Detour index of $TUC_4C_8(S)$ nanotube

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Abstract

The detour $d(i,j)$ between vertices i and j of a graph is the number of edges of the longest path connecting these vertices. The matrix whose (i,j)-entry is the detour between vertices i and j is called the detour matrix. The half sum D of detours between all pairs of vertices (in a connected graph) is the detour index, i.e.,

$$D=\left(\frac{1}{2}\right)\sum_j\sum_i d(i,j).$$

In this paper, we computed the detour index of $TUC_4C_8(S)$ nanotube.

Keywords: Detour index, alternating squares, octagons, nanotubes.

1. Introduction

Fullerenes and nanotubes are promising candidates in the development of nanodevices and superstrong composites. They have aroused both theoretical and experimental interest [5, 6, 7, 9, 14, 15]. 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 [10-12].

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.

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 detour (i.e., the number of edges on the

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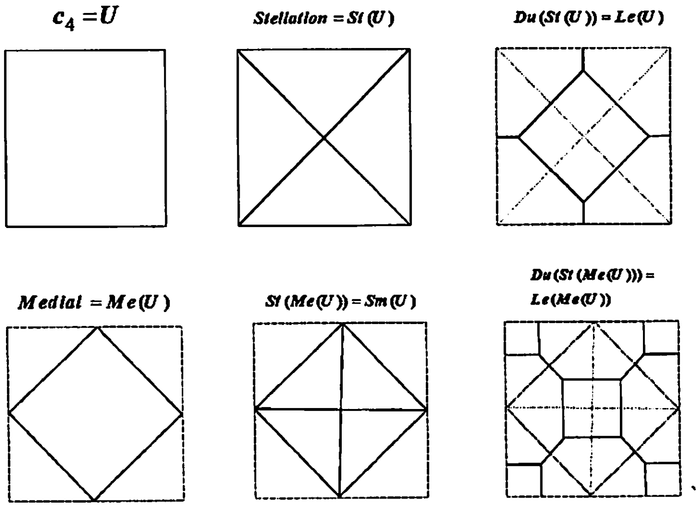
longest path) jointing the two vertices of G. The Detour index [1] D of the graph is the sum of detours over all its distinct vertex pairs (i,j) :

$$D=\frac{1}{2}\sum_j\sum_i d(i,j).$$

Mathematical aspects related to the counting of detours 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.

2. Construction of TUC_4C_8 nanotubes

The C_4C_8 covering is related to the square net tessellating a cylinder [2,4]. Let a square C_4 be the unity polygon U submitted to some well-known operations on a map M [3]. 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 [8].

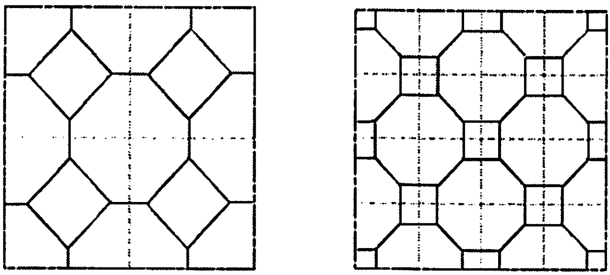


Map operations on the square unity U polygon

Figure 1

Figure 2 shows assemblies of the above leapfrog units.

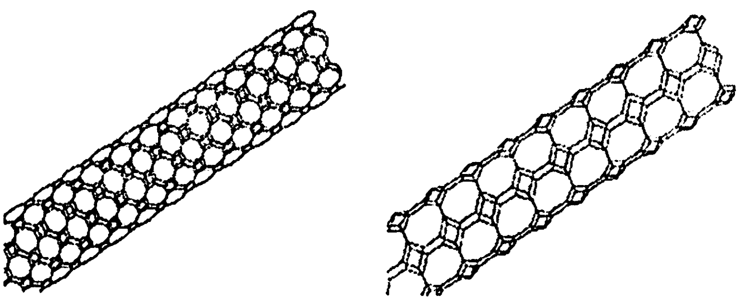
$Du(St(U)) = Le(U)$ $\qquad$ $Du(St(Me(U))) = Dsm(U)$



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

Optimized C_4C_8 nets covering a nanotube are illustrated in Figure 3. Such nanotubes could appear by successive low energy Stone-Wales [13] edge flipping in polyhex nanotubes.

$TUC_4C_8(S)[28,80]$ $\qquad$ $TUC_4C_8(R)[24,64]$

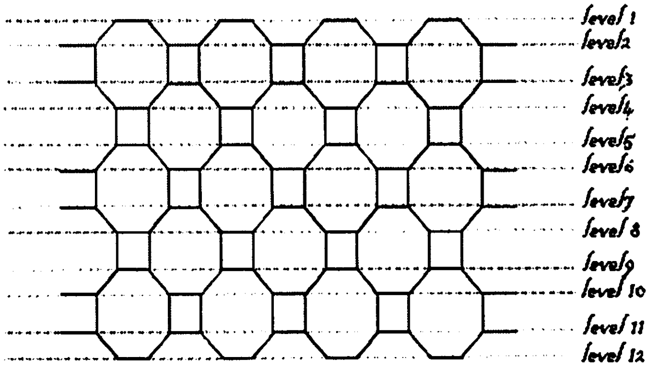


Nanotubes covered by C_4C_8 nets.
Figure 3

In the name $TUC_4C_8(R/S)[c,n]$, the first letter in the brackets is the number of vertices in the cross-section while n denotes the number of cross-sections along the tube. The number of vertices of the nanotube-graph in the molecule is $c \times n$.

3. Detour index of $TUC_4C_8(S)$

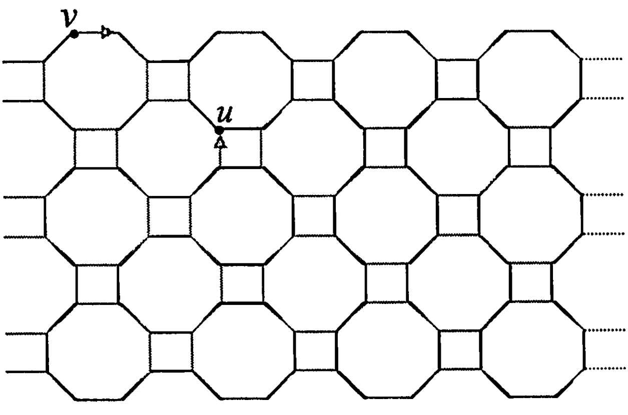
Let us denote by p the number of squares at first row in the tube and by q, m, k the various levels (i.e., the length) of the tube (Figure 4).



$TUC_4C_8(S)$ lattice with $p = 4$, $q = 6$

Figure 4

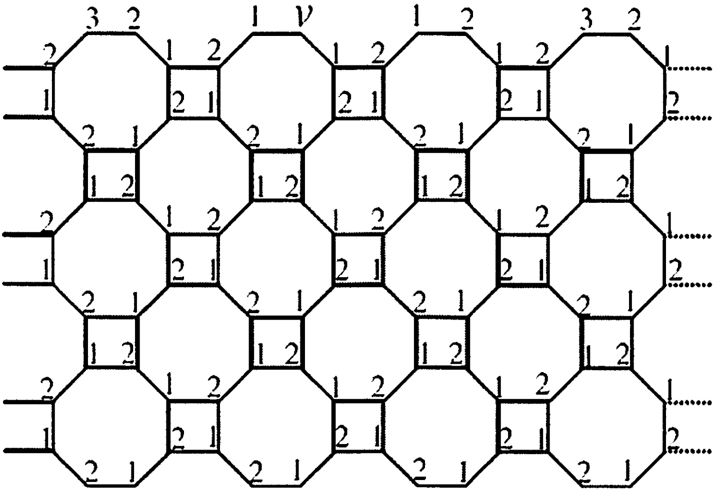
For example, in Figure 5, we marked the detour between vertices v and u ,and detours between other vertices are found similar this way.



Maximum path between vertices v and u .

Figure 5

In Figures 6 and 7, the number m over any vertex, which means $4pq - m$ is the detours from v. Let v be an arbitrary vertex in level 1 (Figure 6),



Detours from vertex v to vertices lying at levels $k = 1,2,..,12$.

Figure 6

Then sum of detours between v and all other vertices lying on same level is given by:
If $p \geq 3$, then:

$$s_1(p) = 8p^2q - 4pq - 5p + 6.$$

And if $p \leq 2$, then:

$$s_1(p) = 8p^2q - 4pq - 3p + 2.$$

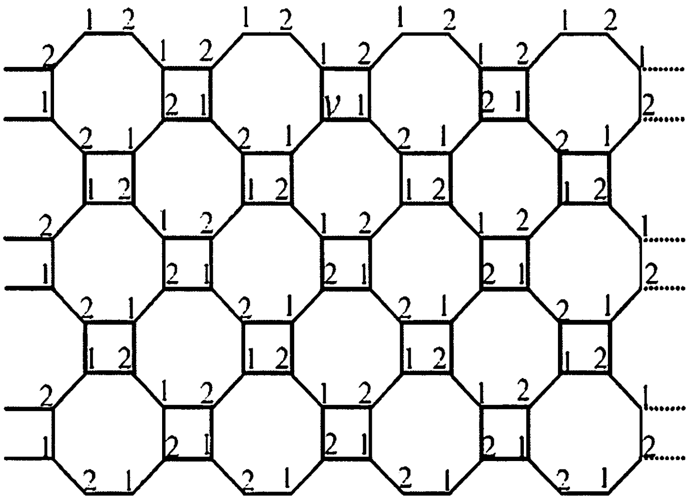
And the sum of detours between v and all other vertices lying at levels $2 \leq k \leq 2q$ is:

$$st_1(p,q) = 16p^2q^2 - 8p^2q - 6pq + 3p.$$

So the total sum of detours between level 1 and all other vertices is:

$$s_1(p,q) = p \cdot s_1(p) + 2p \cdot st_1(p,q) = 32p^3q^2 - 8p^3q - 16p^2q + p^2 + 6p.$$

Now let v be a vertex on level i, $2 \leq i \leq 2q-1$ (For example level 3, see Figure 7).



Detours from vertex v to vertices lying at levels $k = 1, 2, .., 12$.
Figure 7

The sum of detours between v and other vertices lying at same level is given as:

$$s_i(p) = 8p^2q - 4pq - 3p + 2.$$

And the detour sum from v to other vertices lying at levels $i+1 \leq m \leq 2q$ is given as:

$$st_i(p,q) = \sum_{m=i+1}^{2q} (8p^2q - 3p) = 16p^2q^2 - 6pq - (8p^2q - 3p)i.$$

Now sum of detours between level i and all other vertices lying in levels $i \leq k \leq 2q$ is given as:

$$s_i(p,q) = p \cdot s_i(p) + 2p \cdot st_i(p,q).$$

So the total sum of detours between levels $2 \leq i \leq 2q-1$ and all other vertices lying at levels $i \leq j \leq 2q$ is given as:

$$s(p,q) = \sum_{i=2}^{2q-1} s_i(p,q).$$

So we have:

$$s(p,q) = (32p^3q^2 - 20p^2q + 4p)(q-1).$$

If we rotate 180 degree the Figure 6, then the vertices lying at level $2q$ is the same vertices lying at level 1, so we have:

$$s_q(p) = s_1(p).$$

Therefore, the detour index of $TUC_4C_8(S)$ is given as:

If $p \geq 3$, then:

$$D = p \cdot s_1(p) + s_1(p,q) + s(p,q) = (pq)(32p^2q^2 - 20pq + 4) + p(8-4p).$$

If $p \leq 2$, then:

$$D = p \cdot s_1(p) + s_1(p,q) + s_i(p,q) = (pq)(32p^2q^2 - 20pq + 4).$$

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