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Wiener Index of C_4C_8 Nanotubes

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Abstract. A C_4C_8 net is a trivalent decoration made by alternating squares C_4 and octagons C_8. It can cover either a cylinder or a torus. Such a covering can be derived from a square net by the leapfrog operation. This paper presents a method for deriving formulas for calculating the sum of all distances, known as the Wiener index, of the C_4C_8 nanotubes.

INTRODUCTION

Fullerenes and nanotubes are promising candidates in the development of nanodevices and superstrong composites. They have aroused both theoretical and experimental interest.[1-6] Besides the well-known C_{60} and C_{70}, other cages have been isolated in solid-state. Recently, the small cages C_{36} and C_{20} were reported and their halves used for modeling capped narrow nanotubes.[7-9]

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 the graph G is the sum of distances over all its distinct vertex pairs (i,j):

$$W = W(G) = \sum_{(i,j)} d(i,j) \tag{1}$$

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Mathematical aspects related to the counting of distances in nanotubes covered by squares and octagons C_4C_8, as well as the relationship of this covering with the square tiled nanotubes, by the leapfrog operation, will be illustrated in the following.

CONSTRUCTION OF TUC_4C_8 NANOTBES

The C_4C_8 covering is related to the square net tessellating a cylinder.[11,12] Let a square C_4 be the unity polygon U submitted to some well-known operations on a map M.[13,14] It is easily seen that the square stellation, followed by dualisation, leads to the "rhomb"- net (*i.e.*, "bathroom floor" net - Figure 1, first row), which is symbolized as $TUC_4C_8(R)$ $[c,n]$ when it covers a tube (*i.e.*, a cylinder). The medial of U leads to the "square"-net $TUC_4C_8(S)$ $[c,n]$ (the second row in Figure 1). Clearly, the sequence $Du(St(M)) = Le(M)$ is equivalent to the leapfrog Le operation.[14,15]

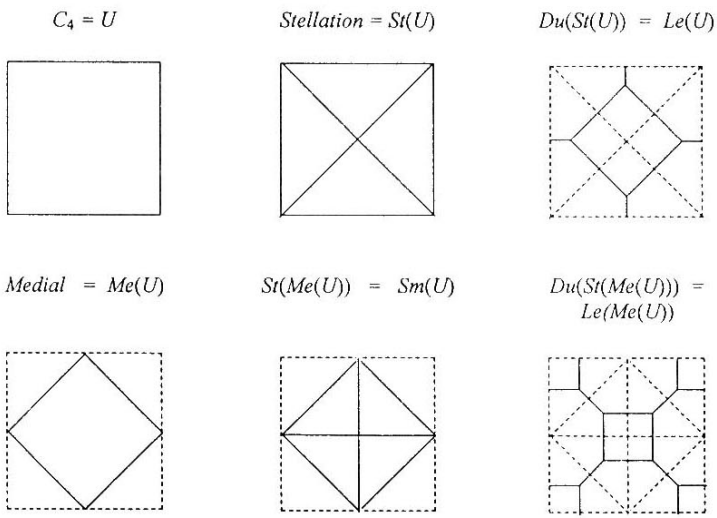

Figure 1. Map operations on the square unity U polygon.

Figure 2 shows assemblies of the above leapfrog units.

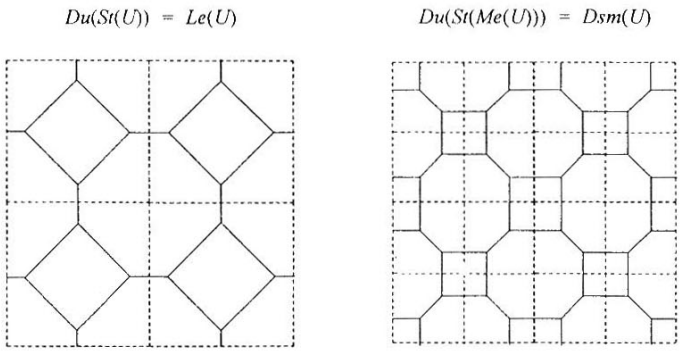

Figure 2. Assemblies of the leapfrog units derived from the square.

Optimized C_4C_8 nets covering a nanotube are illustrated in Figure 3. Such nanotubes could appear by successive low energy Stone-Wales[16] edge flippings in polyhex nanotubes.[17]

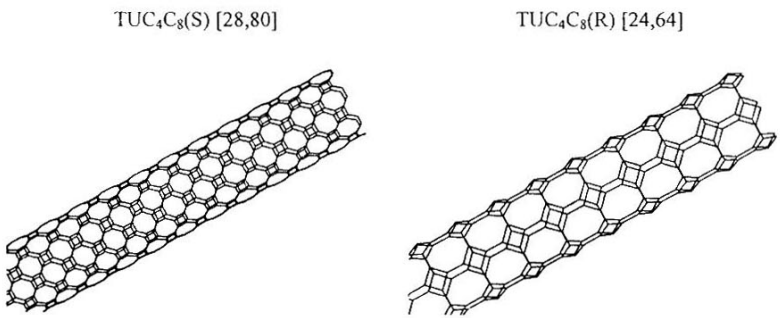

Figure 3. Nanotubes covered by $\mathbf{C_4C_8}$ nets.

In the name TUC_4C_8(R/S) [*c*,*n*], the first letter *c* in the brackets is the number of atoms in the cross-section while *n* denotes the number of cross-sections along the tube. The number of points (*i.e.*, atoms) in the molecule is *c* x *n*.

WIENER INDEX OF C_4C_8 (SQUARE) NANOTUBES

The method for deriving analytical formulas which calculate the Wiener index in C_4C_8 nanotubes is similar to that developed in refs.[18,19]

Method. Let us denote by p the number of squares at level 1 in the tube and by k, m, q the various levels (*i.e.*, the length) of the tube (Figure 4).

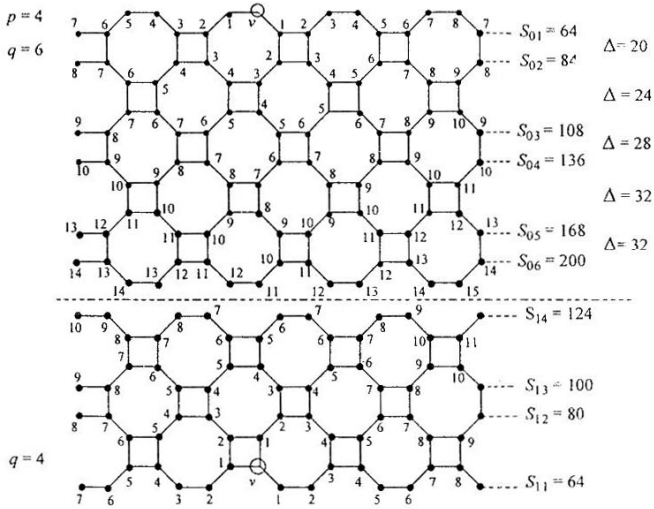

Figure 4. Distance sum from a vertex v to vertices lying at levels k =1..6 and 1..4

The sum from a vertex v lying at level 1 to all other vertices on the same level 1 is given by:

$$s_1(p) = 4p^2 \tag{2}$$

There are two types of vertices: those not located on a square and vertices that lye on a square. For levels in the range $1 \le k \le p+1$, there are two different distance sums from vertex v to all vertices lying at level k:

If v does not belong to a square, then:

$$s_{0k}(p,k) = 4p^2 + 2(k-1)(2p+k) \tag{3}$$

Otherwise,

$$s_{1k}(p,k) = 4p^2 + 2(k-1)(2p+k-2) \tag{4}$$

The distance from all vertices lying at level 1 to vertices at level k, $1 \le k \le p+1$ is given by:

$$s_k(p,k) = p[2 \cdot s_{0k}(p,k) + 2 \cdot s_{1k}(p,k)] = 8p \cdot [2p^2 + (k-1)(2p+k-1)] \tag{5}$$

The distance from level 1 to level $p+1$ is:

$$s_{p+1}(p) = 40p^3 \tag{6}$$

The total distance sum from level 1 to all levels up to m, $1 \le m \le p+1$ is:

$$st_m(p,m) = \sum_{k=1}^{m} s_k(p,k) = 4pm \cdot [4p^2 + \frac{1}{3}(m-1)(2m-1+6p)] \tag{7}$$

The total distance sum from level 1 to levels until $p+1$, is:

$$st_{p+1}(p) = 4p^2(p+1)[4p + \frac{1}{3}(8p+1)] \tag{8}$$

Calculate now the distance sums from all vertices lying on level 1, as follows:

The distance sums to vertices on levels $k > p+1$:

$$sl_k(p,k) = 40p^3 + 32p^2(k-p-1) \tag{9}$$

The total distance sums to all vertices in a tube having the length m, $m>p+1$:

$$stl_m(p,m) = \sum_{k=1}^{p+1} s_k(p,k) + \sum_{k=p+2}^{m} sl_k(p,k) \tag{10}$$

$$stl_m(p,m) = st_{p+1}(p) + 40p^3(m-p-1) + 16p^2(m-p)(m-p-1) \tag{11}$$

By substituting (8) in (11) it becomes:

$$stl_m(p,m) = 4/3 \cdot p^2(12 \cdot m^2 + 6 \cdot m \cdot p - 12m + 2p^2 + 3p + 1) \tag{12}$$

Now we are ready to calculate the Wiener index in a short tube, $TUC_4C_8(S)$ $[4p,q]$ with the length $q \le p+1$, as:

$$W_s(p,q) = \frac{1}{2}[2 \cdot \sum_{m=1}^{q} st_m(p,m) - q \cdot 4p \cdot s_1(p)] \tag{13}$$

and after replacing $st_m(p,m)$ as in (7) and $s_1(p)$, the final formula is:

$$W_s(p,q) = \frac{2}{3} \cdot q \cdot p(q+1)(q^2 + 4 \cdot q \cdot p - q - 4p + 12 \cdot p^2) - 8 \cdot q \cdot p^3 \tag{14}$$

The subtraction of the last term in (12) is reasoned as follows: the reference vertex v may be located at any level m, $1 \le m \le p+1$, each time looking at $TUC_4C_8(S)$ $[4p,q]$ as being obtained by two smaller tubes sharing a common level, namely that containing the vertex v. It is obvious that the actual level of v is counted twice.

If $q = p+1$, the formula (14) for calculating the Wiener index becomes:

$$W_{p+1}(p) = \frac{2}{3} \cdot p^2(p+1)(17 \cdot p^2 + 23p + 2) \tag{15}$$

The Wiener index in a long $TUC_4C_8(S)$ $[4p,q]$, $q > p+1$ is:

$$\begin{aligned} W_l(p,q) &= \frac{1}{2}[2\sum_{m=1}^{p+1} st_m(p,m) + 2 \sum_{m=p+2}^{q} stl_m(p,m) - q \cdot 4p \cdot s_1(p)] \\ &= W_{p+1}(p) + \sum_{m=p+2}^{q} stl_m(p,m) - 8 \cdot p^3 \cdot (q-p-1) \end{aligned} \tag{16}$$

and after replacing $W_{p+1}(p)$ as in (15) and $stl_m(p,m)$ as in (10) the final formula is:

$$W_l(p,q) = \frac{2}{3} \cdot p^2(8 \cdot q^3 - p^3 + 4 \cdot p^2 \cdot q + 6 \cdot p \cdot q^2 - 6 \cdot q + p) \tag{17}$$

Numerical data for Wiener index in tubes $TUC_4C_8(S)$ $[4p,q]$ of various dimensions are given in Tables 1 and 2 (see eqs. (14) and (17)).

Table 1. Wiener index in short tubes, $sTUC_4C_8(S)$ $[4p,q]$, $q \le p+1$

p	q	W	p	q	W
4	2	2336	5	2	4440
4	3	5824	5	4	20800
4	4	11392	5	5	35000
4	5	19520	5	6	54200
6	3	18144	7	3	28168
6	4	34368	7	4	52864
6	5	57120	7	6	132104
6	6	87408	7	7	189336
8	5	126080	7	8	260288
8	6	190016	3	2	1032
8	8	369664	3	3	2664
8	9	489216	3	4	5376

Table 2. Wiener index in long tubes, $ITUC_4C_8(S)$ $[4p,q]$, $q \geq p+1$

p	q	W	p	q	W
3	6	15192	5	6	54200
4	5	19520	5	7	79200
4	6	30720	5	8	110800
4	7	45504	5	9	149800
7	8	260288	5	10	197000
7	9	346528	5	13	395800
8	10	631296	5	20	1296000

Formulas for calculating the Wiener index in $C_4C_8(S)$ tori were given elsewhere.[20]

WIENER INDEX OF C_4C_8(RHOMBOIDAL) NANOTUBES

Method. We denote with p the number of rhombs on the level 1 and with k, m, q the various length of the tube (Figure 5).

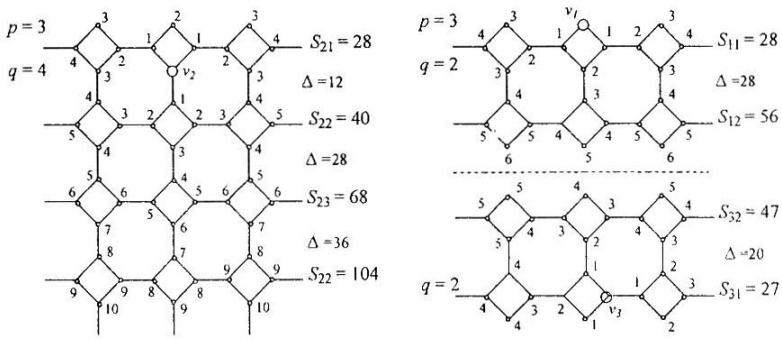

Figure 5. Distance sums from a vertex v to vertices lying at levels k = 1...4 and 1...2

We obtain two formulas: one for the tube length $q \leq [p+1)/2]$ and one for $q \geq [p+1)/2]$.

There are three types of vertices at level 1: vertices lying on the outside part of the rhomb – v_1, vertices that are on the inside part of the rhomb – v_2, and vertices located on an octagon – v_3.

The sum of distances from v_1 and v_2 to all vertices lying at level $k = 1$ is given by:

$$s_{11}(p) = 3 \cdot p^2 + 1 + \frac{[1 + (-1)^p]}{2} \tag{18}$$

The sum from v_3 (which is on the octagon) to all vertices lying at level $k = 1$ is:

$$s_{13}(p) = 3 \cdot p^2 \tag{19}$$

The sum from all vertices on the level 1 to all others vertices at the same level 1 is:

$$s_1(p) = 2 \cdot p(s_{11}(p) + s_{13}(p)) = 2 \cdot p(6 \cdot p^2 + 1 + \frac{[1 + (-1)^p]}{2}) \tag{20}$$

For levels in the range $1 \le k \le \text{int}[(p+1)/2]$, there are three different distance sums from level 1 to level k:

From vertex v_1:

$$s_{1k}(p,k) = 3p^2 + 1 + \frac{[1 + (-1)^p]}{2} + 4(k-1)(2k+p) \tag{21}$$

From vertex v_2:

$$s_{2k}(p,k) = 3p^2 + 1 + \frac{[1 + (-1)^p]}{2} + 4(k-1)(2k+p-4) \tag{22}$$

From vertex v_3:

$$s_{3k}(p,k) = 3p^2 + 4(k-1)(2k+p-2) \tag{23}$$

The distance from all vertices lying at level 1 to vertices at level k, $1 \le k \le \text{int}[(p+1)/2]$ is given by:

$$\begin{aligned} s_{ks}(p,k) &= p[s_{1k}(p,k) + s_{2k}(p,k) + 2 \cdot s_{3k}(p,k)] \\ &= p[12 \cdot p^2 + 3 + (-1)^p + 16(k-1)(2k+p-2)] \end{aligned} \tag{24}$$

The distance sum from level 1 to all levels up to m, where $1 \le m \le \text{int}[(p+1)/2]$ is:

$$st_{ms}(p,m) = \sum_{k=1}^{m} s_{ks}(p,k) = \frac{1}{3} p \cdot m \cdot [36p^2 + 24 \cdot p \cdot m + 32m^2 - 48m - 24p + 25 + 3 \cdot (-1)^p] \tag{25}$$

The Wiener index for short tubes (length q is $1 \le q \le \text{int}[(p+1)/2]$) is calculated as:

$$W_s(p,q) = \frac{1}{2}[2 \cdot \sum_{m=1}^{q} st_{ms}(p,m) - q \cdot s_1(p)] \tag{26}$$

and after replacing $st_{ms}(p,m)$ as in (25) and $s_1(p)$ as in (20), the final formula is

$$W_s(p,q) = \frac{1}{6} \cdot q \cdot p(16 \cdot q^3 + 16 \cdot p \cdot q^2 + 36 \cdot p^2 \cdot q + 3 \cdot q \cdot (-1)^p - 7 \cdot q - 16 \cdot p) \tag{27}$$

For calculating the Wiener index for long tubes, we derived formulas for three different tube length:

Case (i): $q = \text{int}[(p+1)/2] + 1$.

The distance from all vertices lying at level 1 to the last level:

$$s_{klp1}(p) = p[28 \cdot p^2 + 12p[1-(-1)^p] + 3 \cdot (-1)^p - 1] \tag{28}$$

The distance sum from level 1 to all levels up to $m = \text{int}[(p+1)/2] + 1$ is

$$st_{mp1}(p) = p[\frac{28}{3} \cdot p^3 + 27p^2 - 7p^2(-1)^p + \frac{79}{6}p - \frac{17}{2}p \cdot (-1)^p - \frac{1}{2} + \frac{5}{2}(-1)^p] \tag{29}$$

The Wiener index of a tube of length $q = \text{int}[(p+1)/2] + 1$ is

$$W_{p1}(p) = W_s(p, \text{int}[(p+1)/2]) + st_{mp1}(p) - \frac{s_1(p)}{2} \tag{30}$$

$$\begin{aligned} W_{p1}(p) = \frac{p}{24}[&48p^4 + 280p^3 - 56p^3(-1)^p + 507p^2 - 207p^2(-1)^p \\ &+ 302p - 190p(-1)^p - 51[1-(-1)^p]] \end{aligned} \tag{31}$$

Case (ii): $q = \text{int}[(p+1)/2] + 2$.

Analogously, the Wiener index of such tubes is calculated as:

$$\begin{aligned} W_{p2}(p) = \frac{p}{24}[&48p^4 + 504p^3 - 56p^3(-1)^p + 1683p^2 - 375p^2(-1)^p \\ &+ 2058p - 682p(-1)^p - 147[1-(-1)^p]] \end{aligned} \tag{32}$$

Case (iii): $q > \text{int}[(p+1)/2] + 2$.

For tubes of the third length, the distance from all vertices lying at level 1 to vertices at level $k \ge \text{int}[(p+1)/2] + 2$ is:

$$s_{kl}(p,k) = p \cdot [28 \cdot p^2 - 12p(-1)^p + 60p - 2[1-(-1)^p] + 12 \cdot 4 \cdot p[k - \frac{2p+1-(-1)^p+8}{4}]] \tag{33}$$

The distance sum from level 1 to all levels until level m, where $m \ge \text{int}[(p+1)/2] + 2$ is

$$st_{ml}(p,n) = p\cdot[\frac{4}{3}p^3 + 4p^2m + 24pm^2 + 4p^2 - 24pm - 2m[1-(-1)^p] + \frac{31}{6}p - \frac{1}{2}p(-1)^p - \frac{1}{2}(-1)^p + \frac{5}{2}] \tag{34}$$

If we take $l_2 = \mathrm{int}[(p+1)/2]+2 = \frac{2p+1-(-1)^p+8}{4}$ then the Wiener index will be:

$$W_l(p,q) = W_{p2}(p,q) + \sum_{m=l_2+1}^{q} st_{ml}(p,m) - \frac{(q-l_2)\cdot s_1(p)}{2} \tag{35}$$

and after replacing $W_{p2}(p,q)$ from (32), $st_{ml}(p,m)$ from (34) and $s_1(p)$ from (20) the final formula is:

$$W_l(p,q) = \frac{-p}{24}\cdot[4p^4 - 48p^2q^2 - 192pq^3 - 32p^3q + 24\cdot q^2[1-(-1)^p] - p^2 - 3p^2(-1)^p + + 68pq + 12pq(-1)^p - 3[1-(-1)^p]) \tag{36}$$

Table 3. Wiener index in $TUC_4C_8(R)$ Nanotubes,

p	q	$W(p,q)$	p	q	$W(p,q)$
4	2	1952	6	2	6000
4	3	5312	6	3	15228
4	4	11232	6	4	30516
4	5	20480	6	5	53580
4	8	75872	6	6	86148
4	10	143520	6	7	129948
5	1	755	7	2	9268
5	2	3580	7	3	23065
5	3	9355	7	4	45360
5	4	19210	7	5	78407
5	5	34345	7	6	124558
5	8	123430	7	7	186165
5	9	171685	7	10	487242
8	3	33424	9	3	46359
8	4	64768	9	4	88848
8	5	110464	9	5	149895
8	6	173568	9	7	342837
8	7	257152	9	9	656163
8	8	364288	9	10	867690
8	10	661504			

Note that the final formula (36) includes both formula (32) (which calculates $W_{p2}(p)$ for the tube length $q = l_2 = \frac{2p+1-(-1)^p+8}{4}$) and (31) (in the calculation of $W_{p1}(p)$, for the tube length $q = l_1 = [2p+1-(-1)^p+4]/4$).

Examples are given in Table 3 (see eqs. (27) and (36)).

CONCLUSIONS

A C_4C_8 net can be derived from a square net by the leapfrog operation. It was used, in two variants, "square"- C_4C_8 and "rhomb"- C_4C_8 for covering the nanotubes. Formulas for calculating the sum of all distances in such nanotubes are derived and examples are given.

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