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Wiener Index of Zig-zag Polyhex Nanotubes*

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zig-zag polyhex nanotubes

A method for deriving formulas for evaluating the sum of all distances, known as the Wiener index, of the »zig-zag« nanotubes is given. A similar method was applied to the general »square« connected layers.

INTRODUCTION

Carbon nanotubes were discovered in 1991 by Iijima[1] as multi walled structures and in 1993 as single walled carbon nanotubes (briefly denoted SWNT) independently by Iijima's group[2] and Bethune's group[3] from IBM. SWNTs can be seen as a rolled-up graphite sheet in the cylindrical form.

Carbon nanotubes show remarkable mechanical properties. Experimental studies have shown that they belong to the stiffest and elastic known materials.[4-6] These mechanical characteristics clearly predestinate nanotubes for advanced composites.

Thermal conductivity along their axis could exceed that of the type II-a diamond, which has the highest thermal conductivity of any material measured.[7,8]

SWNTs can exhibit either metallic or semiconductor behavior depending only on the diameter and helicity.[9] These properties suggest that nanotubes could lead to a new generation of nanoscopic electronic devices. Experiments are under way in several industrial laboratories.

Let $G = (V, E)$ be a connected graph with the vertex set $V = V(G)$. For vertices $i,j \in V(G)$, we denote by $d(i, j)$ the topological distance (*i.e.*, the number of edges on the shortest path) joining the two vertices of G. The Wiener index[10] W of graph G is the half sum of distances over all its vertex pairs (i,j):

$$W = W(\mathrm{G}) = (1/2) \cdot \sum_{(i,j)} d(i,j) \qquad (1)$$

This paper focuses on $(n, 0)$ zig-zag polyhex SWNTs, proposing a mathematical method for calculating W in the corresponding graphs. Abundant literature appeared on this topic in chemical graph theory (see for example Refs. 11–15). Since the polyhex nanotubes were modeled by one of us (M. V. D.) starting from a cylinder tessellated by squares, the actual method for calculating W was extended for that case.

In the following, our notations[16–18] for tubes will be: $\mathrm{T} = \mathrm{T}(p, q) = \mathrm{TUHC}_6[2p, q]$ and $\mathrm{T'} = \mathrm{T'}(p, q) = \mathrm{TUC}_4[p, q]$ for polyhex and square tubes, respectively (Figure 1).

* Dedicated to Professor Nenad Trinajstić on the occasion of his 65th birthday for his outstanding activity in the field of Chemical Graph Theory.

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$TUHC_6$ [20, q] »zig-zag« TUC_4 [4, q]

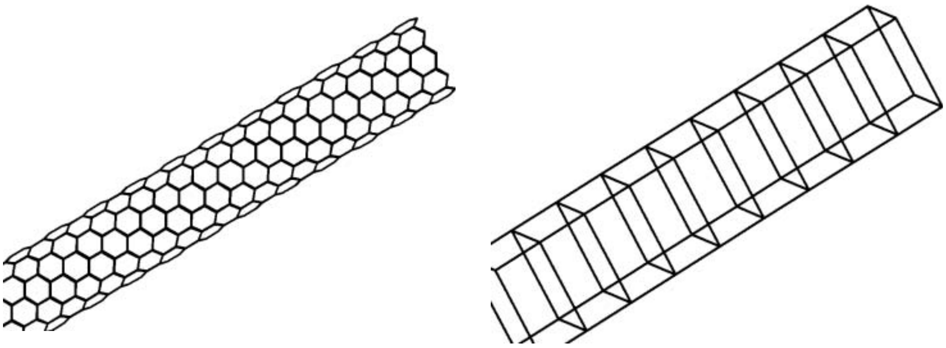


Figure 1. A polyhex (left) and a square (right) lattice covering a cylinder.

Note that graphs T and T' are bipartite (the vertices can be colored white and black so that adjacent vertices have different colors).

The method for calculating the Wiener index $W = W(\mathrm{T}(p, q))$ is described in the following section. Calculation of $W' = W(\mathrm{T}'(p, q))$ is a special case of a more general problem, which is the topic of the third section hereof.

METHOD

Evaluating topological distance in a hexagonal zig-zag lattice can be split with respect to the white and black vertices, as illustrated in Figure 2 ($p = 2$ gives the number of horizontal hexagons and $q = 4$ denotes the number of horizontal »zig-zag« lines).

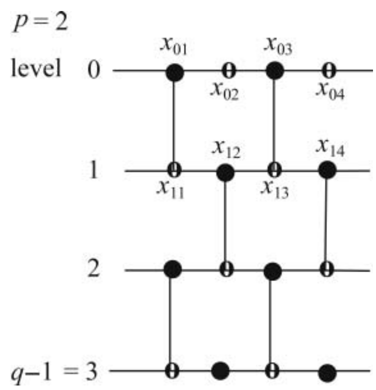


Figure 2. White and black points in a »zig-zag« polyhex net.

The sum of »white« distances, on level k, for $k = 0, 1,..., q - 1$, (distances of one white vertex of level 0 to all vertices of level k) is given as:

$$w_k = \sum_{r=1}^{2p} d(x_{02}, x_{kr}) = \sum_{r=1}^{2p} d(x_{04}, x_{kr}) = \begin{cases} (p+k)^2 + k, & \text{if} \quad 0 \le k < p \\ p(4k+1), & \text{if} \quad p \le k \end{cases} \tag{2}$$

and similarly, for »black« distances (distances of one black vertex of level 0 to all vertices of level k) is given as:

$$b_k = \sum_{r=1}^{2p} d\left(x_{01}, x_{kr}\right) = \sum_{r=1}^{2p} d\left(x_{03}, x_{kr}\right) = \begin{cases} (p+k)^2 - k, & \text{if} \quad 0 \le k < p \\ p(4k-1), & \text{if} \quad p \le k \end{cases} \tag{3}$$

The sum of all white and black distances will be:

$$s_k = w_k + b_k = \begin{cases} 2(p+k)^2, & \text{if} \quad 0 \le k < p \\ 8pk, & \text{if} \quad p \le k \end{cases} \tag{4}$$

The sum of distances at level l is:

$$S(l) = \sum_{k=0}^{l} s_k; \qquad 0 \le l \le q-1 \tag{5}$$

If the reference vertex is on a level l, other than zero, the tube can be built up from two »halves« collapsing at level l. Thus, the distance sum can be written as for $0 \le l \le q - 1$:

$$\varphi(l) = S(l) + S(q-1-l) - S(0); \quad 0 \le l \le q-1 \tag{6}$$

The sum for all l levels is now:

$$\sum_{l=0}^{q-1} \varphi(l) = \varphi(0) + \varphi(1) + \ldots + \varphi(q-1) =$$

$$= S(0) + S(q-1) - S(0) +$$

$$S(1) + S(q-2) - S(0) + \ldots$$

$$S(q-2) + S(1) - S(0) +$$

$$S(q-1) + S(0) - S(0)$$

$$= 2 \cdot \sum_{l=0}^{q-1} S(l) - q \cdot S(0) \tag{7}$$

from which the Wiener index is easily calculated by:

$$W(p,\,q) = \frac{p}{2}\cdot\sum_{l=0}^{q-1}\varphi(l) \tag{8}$$

In the case of short tubes, $0 < q \le p$, the expansion of (8) leads to:

$$W(p,\,q) = \frac{pq}{6}\cdot\left[6p^2q+(4p+q)(q^2-1)\right] \tag{9}$$

while in the case of long tubes, $p \le q$, the Wiener index is evaluated by:

$$W(p,\,q) = \frac{p^2}{6}\cdot\left[p^2(4q-p)+q(8q^2-6)+p\right] \tag{10}$$

For $p = rt$, $q = st$ ($t = 1,2,...$), in short tubes with $r \ge s > 0$, (9) becomes:

$$W(rt,\,st) = \frac{rst^5}{6}\cdot\left[6r^2s+4rs^2+s^3-\frac{4r+s}{t^2}\right] \tag{11}$$

while in the case of long tubes, with $0 < r \le s$, (10) reads:

$$W(rt,\,st) = \frac{r^2t^5}{6}\cdot\left[8s^3+4r^2s-r^3-\frac{6s-r}{t^2}\right] \tag{12}$$

Limits of the above relations, when t goes to infinity, are as follows:

$$\lim_{t\to\infty}\left[W(rt,st)/t^5\right] = rs^2(6r^2+4rs+s^2),\ \text{for } r \ge s \tag{11'}$$

$$\lim_{t\to\infty}\left[W(rt,st)/t^5\right] = r^2(8s^3+4r^2s-r^3),\ \text{for } r \le s \tag{12'}$$

Special cases are:

(i) $q = p$:

$$W(p,\,p) = \frac{p^2}{6}\cdot(11p^3-5p) \approx \frac{11}{6}\cdot p^5 \tag{13}$$

and the limit:

$$\lim_{p\to\infty}\left[W(p,p)/p^5\right] = \frac{11}{6} \tag{13'}$$

(ii) $q = 1$: the tube becomes a simple cycle (on $2p$ vertices) and the formula is:

$$W(p,1) = \frac{p}{6}\cdot(6p^2) = p^3 \tag{14}$$

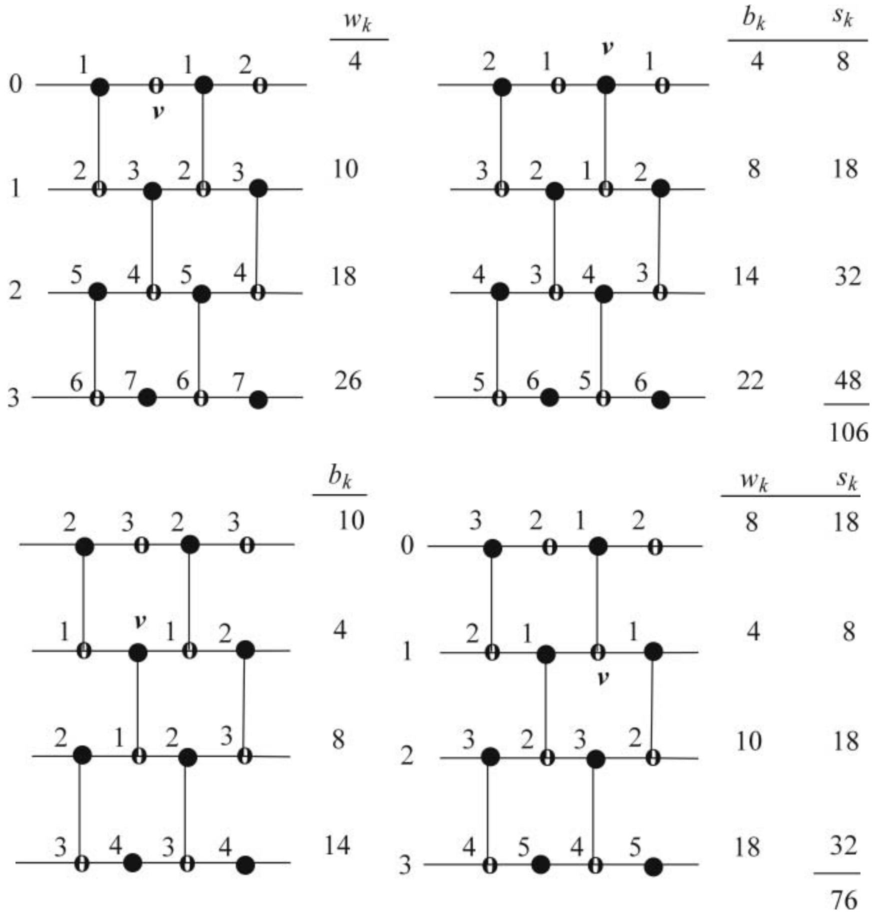


Figure 3. An example of calculating the Wiener index of zig-zag tubes.

$2\cdot(106 + 76) = 364$
$W(2,4) = 2/2\cdot 364 = 364$

(iii) ($p = rq$ (in Eq 9); $s = 1$:

$$W(rq, q) = \frac{rq^2}{6} \cdot \left[6r^2 q^3 + (4rq + q)(q^2 - 1)\right] \quad (15)$$

and its limit:

$$\lim_{q \to \infty} \left[W(rq,q) / q^5\right] = r(6r^2 + 4r + 1) \quad (14')$$

(iv) $q = sp$ (in Eq. 13); $r = 1$:

$$W(p,sp) = \frac{p^2}{6} \cdot \left[p^2 (4sp - p) + sp(8s^2 p^2 - 6) + p\right] =$$

$$\frac{p^5}{6} \cdot \left(4s - 1 + 8s^3 - \frac{6s-1}{p^2}\right) \quad (16)$$

and its limit:

$$\lim_{p \to \infty} \left[W(p,sp) / p^5\right] = \frac{1}{6} \cdot (8s^3 + 4s - 1) \quad (16')$$

An example of calculations is given in Figure 3.

Tables I and II list some values for the Wiener index of T = T(p, q).

TABLE I. Wiener index of short tubes, $q \le p$

p	q	W	p	q	W
9	9	107,649	10	10	182,500
9	8	79,920	10	8	104,320
9	7	57,393	10	6	52,100
9	6	39,474	10	5	34,000
9	5	25,605	10	4	20,400
9	4	15,264	10	3	10,720
9	2	3,258	10	2	4,420

TABLE II. Wiener index of long tubes, $q \ge p$

p	q	W	p	q	W
3	3	423	4	4	1,824
3	8	6,468	4	8	12,000
3	16	49,836	4	16	89,696
5	5	5,625	6	6	14,076
5	10	36,750	6	12	91,620
5	15	117,875	6	18	293,580
5	20	274,000	6	24	682,164
7	7	30,527	8	8	59,648
7	14	198,254	8	16	386,816
7	21	634,893	8	24	1,238,272
7	28	1,474,900	8	32	2,876,160

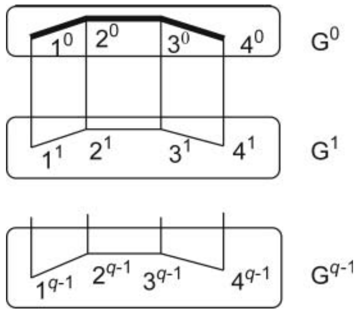


Figure 4. Graph $\widetilde{G}$: layers connected by »squares«, graph G(1^0, 2^0, 3^0, 4^0) is depicted in full line.

Wiener Index in Square Connected Layers

Let G be a graph and G^j its copies, at level $j = 0,1,...q–1$ (Figure 4).

Graph G has the vertex set $V = V(G) = \{1,2,...,n\}$ and $W = W(G)$ denotes its Wiener index.

Let $\widetilde{G}$ be the reunion of G and its q copies, together with the edges joining the copies point by point. Correspondingly, the resulting graph is characterized by $\widetilde{W} = W(\widetilde{G})$; $\widetilde{G}$ has the vertex set $\widetilde{V} = \{j^k;\ j = 1,2,...,n;\ k = 0,1,...,q–1\}$. It is easily seen that, for $i,j = 1,2,...,n$; and $k,l = 0,1,...,q–1\}$, the following relation holds:

$$d(i^l, j^k) = d(i^l, j^l) + d(j^l, j^k) = d(i, j) + |l-k| \quad (17)$$

Let focus our attention on vertex $i = 1,2,...,n$ of G. Then:

$$s_0^i = S^i(0) = s_0^i = \sum_{j=1}^{n} d(i^0, j^0) \quad (18)$$

$$s_k^i = s_0^i + k \cdot n = \sum_{j=1}^{n} d(i^0, j^k)$$

The distance sum at level l will be:

$$S^i(l) = \sum_{k=0}^{l} s_k^i = \sum_{k=0}^{l} (s_0^i + k \cdot n) =$$

$$(l+1) \cdot s_0^i + (l(l+1)/2) \cdot n \quad (19)$$

If the reference vertex is at a level l, other than zero, the lattice can be built up from two »halves« collapsing at level l. Thus, the distance sum can be written as:

$$U^i(l) = S^i(l) + S^i(q-1-l) - S^i(0);\ 0 \le 1 \le (q-1) \quad (20)$$

The sum for all l levels, up to q–1, is now:

$$\sum_{l=0}^{q-1} U^i(l) = 2\sum_{l=0}^{q-1} S^i(l) - q \cdot S^1(0) = 2\sum_{l=0}^{q-1} S^i(l) - q \cdot s_0^i \quad (21)$$

$$\sum_{l=0}^{q-1} S^i(l) = \sum_{l=0}^{q-1} \left[(l+1)s_0^i + (l(l+1)/2) \cdot n\right] =$$

$$\frac{q(q+1)}{6} \cdot \left[3 \cdot s_0^i + n \cdot (q-1)\right] \quad (22)$$

The Wiener index contribution at »vertex i« is:

$$W^i = \sum_{l=0}^{q-1} U^i(l) = \frac{q(q+1)}{6} \cdot \left[3 \cdot s_0^i + n \cdot (q-1)\right] - q \cdot s_0^i = q^2 \cdot s_0^i + 2n \binom{q+1}{3} \quad (23)$$

and the global Wiener index:

$$\widetilde{W} = \frac{1}{2} \sum_{i=1}^{n} W^i = \frac{1}{2} \sum_{i=1}^{n} \left\{ q^2 s_0^i + 2n \binom{q+1}{3} \right\} = \frac{1}{2} \left\{ q^2 \cdot \sum_{i=1}^{n} s_0^i + 2n^2 \binom{q+1}{3} \right\} \quad (24)$$

With $\sum_{i=1}^{n} s_0^i = 2W(G)$, relation (24) becomes:

$$\widetilde{W} = q^2 \cdot W(G) + n^2 \binom{q+1}{3} \quad (25)$$

There are some particular cases of interest:

(v) $G = P_n$: $$W(G) = \binom{n+1}{3} \quad (26)$$

and for

$$\widetilde{G} = P_n \oplus P_m \text{ is}$$

$$\widetilde{W} = W(\widetilde{G}) = m^2 \cdot W(P_n) + n^2 \cdot W(P_m) = m^2 \binom{n+1}{3} + n^2 \binom{m+1}{3}. \quad (27)$$

If $G_1 = P_n$ and $k \geq 2$, then $G_k = P_n \oplus G_{(k-1)}$, and if $q = n$, then (24) transforms into a recurrence relation $W_k = W(G_k)$.

Let $n_k = n(G_k)$ denote the number of vertices of G_k. Clearly, $n_k = n^k$, and

$$W_k = n^2 \cdot W_{(k-1)} + (n_k)^2 \cdot \binom{n+1}{3} \quad (28)$$

For $n = 2$ and G_k, the k-dimensional hypercube will be:

$$W_k = k \cdot 4^{(k-1)} \quad (29)$$

for which the following limit holds:

$$\lim_{k \to \infty} \left[W_k / (k \cdot (n_k)^{(2+1/k)}) \right] = 1/8 \quad (29')$$

Another interesting limit is:

$$\lim_{n \to \infty} \left[W_k / (n_k)^{(2+1/k)} \right] = k/6 \quad (29'')$$

(see also Ref. 15.)

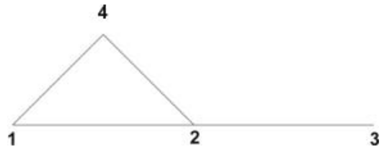
(vi) $G = C_n$:

$W(G) = (n^3 / 8)$ for n even and $W(G) = ((n^3 - n) / 8)$ for n odd.

In the case $q = n$, the global formula is:

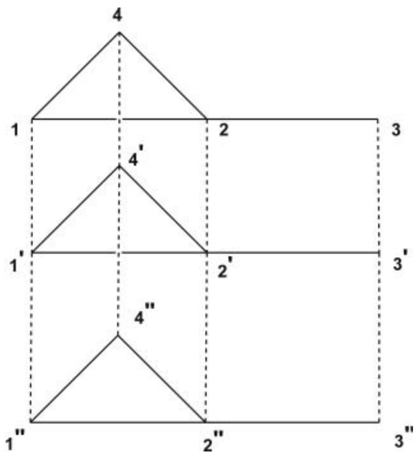
$$\widetilde{W} \sim \left(\frac{1}{8} + \frac{1}{6} \right) \cdot n^5 = \frac{7}{24} \cdot n^5 \quad (30)$$

(vii) Example:



$$n = n(G) = 4$$

$$W(G) = \frac{1}{2}(4+3+5+4) = 8$$



$$q = 3$$

$$\widetilde{G} = G \oplus P_3$$

$$\widetilde{W} = W(\widetilde{G}) = 9 \cdot W(G) + 16 \cdot \binom{4}{3} = 9 \cdot 8 + 16 \cdot 4 = 17 \cdot 8 = 136$$

Table III includes the Wiener index values in square tubes T' = T'(p,q) = TUC_4 [p,q]

TABLE III. Wiener index in tubes T' = TUC_4 [p,q]

p	q	W	p	q	W
4	4	288	5	5	875
4	5	520	5	6	1415
4	6	848	5	7	2135
4	7	1288	5	8	3060
4	8	1856	5	9	4215
4	9	2568	5	10	5625

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SAŽETAK

Wienerov indeks za »zig-zag« poliheksagonalne nanocijevi

Peter E. John i Mircea V. Diudea

Dana je metoda za izvađanje formula za izračunavanje Wienerova indeksa za »zig-zag« poliheksagonalne nanocijevi. Slična je metoda primijenjena na poopćene kvadratično povezane slojeve.