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The Schultz Polynomial of Zigzag Polyhex Nanotubes

MEHDI ELIASI and BIJAN TAERI*
Department of Mathematical Sciences, Isfahan University of Technology, Isfahan 84156-83111, Iran
E-mail: b.taeri@cc.iut.ac.ir

The Schultz polynomial, S(G,x), of a molecular graph G has the property that its first derivative at x=1 is equal to the Schultz index of graph. Ivan Gutman discovered that in the case of G is a tree, S(G,x), has closely related to the Wiener polynomial of G. In this paper, we find the exact expression for Schultz polynomial of $TUHC_6$ [2p; q], the zigzag polyhex nanotubes, and obtain a relation between Schultz and Wiener polynomials of $TUHC_6$ [2p; q].

Key Words: Schultz index, Schultz polynomial, Nanotube.

INTRODUCTION

Topological indices are numerical descriptors that are derived from molecular graphs of chemical compounds. The Wiener index is the oldest topological indices. In 1947 chemist Harold Wiener[1] developed the most widely known topological descriptor, the Wiener index and used it to determine physical properties of types of alkanes known as paraffins. Numerous chemical applications of Wiener index are reported and its mathematical properties are well understood. In the chemical language, the Wiener index is equal to the sum of all shortest carbon carbon bond paths in a molecule. In a graph theoretical language, the Wiener index is equal to the count of all shortest distances in a graph. For a thorough survey in this topic we encourage the reader to consult the reported works[2-4].

Haruo Hosoya[5] introduced a distance-based polynomial, that he called it the Wiener polynomial, related to each connected graph G as:

$$H(G,x) = \tfrac{1}{2}\sum\{x^{d(u,v)} :\ u,v \in V(G), u \neq v\}.$$

The first derivative of H(G,x) at x = 1 is equal to Wiener index of G.

Schultz[6] introduced the following topological index (Schultz index)

$$S(G) = \tfrac{1}{2}\sum\{(\deg(u)+\deg(v))d(u,v) : u,v \in V(G), u \neq v\},$$

where deg(u) is degree of vertex u, *i.e.* the number of the vertices joining to the vertex u.

These indices have many chemical applications[7,8].

Similar to Hosoya, Gutman introduced new polynomial

$$S(G,x) = \tfrac{1}{2}\sum\{(\deg(u)+\deg(v))x^{d(u,v)} : u,v \in V(G), u \neq v\},$$

that the first its derivative at x = 1 is equal to the Schultz index[9]. He obtained some relationships between this polynomial and Wiener polynomial of trees. Sen-Peng *et al.*[10] also did similar work for hexagonal chains.

RESULTS AND DISCUSSION

In 1991 Iijima[11] 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. Diudea[12-16] was the first chemist which considered the problem of computing topological indices of nanostructures. Recently computing topological indices of nanostructures has been the object of many papers[17-27].

In this paper, we give exact expression for Schultz polynomial of $TUHC_6$ [2p; q], zigzag polyhex nanotube (Fig. 1) and obtain a relation between Schultz and Wiener polynomials of $TUHC_6$ [2p; q].

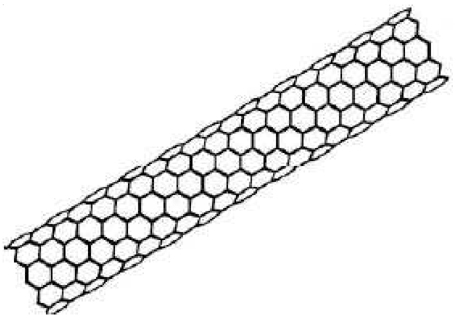

Fig. 1. A $TUHC_6$ [2p; q] nanotube

EXPERIMENTAL

Throughout this paper G: = TUHC [2p; q], (Fig. 1), denotes an arbitrary zig-zag polyhex nanotube in terms of the circumference p and the length q. We also choose a coordinate label for vertices of TUHC [2p; q], as shown in Fig. 2. At first we give an important result on G.

Result 1: For a white vertex of level 0 we have

$$w_k(x) = \sum_{v \in \text{ level } k} x^{d(x_{02},v)}$$

$$= \sum_{v \in \text{ level } k} x^{d(x_{04},v)}$$

$$\vdots$$

$$= \begin{cases} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) & \text{if } 0 \le k < p \\ px^{2k+1} + px^{2k} & \text{if } k \ge p, \end{cases}$$

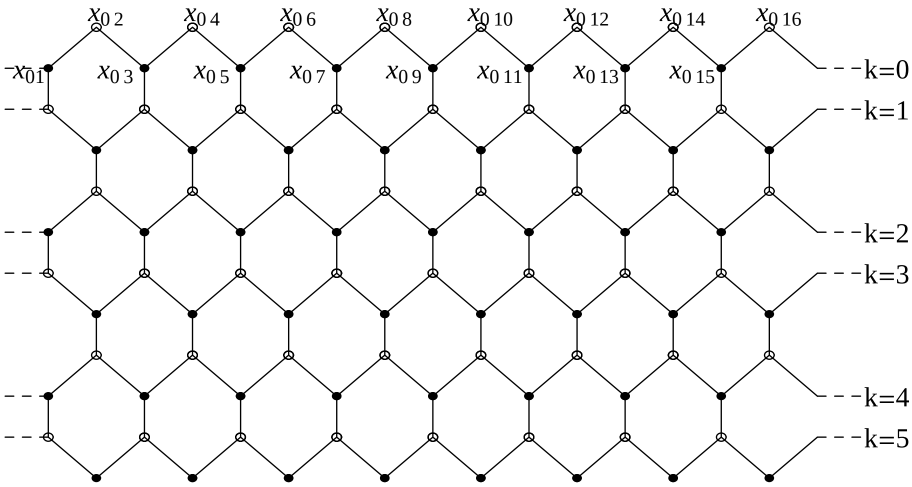

Fig. 2. A zig-zag polyhex nanotube lattice with p=8 and q=6

and for a black vertex of level 0 we have

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

Proof: We compute $b_k(x)$. It suffices to consider x_{01}. For other blacks 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: $k \ge p$ and k is even. In this case for j, where $1 \le j \le p + 1$, we have

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

and obtain p vertices having distance 2k-1 from x_{01} and p vertices having 2k distance

$$
b_k(x) = \sum_{v\in\text{level } k} x^{d(x_{01},v)} = \sum_{j \text{ is even}} x^{d(x_{01},x_{kj})} + \sum_{j \text{ is odd}} x^{d(x_{01},x_{kj})} = px^{2k-1}+px^{2k}.
$$

Case 2: $k \ge p$ and k is odd. In this case for j, where $1 \le j \le p + 1$, we have

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

and we obtain p vertices having distance 2k-1 from x_{01}, and p vertices having 2k distance from x_{01}. So

$$b_k(x)=\sum_{v\in \text{level } k} x^{d(x_{01},v)}=\sum_{j \text{ is even}} x^{d(x_{01},x_{kj})}+\sum_{j \text{ is odd}} x^{d(x_{01},x_{kj})}=px^{2k-1}+px^{2k}.$$

Case 3: k < p. For all p + 1 ≤ j and j > k + 1,

$$d(x_{01},x_{kj})=k+j-1.$$

Thus the summation of $x^{d(x_{01},x_{kj})}$'s (for all j's such that p + 1 ≤ j and j > k + 1) and symmetric of x_{kj}'s is

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

Also if 1 ≤ j ≤ + 1, then

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

By considering these vertices and their symmetric we obtain k+1 vertices having distance 2k and k vertices having 2k-1 distance from x_{01}. Therefore the summation of $x^{d(x_{01},x_{kj})}$'s (for all j's such that 1 ≤ j ≤ k + 1) and symmetric of x_{kj}'s is $S_2=(k+1)x^{2k}+kx^{2k-1}$. Hence

$$\begin{aligned}b_k(x)&=S_1+S_2\\ &=\frac{1}{x-1}(x^{k+p+1}+x^{k+p}-2x^{2k+1})+(k+1)x^{2k}+kx^{2k-1}\\ &=\frac{1}{x-1}(x^{k+p+1}+x^{k+p}+(k-1)x^{2k+1}-x^{2k}-kx^{2k-1}).\end{aligned}$$

In a similar manner we can compute $w_k(x)$.

Result 2:

(a) $d(x_{02},x)=d(x_{04},x)=\cdots=d(x_{0,2p},x)=w_0(x)+w_1(x)+\cdots+w_{q-1}(x)$.

(b) $d(x_{01},x)=d(x_{03},x)=\cdots=d(x_{0,2p-1},x)=b_0(x)+b_1(x)+\cdots+b_{q-1}(x)$.

Proof: By Result 1, we have

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

Thus

$$d(x_{02},x) = d(x_{04},x) = \cdots = d(x_{0,2p},x) = w_0(x) + w_1(x) + \cdots + w_{q-1}(x).$$

The proof of (b) is similar.

For a vertex u of graph G we let $d_G(v,x)$ or sometimes $d(v,x)$, be

$$d_G(u,x) = \sum_{v \in V(G)} x^{d(u,v)}.$$

By this notation we have

Result 3: If $0 \le j \le q - 1$ be an odd number, then

(a) $d(x_{j1},x) = d(x_{j3},x) = \cdots = d(x_{j,2p-1},x) = w_0(x) + w_1(x) + \cdots + w_{q-(j+1)}(x) + b_1(x) + \cdots + b_j(x).$

(b) $d(x_{j2},x) = d(x_{j4},x) = \cdots = d(x_{j,2p},x) = b_0(x) + b_1(x) + \cdots + b_{q-(j+1)}(x) + w_1(x) + \cdots + w_j(x).$

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 Result 2, we have

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

The top part is the graph $TUHC_6[2p; q-1] = \hat{G}_1$ and level 1 of graph G is the first its row and x_{11} is such a black vertex of $\hat{G}_1$. Therefore by Result 2, $d_{\hat{G}_1} = b_0(x) + b_1(x)$ and $d_{\hat{G}_1}(x_{11},x) = d_{\hat{G}_1}(x_{11},x_{13}) = \cdots = d_{\hat{G}_1}(x_{1,2p-11},x) = b_0(x) + b_1(x).$

Since $w_0(x) = b_0(x)$ and $d_G(x_{11},x) = d_{G_1}(x_{11},x) + d_{\hat{G}_1}(x_{11},x) - b_0(x)$, then

$$d_G(x_{11},x) = w_0(x) + w_1(x) + \cdots + w_{q-2}(x) + b_1(x)$$

and such as it. Similarly for x_{12} we can see that

$$d_G(x_{12},x) = d_G(x_{14},x) = \cdots = d_G(x_{1,2p},x) = b_0(x) + b_1(x) + \cdots + b_{q-2}(x) + w_1(x).$$

By repetition of this argument we obtain the result.

Result 4: If $0 \le j \le q - 1$ be an even number, then

(a) $d(x_{j1},x) = d(x_{j3},x) = \cdots = d(x_{j,2p-1},x) = b_0(x) + b_1(x) + \cdots + b_{q-(j+1)}(x) + w_1(x) + \cdots + w_j(x).$

(b) $d(x_{j2},x) = d(x_{j4},x) = \cdots = d(x_{j,2p},x) = w_0(x) + w_1(x) + \cdots + w_{q-(j+1)}(x) + b_1(x) + \cdots + b_j(x).$

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 result 2, we have

$$d_{G_1}(x_{21},x) = d_{G_1}(x_{23},x) = \cdots = d_{G_1}(x_{2,2p-1},x) = b_0(x) + b_1(x) + \cdots + b_{q-3}(x).$$

The top part is the graph $TUHC_6$ [2p; 3]= $\hat{G}_2$ and level 2 of graph G is the first level of $\hat{G}_2$ and x_{21} is such a white vertex of $\hat{G}_2$. Therefore by result 2, we have $d_{\hat{G}_2}(x_{21},x) = w_0(x) + w_1(x) + w_2(x)$ and

$$d_{\hat{G}_2}(x_{21},x) = d_{\hat{G}_2}(x2,x) = \cdots = d_{\hat{G}_2}(x_{2,2p-11},x) = w_0(x) + w_1(x) + w_2(x).$$

Since $w_0(x) = b_0(x)$ and $d_G(x_{21},x) = d_{G_{12}}(x_{21},x) + d_{\hat{G}_2}(x_{21},x) - w_0(x)$, then

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

and similarly

$$d_G(x_{23},x) = \cdots = d_G(x_{1,2p-1},x) = b_0(x) + b_1(x) + \cdots + b_{q-3}(x) + w_1(x) + w_2(x).$$

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

$$d_G(x_{22},x) = d_G(x_{24},x) = \cdots = d_G(x_{2,2p},x) = w_0(x) + w_1(x) + \cdots + w_{q-3}(x) + b_1(x) + b_2(x).$$

By repetition of this argument we can obtain the result.

For all $0 \le j \le q-1$, put

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

and

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

In the following result we find a relation beween Schultz and Wiener polynomials of $TUHC_6[2p; q]$.

Result 5: Let $G=TUHC_6[2p; q]$. Then $S(G,x) = 6H(G,x) - 2p\sum_{i=0}^{q-1} w_i(x).$

Proof: Let A_0 and A_{q-1} be the set of vertices on the levels k = 0 and k = q-1, respectively. We have

$$\begin{aligned}
S(G,x) &= \tfrac{1}{2}\sum_{\{u,v\}\subseteq V(G)}(\deg(u)+\deg(v))x^{d(u,v)} \\
&= \tfrac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}(\deg(u)+\deg(v))x^{d(u,v)} \\
&= \tfrac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\deg(u)x^{d(u,v)} + \tfrac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}\deg(v)x^{d(u,v)} \\
&= \tfrac{1}{2}\sum_{u\in V(G)}\deg(u)\sum_{v\in V(G)}\deg(u)x^{d(u,v)} + \tfrac{1}{2}\sum_{v\in V(G)}\deg(v)\sum_{u\in V(G)}\deg(u)x^{d(u,v)} \\
&= \sum_{u\in V(G)}\deg(u)d(u,x) \\
&= \sum_{u\in V(G)\setminus(A_0\cup A_{q-1})}\deg(u)d(u,x) + \sum_{u\in A_0}\deg(u)d(u,x) + \sum_{u\in A_{q-1}}\deg(u)d(u,x).
\end{aligned}$$

Note that if $u \in V(G)\setminus(A_0 \cup A_{q-1})$, then deg(u)=3. Suppose that $A_{0,b} = \{u \in A_0 \mid u \text{ is black}\}$ and $A_{0,w} = \{u \in A_0 \mid u \text{ is withe}\}$. Then

$$\deg(u) = \begin{cases} 3 & \text{if } u \in A_{0,b} \\ 2 & \text{if } u \in A_{0,w} \end{cases}.$$

The graph G' can be obtained from the graph G such that line q -1 is its first row and line 0 is its last row. Let

$A_{q\text{-}1,b} = \{u \in A_{q-1} \mid u \text{ is black in } G'\}$ and $A_{q\text{-}1,w} = \{u \in A_0 \mid u \text{ is white in } G'\}$.

Then

$$\deg(u) = \begin{cases} 3 & \text{if } u \in A_{q\text{-}1,b} \\ 2 & \text{if } u \in A_{q\text{-}1,w} \end{cases}.$$

Hence

$$\begin{aligned}\sum_{u\in V(G)\setminus(A_0\cup A_{q-1})}\deg(u)d(u,x) &= \sum_{u\in V(G)\setminus(A_0\cup A_{q-1})} d(u,x)\\ &= 3\sum_{u\in V(G)\setminus(A_0\cup A_{q-1})} d(u,x)\\ &= 3\Big(\sum_{u\in V(G)} d(u,x) - \sum_{u\in A_0} d(u,x) - \sum_{u\in A_{q-1}} d(u,x)\Big)\\ &= 3\Big(\sum_{u\in V(G)} d(u,x) - \sum_{u\in A_{0,b}} d(u,x) - \sum_{u\in A_{0,w}} d(u,x) - \sum_{u\in A_{q-1,b}} d(u,x) - \sum_{u\in Aw} d(u,x)\Big).(2)\end{aligned}$$

According to result 2 if $u \in A_{0,b}$ then $d(u,x) = \sum_{i=0}^{q-1} b_i(x)$ and for $u \in A_{0,w}$ we have $d(u,x) = \sum_{i=0}^{q-1} w_i(x)$. Also by considering G' and using result 2, for all $u \in A_{q-1,b}$ we have $d(u,x) = \sum_{i=0}^{q-1} b_i(x)$ and for $u \in A_{q-1,w}$, $d(u,x) = \sum_{i=0}^{q-1} w_i(x)$.

So

$$\begin{aligned}\sum_{u\in V(G)\setminus(A_0\cup A_{q-1})}\deg(u)d(u,x) &= 3\Big(\sum_{u\in V(G)} d(u,x) - p\sum_{i=0}^{q-1} b_i(x) - p\sum_{i=0}^{q-1} w_i(x) - p\sum_{i=0}^{q-1} b_i(x) - p\sum_{i=0}^{q-1} b_i(x) - p\sum_{i=0}^{q-1} w_i(x)\Big)\\ &= 3\sum_{u\in V(G)} d(u,x) - 6p\sum_{i=0}^{q-1} b_i(x) - 6p\sum_{i=0}^{q-1} w_i(x). \qquad (3)\end{aligned}$$

Also

$$\begin{aligned}\sum_{u\in A_0}\deg(u)d(u,x) &= \sum_{u\in A_{0,b}}\deg(u)d(u,x) + \sum_{u\in A_{0,w}}\deg(u)d(u,x)\\ &= 3\sum_{u\in A_{0,b}} d(u,x) + 2\sum_{u\in A_{0,w}} d(u,x)\\ &= 3p\sum_{i=0}^{q\text{-}1} b_i(x) + 2p\sum_{i=0}^{q\text{-}1} w_i(x), \qquad (4)\end{aligned}$$

and similarly

$$\sum_{u\in A_{q-1}} \deg(u)d(u,x) = 3p\sum_{i=0}^{q-1} b_i(x) + 2p\sum_{i=0}^{q-1} w_i(x). \qquad (5)$$

So by (1)-(5) we have

$$S(G,x) = 3\sum_{u\in V(G)} d(u,x) - 2p\sum_{i=0}^{q-1} w_i(x) = 6H(G,x) - 2p\sum_{i-0}^{q-1} w_i(x).$$

Theorem: The Schultz polynomial of G is given by when $q \le p$

$$S(G,x) = -\frac{p}{(x+1)(x-1)^3}(6p(((\tfrac{2}{3}-\tfrac{2}{3}q)x^3 + (2-\tfrac{1}{3}q)x^2 + (\tfrac{2}{3}q+1)x + \tfrac{1}{3}q + \tfrac{1}{3})x^{2q} - \tfrac{5}{3}(x+1)^2(x+\tfrac{1}{5})x^{p+q}$$
$$+ (qx + \tfrac{5}{3}x + \tfrac{1}{3} - q)(x+1)^2x^p - qx^4 + (-\tfrac{2}{3}-q)x^3 - 2x^2 + (q-1)x + q - \tfrac{2}{3}),$$

and when $q > p$

$$S(G,x) = \frac{1}{(x-1)^3(x+1)}6p(((-q+p-1)x^2 - \tfrac{5}{3}x + q - p - \tfrac{4}{3})x^{2p+1} + (x+1)^2(qx^2 + \tfrac{5}{3}x - q + \tfrac{1}{3})x^p$$
$$- \tfrac{2}{3}p(x+\tfrac{1}{2})(x^2-1)x^{2q} - qx^4 + (-\tfrac{2}{3}-q)x^3 - 2x^2 + (q-1)x - \tfrac{1}{3} + q)).$$

Proof: We compute $\sum_{u\in V(G)} d(u,x)$ and $\sum_{i=0}^{q-1} w_i(x)$. Let

$$A_1 = \{i \mid 1 \le i \le 2p \text{ and } i \text{ is evan}\},\ A_2 = \{i \mid 1 \le i \le 2p \text{ and } i \text{ is odd}\}$$

and

$$A_2 = \{j \mid 1 \le j \le q\text{-}1 \text{ and } j \text{ is evan}\},\ A_2 = \{j \mid 1 \le i \le q\text{-}1 \text{ and } j \text{ is odd}\}.$$

Then we have

$$\sum_{u\in V(G)} d(u,x) = \sum_{x_{ji}\in V(G)} d(x_{ji},x)$$
$$= \sum_{j\in B_1}\sum_{i\in A_1} d(x_{ji},x) + \sum_{j\in B_1}\sum_{i\in A_2} d(x_{ji},x) + \sum_{j\in B_2}\sum_{i\in A_1} d(x_{ji},x) + \sum_{j\in B_2}\sum_{i\in A_2} d(x_{ji},x)$$
$$= \sum_{j\in B_1}\sum_{i\in A_1} f(j,x) + \sum_{j\in B_1}\sum_{i\in A_2} g(j,x) + \sum_{j\in B_2}\sum_{i\in A_1} g(j,x) + \sum_{j\in B_2}\sum_{i\in A_2} g(j,x)$$
$$= \sum_{j\in B_1} f(j,x)\sum_{i\in A_1} 1 + \sum_{j\in B_1} g(j,x)\sum_{i\in A_2} 1 + \sum_{j\in B_2} g(j,x)\sum_{i\in A_1} 1 + \sum_{j\in B_2} f(j,x)\sum_{i\in A_2} 1$$
$$= \sum_{j\in B_1} pf(j,x) + \sum_{j\in B_1} pg(j,x) + \sum_{j\in B_2} pg(j,x) + \sum_{j\in B_2} pf(j,x)$$
$$= p[\sum_{j\in B_1}(f(j,x)+g(j,x)) + \sum_{j\in B_2}(f(j,x)+g(j,x))]$$
$$= p\sum_{j=0}^{q-1}(f(j,x)+g(j,x)).$$

Suppose that $q \le p$. Then by Lemma 1, for each $0 \le k \le q-1$ we have

$$b_k(x) = \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1}),$$

and

$$w_k(x) = \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}).$$

So

$$\sum_{u \in V(G)} d(u,x) = \frac{-2p}{(x-1)^3}((x+1)(qx^2 + 2x - 2x^{q+1} - q)x^p - x((q-1)x - q - 1)x^{2q} - qx^3 - x - x^2 + q)$$

$$\sum_{i=0}^{q-1} w_i(x) = \frac{1}{(x-1)^2(x+1)}(x^{p+q+2} + (q-1)x^{2q+2} + 2x^{p+q+1} - x^{2q+1} - (1+q)x^{2q} + x^{p+q} + x^2 - x^{p+2} + 1 - 2x^{p+1} - x^p)$$

and the result follows.

Now suppose that q > p. Let

$$C_1 := \{0 \le j \le p-1 \,|\, 0 \le q-(j+1) \le p-1\},\ C_2 := \{0 \le j \le p-1 \,|\, p \le q-(j+1) \le q-1\},$$
$$C_3 := \{p \le j \le q-1 \,|\, 0 \le q-(j+1) \le p-1\},\ C_4 := \{p \le j \le q-1 \,|\, p \le q-(j+1) \le q-1\}.$$

We note that if $C_1 \ne \varnothing$ then 2p > q. also if $C_4 \ne \varnothing$, then 2p < q. Therefore first suppose that $C_1 \ne \varnothing$, so $C_4 = \varnothing$ and 2p > q. Thus by result 1,

$$j \in C_1 \Rightarrow f(j,x) = \sum_{k=0}^{q-(j+1)} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) + \sum_{k=1}^{j} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1})$$

$$j \in C_2 \Rightarrow f(j,x) = \sum_{k=0}^{p-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) + \sum_{k=p}^{q-(j+1)}(px^{2k+1} + px^{2k}) + \sum_{k=1}^{j} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1})$$

$$j \in C_3 \Rightarrow f(j,x) = \sum_{k=0}^{q-(j+1)} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) + \sum_{k=1}^{p-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1}) + \sum_{k=p}^{j}(px^{2k-1} + px^{2k}).$$

$$j \in C_1 \Rightarrow g(j,x) = \sum_{k=0}^{j-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) + \sum_{k=1}^{q-(j+1)} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1})$$

$$j \in C_2 \Rightarrow g(j,x) = \sum_{k=0}^{j} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) +$$
$$\sum_{k=1}^{p-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1}) + \sum_{k=p}^{q-(j+1)}(px^{2k-1} + px^{2k})$$
$$j \in C_3 \Rightarrow g(j,x) = \sum_{k=0}^{p-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) +$$
$$\sum_{k=p}^{j}(px^{2k+1} + px^{2k}) + \sum_{k=1}^{q-(j+1)} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + (k-1)x^{2k+1} - x^{2k} - kx^{2k-1}).$$

So

$$\sum_{u \in V(G)} d(u,x) = \frac{-2p}{(x-1)^3}(x((p-1-q)x + q - p - 1)x^{2p} + (x+1)(qx^2 + 2x - q)x^p - px^{2q+1}(x-1) - x^2 - x - qx^3 + q).$$

Also in this case since $p \le q$, then by result 1 we have

$$\sum_{i=0}^{q-1} w_i(x) = \sum_{k=0}^{p-1} w_k(x) + \sum_{k=p}^{q-1} w_k(x)$$
$$= \sum_{k=0}^{p-1} \frac{1}{x-1}(x^{k+p+1} + x^{k+p} + kx^{2k+2} - x^{2k+1} - (k+1)x^{2k}) + \sum_{k=p}^{q-1}(px^{2k+1} + px^{2k})$$
$$= \frac{1}{(x+1)(x-1)^2}(x^{2p+1} - (x+1)^2 x^p + (px^2 - p)x^{2q} + x^2 + x + 1).$$

Therefore

$$S(G,x) = \frac{1}{(x-1)^3(x+1)}(6p(((-q+p-1)x^2 - \tfrac{5}{3}x + q - p - \tfrac{4}{3})x^{2p+1} + (x+1)^2(qx^2 + \tfrac{5}{3}x - q + \tfrac{1}{3})x^p$$
$$- \tfrac{2}{3}p(x + \tfrac{1}{2})(x^2 - 1)x^{2q} - qx^4 + (-\tfrac{2}{3} - q)x^3 - 2x^2 + (q-1)x - \tfrac{1}{3} + q)).$$

We can proof other conditions by this method.

Now differentiation of Schultz polynomial of G and letting x=1 we obtain the Schultz index of G.

Corollary: The Schultz index of G is given by when $q \le p$

$$S(G) = \tfrac{1}{3}pq(2 + 3q^3 - 3q - 6p - 6p^2 - 6pq - 2q^2 + 18p^2q + 12pq^2),$$

and when $p < q$

$$S(G) = \tfrac{1}{3}p^2(2 + 3p - 2p^2 - 12q + 12p^2q - 12q^2 - 3p^3 - 24q^3).$$

Conclusion

We developed a method which is usually useful for calculating Schultz polynomials of C_6 nanotubes. As a consequence of calculating Schultz polynomial of zigzag polyhex nanotubes we computed Schultz index of such nanotubes.

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