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Szeged Index of $TUC_4C_8(R)$ Nanotubes

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Abstract

Let G be a graph. If (i, j) is an edge between vertices i and j of G and $N(i)$ denote the number of vertices of G lying closer to vertex i than to j and $N(j)$ denote the number of vertices of G lying closer to vertex j than to i, the Szeged index of G is defined as $Sz(G) = \sum_{(i,j)} N(i)N(j)$, where (i, j) go over all edges of G. In this paper we derive an exact expression for Szeged index of $TUC_4C_8(R)$ nanotubes.

1. Introduction. In 1991 Iijima [1] 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.

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 Wiener index is oldest topological indices . In 1947 chemist Harold Wiener [3] developed the most widely known topological descriptor, the Wiener index, and used in to determine physical properties of types of alkanes known as paraffins. Numerous of its chemical applications were reported and its mathematical properties are well understood [5]-[9].

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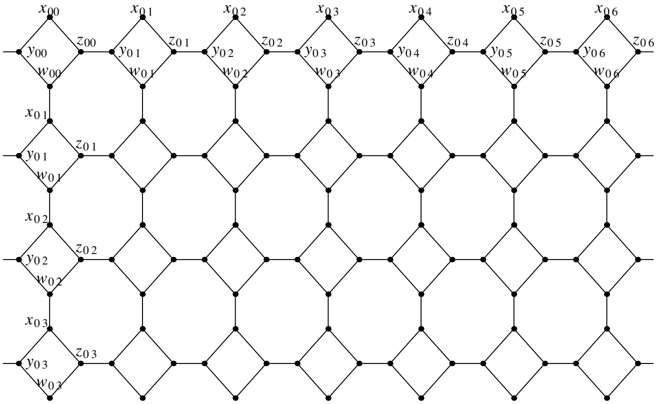

Figure 1: A $TUC_4C_8(R)$ Lattice with $p = 7$ and $q = 4$.

Let G be a connected graph, the set of vertices and edges of will be denoted by $V(G)$ and $E(G)$, respectively. If e is an edge of G, connecting the vertices i and j of G then we write $e = ij$. The distance between a pair of vertices i and i of G is denoted by $d(i, j)$. For an edge $e = ij$, let $N(i)$ be the number vertices of G lying closer to i than to j and $N(j)$ be the number of vertices of G lying closer to j than to i, that is

$$N(i) = |\{u \in V(G) \mid d(u, i) < d(u, j)\}| \quad \text{and} \quad N(j) = |\{u \in V(G) \mid d(u, j) < d(u, i)\}|.$$

The summation $\sum_{ij \in E(G)} N(i)N(j)$ is defined as Szeged index of G.

The Szeged index has been defined by Khadikar, *et. al.* [23] and studied in many papers, see for example [19]-[25].

In a series of papers, Diudea and coauthors [10]-[18] computed the Wiener index of some nanotubes. In this paper we find an exact expression for Szeged index of $TUC_4C_8(R)$ nanotube. For this nanotubes and obtain a formula for Szeged index in short and long cases.

2. Szeged index of $TUC_4C_8(R)$

In this section we derive an exact formula for the Szeged index of $T(p, q) := TUC_4C_8(R)$. For this purpose we choose a coordinate label for vertices of $T(p, q)$ as shown in figure 1.

In Appendix we include a MATHEMATICA [4] program to produce the graph of $T(p, q)$ and computing the Szeged index of the graph. If $[\frac{p+1}{2}] > q$ (where $[a]$ denotes the integer part of real number a), then the nanotube is called short and if $q \geq [\frac{p+1}{2}]$ the nanotube is called long. Throughout the paper we fix $p_1 = [\frac{p+1}{2}]$. Firstly we consider the short case. To compute Szeged index in short case, as the first step, for the edge $x_{i0}y_{i0}$ we find a set of vertices that lying closer to x_{i0} than to y_{i0}. In the following Lemma we obtain a method for computing the distance between two vertices of the lattice.

Lemma 1. Let $0 \le r \le k$, $a_{ij}, b_{ij} \in \{x_{ij}, y_{ij}, z_{ij}, w_{ij}\}$ and $d(a_{r0}, b_{r0}) = \alpha$. Then

$$d(a_{kt}, b_{r0}) = \begin{cases} 3(k-t)+t+\alpha & \text{if } \ 0 \le t < k-r < p_1 \ \text{ or } \ a_{kt} = y_{tt}, w_{tt} \\ 3t+(k-t)+\alpha & \text{if } \ k-r < t \le p < p_1 \ \text{ or } \ a_{kt} = z_{tt}, x_{tt} \end{cases}$$

Proof: Suppose $0 \le t < k-r < p_1$ or $a_{kt} = y_{tt}, w_{tt}$. Each row contains three vertices and every path from a_{kt} to b_{r0} must moves left t columns and moves up at least $k-r$ rows. Thus the length of a shortest path from a_{kt} to a_{r0} is $3(k-r)+t$. Therefore $d(a_{kt}, b_{r0}) = 3(k-r)+t+\alpha$, where α is the distance between a_{r0} and b_{r0}.

Now suppose $k-r < t < p_1$ or $a_{kt} = z_{tt}, x_{tt}$. A shortest path from a_{kt} to a_{r0} most move left t columns contains three vertex and moves up $k-r$ row contains one vertex. So the length of this path is $3t+(k-r)+\alpha$. □

Now we compute $N(x_{kt})$ and $N(y_{kt})$ for all edges which are not vertical or horizontal in $T(p,q)$. For an edge uv of G we denote by G^k_u the set of vertices of kth row lying closer to u that to v and denote by $N_k(u)$ the number of elements of G^k_u.

Lemma 2. Let $0 \le i < q$ and $x_{i0}y_{i0}$ be the edge between x_{i0} and y_{i0} in a short $T(p,q)$. Then $N_k(x_{i0}) = 2p+4i-4k-1$ and $N_k(y_{i0}) = \begin{cases} 4pq - N_k(x_{i0}) & \text{if } \ p \ \text{ is even} \\ 4pq - N_k(x_{i0}) - q & \text{if } \ p \ \text{ is odd} \end{cases}$

Proof: Let $a_{kt} \in \{x_{kt}, y_{kt}, z_{kt}, w_{kt}\}$ be an arbitrary vertex in the kth row. We consider two cases:

Case 1. If $0 \le t < p_1$. Let $0 \le t < k-i < p_1$. By Lemma 1, we have $d(a_{kt}, x_{i0}) = 3(k-i)+t+\alpha_1$ and $d(a_{kt}, y_{i0}) = 3(k-i)+t+\alpha_2$, where $d(a_{i0}, x_{k,0}) = \alpha_1$ and $d(a_{i0}, y_{i0}) = \alpha_2$. So $\alpha_1 = \alpha_2 + 1$ and $a_{kt} \in G^k_{y_{i0}}$. Similarly if $a_{kt} = w_{tt}, y_{tt}$, then by Lemma 1, $a_{kt} \in G^k_{y_{i0}}$.
Now let $k-i < t \le p_1$. By Lemma 1, $d(a_{kt}, x_{i0}) = 3t+(k-i)+\alpha_1$ and $d(a_{kt}, y_{i0}) = 3t+(k-i)+\alpha_2$, where $d(a_{i0}, x_{i0}) = \alpha_1$ and $d(a_{i0}, y_{k0}) = \alpha_2$. If p is even, $\alpha_2 = \alpha_1+1$ and $a_{kt} \in G^k_{x_{i0}}$ and similarly if $a_{kt} = x_{tt}, z_{tt}$, then $a_{kt} \in G^k_{x_{i0}}$. Thus $G^k_{x_{i0}}$ has $p/2-k+i$, $2(p/2-k+i)-1$ and $p/2-k+i-1$ vertices of the form x_{kt}, y_{kt} and z_{kt} respectively. If p is odd, then as in the even case, $a_{kt} \in G^k_{x_{i0}}$, for $a_{kt} \ne z_{k,\frac{p-1}{2}}$, because $d(z_{k,\frac{p-1}{2}}, x_{i0}) = d(z_{k,\frac{p-1}{2}}, y_{i0}) = 3(p_1-1)+k-i+1$. Thus $z_{k,\frac{p-1}{2}} \notin G^k_{x_{i0}}$ and $z_{k,\frac{p-1}{2}} \notin G^k_{y_{i0}}$. So $G^k_{x_{i0}}$ has p_1-k+i, $2(p_1-k+i-1)$ and $p_1-k+i-1$ vertices of the form x_{kt}, y_{kt} and z_{kt} respectively.

Case 2. $p_1 \le t < p$. By symmetry of $T(p,q)$ we have

$$d(a_{kt}, x_{i0}) = d(a_{kt}, x_{ip-1}) + d(x_{ip-1,x_{i0}}) = d(a_{k,p-t-1}, x_{i0}) + 3$$

and

$$d(a_{kt}, y_{i0}) = d(a_{kt}, y_{i,p-1}) + d(y_{i,p-1}, x_{i0}) = d(a_{k,p-t-1}, y_{i0}) + 3.$$

So if p is even for $a_{kt} \ne y_{k,p/2}$, $a_{kt} \in G^k_{y_{i0}}$ and $y_{k,p/2} \in G^k_{x_{i0}}$. Also if p is odd, then for all of the a_{kt}, we have $a_{kt} \in G^k_{y_{i0}}$.

Now by two cases above, if p is even, then

$$N_k(x_{i0}) = \left(\frac{p}{2} - k + i\right) + 2\left(\frac{p}{2} - k + i\right) - 1 + \left(\frac{p}{2} - k + i - 1\right) + 1 = 2p - 4k + 4i - 1,$$

and $N_k(y_{i0}) = 4pq - N_k(x_{i0})$, for all $0 \le k < q$. Also if p is odd, then $N_k(y_{i0}) = 4pq - N_k(x_{i0}) - q$ and for all $0 \le k \le q-1$, we have

$$N_k(x_{i0}) = (p_1 - k + i) + 2(p_1 - k + i - 1) + (p_1 - k + i - 1) = 2p - 4k + 4i - 1.$$

Therefore the proof is complete. □

By symmetry of $T(p,q)$ for each $0 \le i < q$, the number $N(x_{i0})$, with respect to the edge $x_{i0}y_{i0}$, is equal to $N(x_{st})$, $0 \le s < q$, with respect to the edge $x_{st}y_{st}$. Similarly for edges $x_{i0}y_{i0}$ and $x_{q-i-1,0}y_{q-i-1,0}$ we have $N(x_{i0}) = N(x_{q-i-1,0})$. Therefore for each $0 \le t < p$ and $0 \le i < q$, $N(x_{it}) = N(x_{q-i-1,t})$ with respect to the edges $x_{it}y_{it}$ and $x_{q-i-1,t}y_{q-i-1,t}$.
In two lemma below we compute $N(a_{kt})$ for horizontal and vertical edges in $T(p,q)$.

Lemma 3. Let p be an even integer. Then if $0 \le k < q$ and $0 \le t < p$, for edge $z_{kt}y_{k,t+1}$ in $T(p,q)$, $N(z_{kt}) = N(y_{k,t+1}) = 2pq$. If p is an odd integer and $q < p_1$ then $N(z_{kt}) = N(y_{k,t+1}) = q(2p-1)$.
Proof. By symmetry of $T(p,q)$, $N(z_{00}) = N(z_{kt})$ and $N(y_{01}) = N(y_{k,t+1})$, so we compute $N(z_{00})$ and $N(y_{01})$, for edge $z_{00}y_{01}$. If p is an even integer, then for $1 \le t \le p/2$ and $0 \le k < q$ we have $d(a_{kt}, y_{01}) + 1 = d(a_{kt}, z_{00})$. Thus $a_{kt} \in G_{y_{01}}$. Therefore the number of element of $N(y_{01})$ in kth row is $p/2 + p + p/2$. So $N_k(y_{01}) = 2p$ and $N(y_{01}) = q(p/2 + p + p/2) = 2pq$. For other vertices of graph we have $d(a_{kt}, y_{01}) = d(a_{kt}, z_{00}) + 1$. So $a_{kt} \in G_{z_{00}}$. Since the number of all vertices of $T(p,q)$ is $4pq$ we have $N(z_{00}) = 4pq - 2pq = 2pq$.
Now if p is odd and $q < p_1$, then for $0 \le k < q$, we have $d(x_{k,p_1+1}, y_{01}) = d(x_{k,p_1+1}, z_{00}) = 3(p_1 - 1) + 2 + k$ and $d(w_{k,p_1+1}, y_{01}) = d(x_{k,p_1+1}, z_{00}) = 3(p_1 - 1) + 2 + k$. Thus $2q$ of the vertices have equal distances from y_{01} and z_{00}. For $4pq - 2q$ remaining vertices of the graph, as in the previous case, we have $a_{kt} \in G_{y_{01}}$, for all $1 \le t \le (p-1)/2$ and $0 \le k < q$. So $N(y_{01}) = 2pq - q = q(2p-1)$ and $N(z_{kt}) = N(y_{k,t+1})$. Therefore the proof of lemma is complete. □

Lemma 4. Let $0 \le k < q$ and $0 \le t < p$ then for edge $x_{k+1,t}w_{kt}$ in $T(p,q)$, $N(x_{k+1,t}) = 4(k+1)p$ and $N(w_{kt}) = 4p(q-k-1)$.
Proof. Since $N(x_{i+1,t}) = N(x_{i+1,0})$ and $N(w_{it}) = N(w_{i0})$, we may compute $N(x_{i+1,0})$ and $N(w_{i0})$ for all edges $x_{i+1,0}w_{i0}$, where $0 \le i < q$. For $0 \le t < p$ and $0 \le k \le i$, we have $d(a_{kt}, w_{i0}) + 1 = d(a_{kt}, x_{i+1,0})$. So $a_{kt} \in G_{w_{i0}}$. Therefore $N(w_{i0}) = 4p(i+1)$ and $N(x_{i+1,0}) = 4pq - 4p(k+1) = 4p(q-k-1)$. □

Now we can compute the Szeged index of short $T(p,q)$ where $p_1 > q$.

Theorem 1. The Szeged index of short $TUC_4C_8(R)$ is given by the following equation

$$Sz(G) = \begin{cases} \frac{p}{3}(p^2(68q^3 - 8q) + 4q^3 - 16q^5) & \text{if } p \text{ is even} \\ \\ \frac{p}{3}(p^2(68q^3 - 8q) - 36q^3p + 19q^3 - 16q^5) & \text{if } p \text{ is odd} \end{cases}$$

Proof. Since $q < p_1$, by Lemma 2, for $0 \le i < q$ we have

$$N(x_{i0}) = \sum_{k=0}^{q-1}\Big(2p + 4i - 4k - 1\Big) = q(2p + 4i + 1) - 2q^2.$$

By definition of the Szeged index and using the symmetry of $T(p,q)$, $Sz(G)$ can be computed as follows

$$\begin{aligned} Sz(G) &= \sum_{k=0}^{q-1}\sum_{t=0}^{p-1} N(x_{kt})N(y_{kt}) + \sum_{k=0}^{q-1}\sum_{t=0}^{p-1} N(x_{kt})N(z_{kt}) + \sum_{k=0}^{q-1}\sum_{t=0}^{p-1} N(w_{kt})N(y_{kt}) + \\ &\quad \sum_{k=0}^{q-1}\sum_{t=0}^{p-1} N(w_{kt})N(z_{kt}) + \sum_{k=0}^{q-2}\sum_{t=0}^{p-1} N(w_{kt})N(x_{k+1,t}) + \\ &\quad \sum_{k=0}^{q-1}\sum_{t=0}^{p-2} N(z_{kt})N(y_{k,t+1}) + \sum_{k=0}^{q-1} N(z_{k,p-1})N(y_{k0}) \\ &= p\sum_{k=0}^{q-1} N(x_{k0})N(y_{k0}) + p\sum_{k=0}^{q-1} N(x_{k0})N(z_{k0}) + p\sum_{k=0}^{q-1} N(w_{q-k-1,0})N(y_{q-k-1,0}) + \\ &\quad p\sum_{k=0}^{q-1} N(w_{q-k-1,0})N(z_{q-k-1,0}) + p\sum_{k=0}^{q-2} N(w_{kt})N(x_{k+1,t}) + p\sum_{k=0}^{q-1} N(z_{k0})N(y_{k1}) \\ &= 4p\sum_{k=0}^{q-1} N(x_{k0})N(y_{k0}) + p\sum_{k=0}^{q-2} N(w_{kt})N(x_{k+1,t}) + p\sum_{k=0}^{q-1} N(z_{k0})N(y_{k1}). \end{aligned}$$

Suppose that p is even. By Lemma 2, 3 and 4 we have

$$\begin{aligned} Sz(G) &= 4p\sum_{i=0}^{q-1}(q(2p + 4i + 1) - 2q^2)(4pq - q(2p + 4i + 1) + 2q^2) \\ &\quad +p\sum_{k=0}^{q-2} 4p(k + 1)4p(q - k - 1) + pq(2pq)(2pq) \\ &= \Big(16p^3q^3 - \frac{16}{3}pq^5 + \frac{4}{3}pq^3\Big) + \Big(-\frac{8}{3}p^3q + \frac{8}{3}p^3q^3\Big) + (4p^3q^3) \\ &= \frac{p}{3}\Big(p^2(68q^3 - 8q) + (4q^3 - 16q^5)\Big) \end{aligned}$$

Now suppose that p is odd. So

$$\begin{aligned} Sz(G) &= 4p\sum_{i=0}^{q-1}(q(2p + 4i + 1) - 2q^2)(4pq - q(2p + 4i + 1) + 2q^2 - q) \\ &\quad +p\sum_{k=0}^{q-2} 4p(k + 1)4p(q - k - 1) + pq(q(2p - 1))(q(2p - 1)) \end{aligned}$$

$$= \left(16p^3q^3 - \frac{16}{3}pq^5 + \frac{16}{3}pq^3 - 8q^3p^2\right) + \left(-\frac{8}{3}p^3q + \frac{8}{3}p^3q^3\right) + (q^3p(2p-1)^2)$$
$$= \frac{p}{3}\left(p^2(68q^3 - 8q) - 36q^3p + 19q^3 - 16q^5\right).$$

This completes the proof. □

Now we consider long $T(p,q) = TUC_4C_8(R)$ nanotube ($q \geq p_1$). If p is an even integer, Lemma 3 and Lemma 4 are valid, and we use these for horizontal and vertical edges of the graph. For oblique edges we may compute $N(x_{i0})$, $N(y_{i0})$ with respect to the edge $x_{i0}y_{i0}$ and $N(z_{i0})$, $N(y_{i1})$ with respect to the edge $z_{i0}y_{i1}$, for all $0 \leq i < q-1$.

In the following lemma we consider horizontal edges, when p is odd.

Lemma 5. Suppose that p is odd, $0 \leq k < q$ and $0 \leq t < p$. For edge $z_{kt}y_{k,t+1}$ in $T(p,q)$, if $p_1 \leq q < p$ then

$$N(z_{kt}) = N(y_{k,t+1}) = \begin{cases} 2q(p-1) + p_1 + k & \text{if} \quad 0 \leq k < q - p_1 \\ 2qp - q & \text{if} \quad q - p_1 \leq k < p_1 \\ q(2p-1) + p_1 - k - 1 & \text{if} \quad p_1 \leq k < q, \end{cases}$$

and if $q \geq p$ then

$$N(z_{kt}) = N(y_{k,t+1}) = \begin{cases} 2q(p-1) + p_1 + k & \text{if} \quad 0 \leq k < p_1 \\ 2q(p-1) + 2p_1 - 1 & \text{if} \quad p_1 \leq k < q - p_1 \\ q(2p-1) + p_1 - k - 1 & \text{if} \quad q - p_1 \leq k < q \end{cases}$$

Proof. By symmetry of $T(p,q)$, for all $0 \leq t < p$ and for edges $z_{st}y_{s,t+1}$, we have $N(z_{st}) = N(y_{s,t+1})$. So we may compute $N(z_{s0}) = N(y_{s1})$, for a fixed integer $0 \leq s < q$.

As in the proof of Lemma 3, for $0 \leq k < q$, we have $d(x_{k,p_1+1}, y_{s1}) = d(x_{k,p_1+1}, z_{s0})$ and $d(w_{k,p_1+1}, y_{s1}) = d(w_{k,p_1+1}, z_{s0})$. We denote these vertices by b_{kp_1}.
If $|k-s| \geq p_1$, then $d(y_{k,p_1+1}, y_{s1}) = d(y_{k,p_1+1}, z_{s0}) = 4(p_1-1) + 3(k-s-p_1+1)$ and $d(z_{k,p_1+1}, y_{s1}) = d(z_{k,p_1+1}, z_{s0}) = 4(p_1-1) + 3(k-s-p_1+1)$. We denote these vertices by c_{kp_1}.
If $a_{kt} \neq b_{kp_1}$ or $a_{kt} \neq c_{kp_1}$, then $a_{kt} \in G_{y_{s1}}$ or $a_{kt} \in G_{z_{s0}}$.

Now suppose that $q < p$. We distinguish three cases:

Case 1. $0 \leq s < q - p_1$. In this case the number of vertices b_{kp_1} is $2q$ and number of vertices c_{kp_1} is $2(q-p_1-s)$. So $N(z_{s0}) = N(y_{s1}) = \frac{4pq-2q-2(q-p_1-s)}{2} = 2q(p-1) + p_1 + s$.

Case 2. $q - p_1 \leq s < p_1$. In this case the number of vertices b_{kp_1} is also $2q$ and there isn't any vertex c_{kp_1}. So $N(z_{s0}) = N(y_{s1}) = \frac{4pq-2q}{2} = 2qp - q$.

Case 3. $p_1 \leq s < q$. In this the case number of vertices b_{kp_1} is also $2q$ and number of vertices c_{kp_1} is $2(q-p_1-(q-s-1))$. So $N(z_{s0}) = N(y_{s1}) = \frac{4pq-2q-2(q-p_1-(q-s-1))}{2} = q(2p-1)+p_1-s-1$.

Now suppose $q \geq p$. As in the case $q < p$ we distinguish three cases:

Case 1. $0 \leq s < p_1$. As above, we have $N(z_{s0}) = N(y_{s1}) = 2q(p-1) + p_1 + s$.

Case 2. $p_1 \leq s < q - p_1$. In this case the number of edges b_{kp_1} is $2q$ and number of vertices

c_{kp_1} is $2(q-p_1-(p_1-1))$, so $N(z_{s0}) = N(y_{s1}) = \frac{4pq-2q-2(q-p_1-(p_1-1))}{2} = 2q(p-1)+2p_1-1$.

Case 3. $q-p_1 \leq s < q$. As above, we have $N(z_{s0}) = N(y_{s1}) = q(2p-1)+p_1-s-1$.

Therefore the proof of Lemma is completed. □

Now we consider oblique edges of the graph. By Lemma 2, $N_k(x_{i0}) = 2p-4k+4i-1$. In two cases below we compute $N(x_{i0})$:

If $0 \leq i < p_1$. Since $N_k(x_{i0}) = 2p-4k+4i-1$ we can consider p_1+i row of the graph $T(p,q)$ where have at least one element in $G_{x_{i0}}$.

Thus if $p_1+i \leq q$:

$$N(x_{i0}) = \sum_{k=0}^{p_1+i-1}(2p+4i-4k-1) = \frac{1}{2}(p^2+(4i+1)p+4i^2+2i) \tag{1}$$

If p is even $N(y_{i0}) = 4qp - N(x_{i0})$. If p is odd for $0 \leq k \leq p_1+i-1$, $d(z_{kp_1}, y_{i0}) = d(z_{kp_1}, x_{i0})$ so $z_{kp_1} \notin G_{x_{i0}}$ and $z_{kp_1} \notin G_{y_{i0}}$. then $N(y_{i0}) = 4qp - N(x_{i0}) - p_1 - i$.

If $p_1+i > q$ we can consider at most $q-1$ row of the graph where have at least one element in $G_{x_{i0}}$. So

$$N(x_{i0}) = \sum_{k=0}^{q-1}(2p+4i-4k-1) = q(2p+4i+1)-2q^2 \tag{2}$$

If p is even $N(y_{i0}) = 4qp - N(x_{i0})$ but if p is odd for $0 \leq k \leq q-1$, $z_{kp_1} \notin G_{x_{i0}}$ and $z_{kp_1} \notin G_{x_{i0}}$. Then $N(y_{i0}) = 4qp - N(x_{i0}) - q$.

If $i \geq p_1$. As in pervious case, we can consider p_1+i row of $T(p,q)$ where have at least one element in $G_{x_{i0}}$. By lemma 4 each row of graph has at most $p+2p+p = 4p$ element in $G_{x_{i0}}$. So if $p_1+i \leq q$ then for $i-p_1 \leq k < p_1+i$, k-th row has $2p-4k+4i-1$ element in $G_{x_{i0}}$ but for $0 \leq k \leq i-p_1-1$, k-th row has $4p$ element in $G_{x_{i0}}$. Let $p_2 = \begin{cases} \frac{p}{2} & \text{if } p \text{ is even} \\ \frac{p-1}{2} & \text{if } p \text{ is odd .} \end{cases}$ Then

$$N(x_{i0}) = \sum_{k=0}^{i-p_2-1} 4p + \sum_{k=i-p_2}^{p_1+i-1}(2p+4i-4k-1) = p(4i+1) \tag{3}$$

In this case if p is odd, then for all $i-p_2 \leq k \leq p_1+i-1$, we have $z_{kp_1} \notin G_{x_{i0}}$ and $z_{kp_1} \notin G_{y_{i0}}$. Thus $N(y_{i0}) = 4qp - N(x_{i0}) - p$.

If $p_1+i > q$, as in the pervious case we have

$$\begin{aligned} N(x_{i0}) &= \sum_{k=0}^{i-p_2-1} 4p + \sum_{k=i-p_2}^{q-1}(2p+4i-4k-1) \\ &= q(2p+4i+1) - 2q^2 - \frac{1}{2}(p^2 - p(4i+1) + 4i^2 + 2i) \end{aligned} \tag{4}$$

If p is odd, then for all $i-p_2 \leq k \leq q-1$, we have $z_{kp_1} \notin G_{x_{i0}}$ and $z_{kp_1} \notin G_{y_{i0}}$. Thus $N(y_{i0}) = 4qp - N(x_{i0}) - (q+p_2-i)$.

Now suppose that p is an even integer. Then $p_1 = p/2$ and $N(y_{i0}) = 4pq - N(x_{i0})$. Thus if $q < p$ by (1), (2) and (4) we have

$$\begin{aligned}
\sum_{i=0}^{q-1} N(x_{i0})N(y_{i0}) &= \sum_{i=0}^{p/2} N(x_{i0})N(y_{i0}) + \sum_{i=p/2+1}^{q-1} N(x_{i0})N(y_{i0}) \\
&= \sum_{i=0}^{q-p/2} \left(\frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right)\left(4pq - \frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right) \\
&\quad + \sum_{i=q-p/2+1}^{p/2} (q(2p+4i+1) - 2q^2)(4pq - q(2p+4i+1) + 2q^2) + \\
&\quad \sum_{i=p/2+1}^{q-1} \left(q(2p+4i+1) - 2q^2 - \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \times \\
&\quad \left(4pq - q(2p+4i+1) + 2q^2 + \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \\
&= \frac{1}{60}\Big(3q^5 - 40qp^4 + (160q^2 - 5)p^3 + 40qp^2 + (80q^4 - 60q^2 + 2)p \\
&\quad + 20q^3 - 16q^5 - 4q\Big) \qquad (5)
\end{aligned}$$

and if $q \geq p$, then by (1), (3) and (4) we have

$$\begin{aligned}
\sum_{i=0}^{q-1} N(x_{i0})N(y_{i0}) &= \sum_{i=0}^{p/2} N(x_{i0})N(y_{i0}) + \sum_{i=p/2+1}^{q-1} N(x_{i0})N(y_{i0}) \\
&= \sum_{i=0}^{p/2} \left(\frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right)\left(4pq - \frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right) + \\
&\quad \sum_{i=p/2+1}^{q-p/2} (p(4i+1))(4pq - p(4i+1)) \\
&\quad + \sum_{i=q-p/2+1}^{q-1} \left(q(2p+4i+1) - 2q^2 - \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \times \\
&\quad \left(4pq - q(2p+4i+1) + 2q^2 + \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \\
&= \frac{p}{60}\Big(-13p^4 + 40qp^3 + 15p^2 + (160q^3 - 20q)p - 2\Big) \qquad (6)
\end{aligned}$$

Now if p is an odd integer then $p_1 = \frac{p+1}{2}$. If $q < p$ then by (1),(2) and (4) we have

$$\begin{aligned}
\sum_{i=0}^{q-1} N(x_{i0})N(y_{i0}) &= \sum_{i=0}^{\frac{p+1}{2}} N(x_{i0})N(y_{i0}) + \sum_{i=\frac{p+1}{2}+1}^{q-1} N(x_{i0})N(y_{i0}) \\
&= \sum_{i=0}^{q-\frac{p+1}{2}} \left(\frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right) \times
\end{aligned}$$

$$
\begin{aligned}
& \left(4pq - \frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i] - \frac{p+1}{2} - i\right) \\
& + \sum_{i=q-\frac{p+1}{2}+1}^{\frac{p-1}{2}} (q(2p+4i+1) - 2q^2)(4pq - q(2p+4i+1) + 2q^2 - q) + \\
& \sum_{i=\frac{p+1}{2}}^{q-1} \left(q(2p+4i+1) - 2q^2 - \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \times \\
& \left(4pq - q(2p+4i+1) + 2q^2 + \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i] - \left(\frac{p-1}{2} + q - i\right)\right) \\
= & \frac{1}{60}\Big(3p^5 - 40qp^4 + (160q^2 + 30q - 10)p^3 + (-120q^2 + 40q)p^2 + (80q^4 - 30q + 7)p \\
& -16q^5 + 16q\Big) \qquad (7)
\end{aligned}
$$

and if $q \geq p$, then

$$
\begin{aligned}
\sum_{i=0}^{q-1} N(x_{i0})N(y_{i0}) = & \sum_{i=0}^{\frac{p-1}{2}} N(x_{i0})N(y_{i0}) + \sum_{i=\frac{p+1}{2}}^{q-1} N(x_{i0})N(y_{i0}) \\
= & \sum_{i=0}^{\frac{p-1}{2}} \left(\frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i]\right) \times \\
& \left(4pq - \frac{1}{2}[p^2 + p(4i+1) + 4i^2 + 2i] - \frac{p+1}{2} - i\right) \\
& + \sum_{i=\frac{p+1}{2}}^{q-\frac{p+1}{2}} (p(4i+1))(4pq - p(4i+1) - p) + \\
& \sum_{i=q-\frac{p-1}{2}}^{q-1} \left(q(2p+4i+1) - 2q^2 - \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i]\right) \times \\
& \left(4pq - q(2p+4i+1) + 2q^2 + \frac{1}{2}[p^2 - p(4i+1) + 4i^2 + 2i - (q + \frac{p-1}{2} - i)]\right) \\
= & \frac{p}{60}\Big(-13p^4 + 40qp^3 + (30q - 10)p^2 + (160q^3 - 120q^2 + 40q)p - 30q + 23\Big) \qquad (8)
\end{aligned}
$$

Now we can compute the Szeged index of long $TUC_4C_8(R)$ nontubes $\left(q > p_1 = \frac{p+1}{2}\right)$.

Theorem 2. If p is an even integer, then the Szeged index of long $G = TUC_4C_8(R)$ is given by the following equation:

$$
Sz(G) = \begin{cases} \frac{p}{60}\Big(12q^5 - 160qp^4 + (640q^2 - 20)p^3 + 400q^3p^2 + \\ \qquad (320q^4 - 240q^2 + 8)p - 64q^5 + 80q^3 - 16q\Big) & \text{if } q < p \\ \\ \frac{p^2}{15}\Big(-13p^4 + 40qp^3 + 15p^2 + (260q^3 - 60q)p - 2\Big) & \text{if } q \geq p \end{cases}
$$

and if p is an odd integer then

$$Sz(G) = \begin{cases} \frac{p}{60}\Big(12p^5 - 160qp^4 + (640q^2 + 60q - 45)p^3 + (400q^3 - 240q^2 + 60q)p^2 + \\ (320q^4 - 480q^3 - 180q^2 - 60q + 33)p - 64q^5 + 220q^3 + 24q\Big) & \text{if } q < p \\ \\ \frac{p}{60}\Big(- 52p^5 + 160qp^4 + (60q - 65)p^3 + (1040q^3 - 240q^2 + 120q)p^2 - \\ \quad (480q^3 + 240q^2 + 60q - 117)p + 240q^3 - 60q\Big) & \text{if } q \geq p \end{cases}$$

Proof. First we assume that p is an even integer. As in the proof of Theorem 1, we have

$$Sz(G) = 4p\sum_{k=0}^{q-1} N(x_{k0})N(y_{k0}) + p\sum_{k=0}^{q-2} N(w_{kt})N(x_{k+1,t}) + p\sum_{k=0}^{q-1} N(z_{k0})N(y_{k1}).$$

Let $q < p$ by Lemma 2,3 and (5) we have

$$\begin{aligned} Sz(G) &= 4p\sum_{k=0}^{q-1} N(x_{k0})N(y_{k0}) + p\sum_{k=0}^{q-2} 4p(k+1)4p(q-k-1) + pq(2pq)(2pq) \\ &= \left(\frac{4p}{60}\Big(3q^5 - 40qp^4 + (160q^2 - 5)p^3 + 40qp^2 + \right. \\ &\qquad \left.(80q^4 - 60q^2 + 2)p + 20q^3 - 16q^5 - 4q\Big)\right) + \left(- \frac{8}{3}p^3q + \frac{8}{3}p^3q^3\right) + 4p^3q^3 \\ &= \frac{p}{60}\Big(12q^5 - 160qp^4 + (640q^2 - 20)p^3 + 400q^3p^2 + \\ &\qquad (320q^4 - 240q^2 + 8)p - 64q^5 + 80q^3 - 16q\Big) \end{aligned}$$

Now suppose that $q \geq p$. By Lemma 3 , 4 and (6) we have

$$\begin{aligned} Sz(G) &= 4p\sum_{k=0}^{q-1} N(x_{i0})N(y_{i0}) + p\sum_{k=0}^{q-2} 4p(k+1)4p(q-k-1) + pq(2pq)(2pq) \\ &= \left(\frac{4p^2}{60}\Big(- 13p^4 + 4qp^3 + 15p^2 + (160q^3 - 20q)p - 2\Big)\right) + \left(- \frac{8}{3}p^3q + \frac{8}{3}p^3q^3\right) + 4p^3q^3 \\ &= \frac{p^2}{15}\Big(- 13p^4 + 40qp^3 + 15p^2 + (260q^3 - 60q)p - 2\Big) \end{aligned}$$

Now if p is an odd integer if $q < p$ by (7) and Lemma 5,

$$\begin{aligned} Sz(G) &= 4p\sum_{k=0}^{q-1} N(x_{k0})N(y_{k0}) + p\sum_{k=0}^{q-2} N(w_{kt})N(x_{k+1,t}) + p\sum_{k=0}^{q-1} N(z_{k0})N(y_{k1}) \\ &= 4p\sum_{k=0}^{q-1} N(x_{i0})N(y_{i0}) + p\sum_{k=0}^{q-2} 4p(k+1)4p(q-k-1) + \\ &\qquad p\sum_{k=0}^{q-p_1-1} (2q(p-1) + p_1 + k)^2 + p\sum_{k=q-p_1}^{p_1-1} (2pq - q)^2 + \end{aligned}$$

$$
\begin{aligned}
& p\sum_{k=p_1}^{q-1}(q(2p-1)+p_1-k-1)^2 \\
= \; & \frac{4p}{60}\Bigg(3q^5-40qp^4+(160q^2+30q-10)p^3+(-120q^2+40q)p^2+(80q^4-30q+7)p \\
& -16q^5+16q\Bigg)+\Bigg(-\frac{8}{3}p^3q+\frac{8}{3}p^3q^3\Bigg) \\
& +p\Bigg(-p^3\Bigg(q+\frac{1}{12}\Bigg)+p^2(4q^3+4q^2+q)-p\Bigg(8q^3+3q^2-q-\frac{1}{12}\Bigg)+\frac{11}{3}q^3-\frac{2}{3}q\Bigg) \\
= \; & \frac{p}{60}\Bigg(12p^5-160qp^4+(640q^2+60q-45)p^3+(400q^3-240q^2+60q)p^2+ \\
& (320q^4-480q^3-180q^2-60q+33)p-64q^5+220q^3+24q\Bigg)
\end{aligned}
$$

For $q \geq p$ by Lemma 5 and (8):

$$
\begin{aligned}
Sz(G) \; = \; & 4p\sum_{k=0}^{q-1}N(x_{k0})N(y_{k0})+p\sum_{k=0}^{q-2}N(w_{kt})N(x_{k+1,t})+p\sum_{k=0}^{q-1}N(z_{k0})N(y_{k1}) \\
= \; & 4p\sum_{k=0}^{q-1}N(x_{i0})N(y_{i0})+p\sum_{k=0}^{q-2}4p(k+1)4p(q-k-1)+p\sum_{k=0}^{p_1-1}(2q(p-1)+p_1+k)^2 \\
& +p\sum_{k=p_1}^{q-p_1-1}(2q(p-1)+2p_1-1)^2+p\sum_{k=q-p_1}^{q-1}(q(2p-1)+p_1-k-1)^2 \\
= \; & \frac{p}{60}\Bigg(-13p^4+40qp^3+(30q-10)p^2+(160q^3-120q^2+40q)p-30q+23\Bigg)+ \\
& \Bigg(-\frac{8}{3}p^3q+\frac{8}{3}p^3q^3\Bigg)+p\Bigg(-p^3\Bigg(q+\frac{5}{12}\Bigg)+p^2(4q^3+4q^2+2q) \\
& -p\Bigg(8q^3+4q^2-q-\frac{5}{12}\Bigg)+4q^3-q\Bigg) \\
= \; & \frac{p}{60}\Bigg(-52p^5+160qp^4+(60q-65)p^3+(1040q^3-240q^2+120q)p^2- \\
& (480q^3+240q^2+60q-117)p+240q^3-60q\Bigg).
\end{aligned}
$$

This completes the proof of the Theorem. □

In Tables (1),(2) and (3) the numerical data for Szeged index in tubes $T(p,q)=TUC_4C_8(R)$ of various dimensions are given.

p	q	$Sz(G)$	p	q	$Sz(G)$
5	2	19000	10	3	591400
6	2	37056	10	4	1386240
7	2	54824	11	3	752345
7	3	183421	11	5	3397295
8	2	88832	12	2	302208
8	3	299168	12	3	1028592
9	2	119448	12	5	4674960
9	3	403947	13	4	2968160
9	4	942048	13	6	9761960
10	2	174400	13	9	30738045

Table 1: Szeged index of short $T(p,q) = TUC4C8(R)$ nanotubes , $q < p_1$

p	q	$Sz(G)$	p	q	$Sz(G)$
3	2	3528	9	6	3007746
4	3	34080	9	7	4655997
5	4	140090	10	6	4473400
6	3	122904	10	7	6929560
6	4	280104	10	8	10119560
6	5	528216	10	9	14143320
7	5	793485	11	9	18143631
8	5	1314688	11	10	24558292
8	6	2206016	12	8	18033504
8	7	3418240	12	9	25180320

Table 2: Szeged index in long $T(p,q) = TUC4C8(R)$ nanotubes, $q < p$

p	q	$Sz(G)$	p	q	$Sz(G)$
3	3	11331	7	7	2068045
4	4	77600	7	8	3035620
4	6	251168	8	10	9504896
4	8	584480	8	12	16136320
4	10	1130784	10	10	19103320
5	5	265055	11	11	32136511
5	6	448420	11	12	41241794
6	6	888792	11	15	78586827
6	8	2036760	12	12	57069600
6	10	3903576	12	14	88814112

Table 3: Szeged index in long $T(p,q) = TUC4C8(R)$ nabotubes, $q \geq p$

Appendix

In this appendix we include a MATHEMATICA [4] program to produce the graph of $T(p,q)$ and computing the Szeged index of the graph.

```
 << Graphics`Arrow`
 << DiscreteMath`Combinatorica`
rect[x_,y_]:={{{x,y+1},{x-1,y}},{{x-1,y},{x,y-1}},{{x,y-1},{x+1,y}},
               {{x+1,y},{x,y+1}},{{x,y-1},{x,y-2}}};
lin[x_,y_]:= {{x+1,y},{x+2,y}};
c48[p_,q_]:=Join[Flatten[Table[rect[x,y],{y,3q-3,3,-3},{x,0,3p-3,3}],2],
             Flatten[Table[lin[x,y],{y,3q-3,3,-3},{x,0,3*p-6,3}],1],
             Table[{{-1,y},{3p-2,y}},{y,3,3q-3,3}],
             Flatten[Table[Take[rect[x,0],{1,4}],{x,0,3p-3,3}],1],( *last piece*)
             Table[lin[x,0],{x,0,3*p-6,3}],        (*last piece*)
             {{{-1,0},{3p-2,0} } }  ]              (*last piece*)
p=7;q=4;
w=c48[p,q];
Show[Graphics[Map[Line,w]]]
(* generating the graph *)
drawgraph[edgs_]:=Module[{vert,G,n,t,e,vv},
          vert=Union[Flatten[w,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[w];  (* Show graph*)
(* computing the Szeged index  *)
szeged[G_,ed_]:=Module[{vert,t,i,j,ni,nj,L1,L2},
         ni=0;nj=0;
         vert=Union[Flatten[Edges[G],1]];
         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];
                  ]
(* The Szeged index of the graph *)
 edgs=Edges[K];
Sum[szeged[K,edgs[[i]]],{i,1,Length[edgs]}]
```

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