and A. Graovac, Generation and Graph-Theoretical Properties of C_4-Tori, MATCH Commun. Math. Comput. Chem. **44** (2001) 93-102.

[20] M. V. Diudea, I. Silaghi-Dumitrescu and B. Parv, Toranes Versus Torenes, MATCH Commun. Math. Comput. Chem. **44** (2001) 117-133.

[21] M. V. Diudea and P. E. John, Covering polyhedral tori, MATCH Commun. Math. Comput. Chem. **44** (2001) 103-116.

[22] M. V. Diudea, Graphenes from 4-valent tori, Bull. Chem. Soc. Jpn. **75** (2002) 487-492.

[23] M. V. Diudea, Hosoya Polynomial in Tori, MATCH Commun. Math. Comput. Chem. **45** (2002) 109-122.

[24] M. V. Diudea, M. Stefu, B. Parv and P. E. John, Wiener Index of Armchair Polyhex Nanotubes, Croat. Chem. Acta, **77** (2004) 111-115.

[25] A. R. Ashrafi and A. Loghman, PI Index of Zig-zag Polyhex Nanotubes, MATCH Commun. Math. Comput. Chem. **55** (2006) 447-452.

[26] A. R. Ashrafi and S. Yousefi, Computing the Wiener Index of a TUC_4C_8(S) Nanotorus, MATCH Commun. Math. Comput. Chem. **57** (2007) 403-410.

[27] A. Heydari and B. Taeri, Szeged Index of $TUC_4C_8(R)$ Nanotubes, MATCH Commun. Math. Comput. Chem. **57** (2007) 665-676.

[28] A. Heydari and B. Taeri, Wiener and Schultz Indices of $TUC_4C_8(R)$ Nanotubes, J. Comput. Theor. Nano Sci. **4** (2007) 158-167.

[29] A. Heydari and B. Taeri, Wiener and Schultz Indices of $TUC_4C_8(S)$ Nanotubes, MATCH Commun. Math. Comput. Chem. **57** (2007) 665-676.

[30] S. Yousefi and A. R. Ashrafi, An exact expression for the Wiener index of a polyhex nanotorus, MATCH Commun. Math. Comput. Chem. **56** (2006) 169-178.

[31] E. Eliasi and B. Taeri, Szeged and Balaban indices of zig-zag polyhex nanutubes, MATCH Commun. Math. Comput. Chem. **56** (2006) 383-402.

[32] A. Heydari and B. Taeri, Szeged index of $TUC_4C_8(R)$ nanotubes, MATCH Commun. Math. Comput. Chem. **57** (2007) 463-477.

[33] M. Diudea and M. Stefu, Wiener index of C_4C_8 nanotubes, MATCH Commun. Math. Comput. Chem. **50** (2004) 133-144.

[34] M. Diudea, B. Parv, P. E. John, O. Ursu and A. Graovac, Distance counting in tori. MATCH Commun. Math. Comput. Chem. **49** (2003) 23-36.

[35] M. Diudea, Hosoya polynomial in tori. MATCH Commun. Math. Comput. Chem. **45** (2002) 109-122.

[36] E. Eliasi and B. Taeri, Balaban index of zigzag polyhex nanotorus, J. Comput. Theor. Nano Sci. Accepted for publication.

[37] F. Harary, Graph Theory, Addison-Welesly, 1972.

[38] S. Wolfram. The Mathematica Book, Cambridge University Press and Wolfram Media, Cambridge, 1999.