A New Method for Computation of The Wiener Index of $C_4C_8(S)$ Nanotorus

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Abstract

Let G be a simple connected graph. The Wiener index of G is defined as

$$W(G) = \frac{1}{2} \sum_{\{i,j\} \subseteq V(G)} d(i,j)$$

in which $V(G)$ is the set of all vertices of G and $d(i,j)$ is the distance between vertices i and j of the graph. Ashrafi and yousefi (see A. R. Ashrafi and S. Yousefi, Computing the Wiener Index of a $TUC_4C_8(S)$ Nanotorus, MATCH Commun. Math. Comput. Chem., 57(2)(2007), 403-410) computed the Wiener index of the $TUC_4C_8(S)$ Nanotorus. In this paper we use a new method to compute the Wiener index of these Nanotorus.

1 Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labelling or pictorial representation of a graph. Topological indices are one of the descriptors of molecules that play an important role in structure property and structure activity studies, particularly when multivariate regression analysis, artificial neural networks, and pattern recognition are used as statistical tools. One of the topics of continuing interest in structure-property studies is to arrive at simple correlations between the selected properties and the molecular structure [4]-[9].

Wiener index is one of the most studied topological indices and is connected to the problem of distances in graph. Harold Wiener [9] in 1947 introduced the notion of path number of a graph as the sum of the distances between two carbon atoms in the molecules, in terms of carbo-carbon bound.

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 j of G is denoted by $d(i,j)$. The degree of a vertex $i \in V(G)$ is the number of vertices joining to i and denoted by $v(i)$. The (i,j) entry of the adjacency matrix of G is denoted by $A(i,j)$.

The Wiener index of the graph G is the half sum of distances over all its vertex pairs (i,j): $W(G) = \frac{1}{2}\sum_{i,j} d(i,j)$. The sum distance of a vertex u of G is defined as

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

So we have

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} d(u).$$

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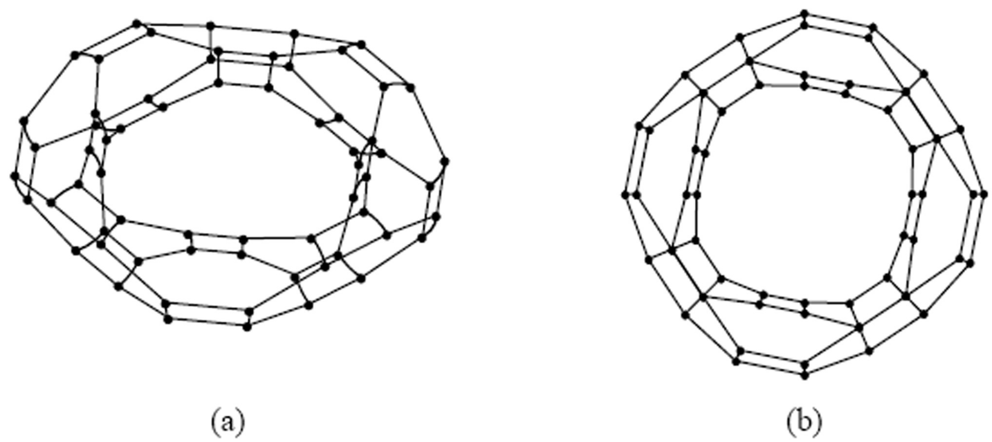

Figure 1: A C4C8(S) Nanotorus (a) Side view (b) Top view.

Recently computing topological indices of nano structures have been the object of many papers. In a series of papers, Ashrafi and Taeri and coauthors [1]-[4] studied the topological indices of some chemical graphs related to Nanotorus. The Wiener index of graphs with different structure may be obtained by various methods [2]-[4]. Ashrafi and Yousefi compute Wiener index of $C_4C_8(S)$ nanotorus by considering vertices on one square of this graph as a collection of vertices which have same distance from a certain vertex of the graph. In this paper we compute this topological index by calculation summation of distance and square distance between a vertex and vertices which placed on same row of the graph.

2. Main results

In this section we derive an exact formula for the hyper Wiener index of graph $C_4C_8(S)$ Nanotorus. For this purpose first we choose a coordinate label for vertices of this graph as shown in Figure 2. Let the graph has q row and $2p$ column of vertices (q and p are positive even integer). In this case we denote the graph by $T(p,q)$. If $q \leq p$ the graph of $T(p,q)$ is called short and if $q > p$, then the graph is called long.

To compute sum distance of vertices of the graph we consider vertices x_{0p} and y_{0p} in the first row of the graph and obtain distance between these vertices and other vertices of the graph. The obtained results can be used for other vertices by symmetry of the graph. Let $d_x(k)$ denotes the summation of distances between vertex x_{0p} and all of the vertices placed in kth row of the graph. Thus

$$d_x(k) = \sum_{t=0}^{p-1} \Big(d(x_{kt}, x_{0p}) + d(y_{kt}, x_{0p}) \Big).$$

Similarly we define $d_y(k)$ as follow:

$$d_y(k) = \sum_{t=0}^{p-1} \Big(d(x_{kt}, y_{0p}) + d(y_{kt}, y_{0p}) \Big).$$

By using of two following Lemma which was proved in [2] we can compute $d_x(k)$ and $d_y(k)$ for $0 \leq k < q$.

Lemma 1. Let $1 \leq k < q$, $0 \leq t < 2p$ and $R_x(k) = (d(x_{kt}, x_{0p}) + d(y_{kt}, x_{0p})) - (d(x_{k-1,t}, x_{0p}) + d(y_{k-1,t}, x_{0p}))$. If p

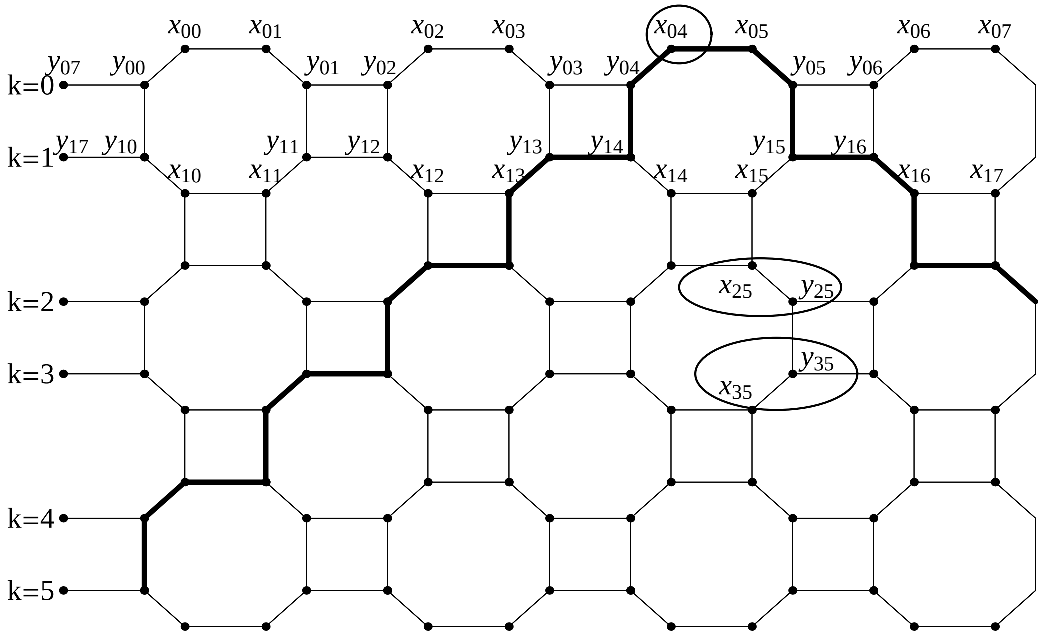

Figure 2: A $C_4C_8(S)$ Lattice with $p = 4$ and $q = 6$.

is an even integer then

$$R_x(k) = \begin{cases} 4 & \text{if } p - k + 1 \leq t \leq p + k \\ 2 & \text{otherwise.} \end{cases}$$

If p is an odd integer then

$$R_x(k) = \begin{cases} 4 & \text{if } p - k \leq t \leq p + k - 1 \\ 2 & \text{otherwise.} \end{cases}$$

As in Lemma 1, we can compute the subtraction of the summation of distances between y_{0p} and k-th row of graph from the summation of the distances between y_{0p} and $(k-1)$-th row of the graph.

Lemma 2. Let $2 \leq k < q$, $0 \leq t < 2p$ and $R_y(k) = (d(x_{kt}, y_{0p}) + d(y_{kt}, y_{0p})) - (d(x_{k-1,t}, y_{0p}) + d(y_{k-1,t}, y_{0p}))$. If p is an even integer then

$$R_y(k) = \begin{cases} 4 & \text{if } p - k + 1 \leq t \leq p + k - 2 \\ 2 & \text{otherwise.} \end{cases}$$

If p is an odd integer then

$$R_y(k) = \begin{cases} 4 & \text{if } p - k + 2 \leq t \leq p + k - 1 \\ 2 & \text{otherwise.} \end{cases}$$

Now we can compute $d_x(k$ and $d_y(k$ by using Lemma 1 and 2 as follow.

Lemma 3. Let $0 \leq k < q$, then

$$d_x(k) = \begin{cases} 4p^2 + 4kp + 2(k^2 + k) & \text{if } k \leq p \\ \\ 2p^2 + 8kp + 2p & \text{if } k > p \end{cases}$$

and

$$d_y(k) = \begin{cases} 4p^2 + 4kp + 2(k^2 - k) & \text{if } k \leq p \\ \\ 2p^2 + 8kp - 2p & \text{if } k > p. \end{cases}$$

Proof: Let $k = 0$. Then for vertices $a_{0t} \in \{x_{0t}, y_{0t}\}$ in the first row of the graph, we have

$$\sum_{t=0}^{2p-1} d(a_{0t}, x_{0p}) = \sum_{t=0}^{2p-1} d(a_{0t}, y_{0p}) = (1 + 2 + \cdots + 2p) + (1 + 2 + \cdots + 2p - 1) = 4p^2.$$

So $d_x(0) = d_y(0) = 4p^2$.

Now suppose that $k \leq p$. Then

$$d_x(k) = d_x(0) + (d_x(1) - d_x(0)) + (d_x(2) - d_x(1)) + \cdots + (d_x(k) - d_x(k-1))$$

By Lemma 1, the number of vertices satisfying the condition $p - i + 1 \leq t \leq p + i$, is $2i$ and for those vertices, $R_x(k) = 4$ and for other $2p - 2i$ remaining vertices of this row we have $R_x(k) = 2$. So

$$\begin{aligned} d_x(k) &= 4p^2 + (4 \times 2 + 2(2p - 2) + (4 \times 4 + 2(2p - 4)) + \cdots + (4 \times 2k + 2(2p - 2k) \\ &= 4p^2 + 4(2 + 4 + \cdots + 2k) + 2((2p - 2) + (2p - 4) + \cdots + (2p - 2k)) \\ &= 4p^2 + 8\sum_{i=1}^{k} i + 4\sum_{i=1}^{k}(p - i) \\ &= 4p^2 + 4kp + 2(k^2 + k). \end{aligned}$$

With a similar argument, using Lemma 2, we have

$$\begin{aligned} d_y(k) &= d_y(0) + (d_y(1) - d_y(0)) + (d_y(2) - d_y(1)) + \cdots + (d_y(k) - d_y(k-1)) \\ &= 4p^2 + 4(0 + 2 + \cdots + 2(k-1)) + 2((2p - 0) + (2p - 2) + \cdots + (2p - 2k + 2)) \\ &= 4p^2 + 8\sum_{i=1}^{k-1} i + 4\sum_{i=1}^{k-1}(p - i) \\ &= 4p^2 + 4kp + 2(k^2 - k). \end{aligned}$$

Now let $k > p$. Then all of vertices satisfy the condition $p - i + 1 \leq t \leq p + i$. So by Lemma 1, we have

$$\begin{aligned} d_x(k) &= d_x(p) + (d_x(p+1) - d_x(p)) + (d_x(p+2) - d_x(p+1)) + \cdots \\ &\quad +(d_x(p+k) - d_x(p+k-1)) \\ &= (10p^2 + 2p) + 4(2p)(k-p) \\ &= 2p^2 + 8kp + 2p. \end{aligned}$$

Similarly we have

$$\begin{aligned} d_y(k) &= d_y(p) + (d_y(p+1) - d_y(p)) + (d_y(p+2) - d_y(p+1)) + \cdots \\ &\quad +(d_y(p+k) - d_y(p+k-1)) \\ &= (10p^2 - 2p) + 4(2p)(k-p) \\ &= 2p^2 + 8kp - 2p. \end{aligned}$$

This completes the proof. □

Now we can compute quantity of expression $\sum_{\{i,j\}\subseteq V(G)} d(i,j)$ for graph of $G = C_4C_8(S)$ Nanotorus which equal to Wiener index of this graph.

Theorem 1. The Wiener index of $G := C_4C_8(S)$ Nanotubes given by

$$W(G) = \begin{cases} \dfrac{pq^2}{3}(24p^2 + 6qp + q^2 - 4), & \text{if } q \leq p \\[2ex] \dfrac{4p^2q}{3}(2p^2 + 3qp + 3q^2 - 2), & \text{if } q > p. \end{cases}$$

Proof: Let $q \leq p$, by Lemma 3 we have

$$\begin{aligned} \sum_{\{i,j\}\subseteq V(G)} d(i,j) &= pq \sum_{k=0}^{q/2-1} d_x(k) + \sum_{k=1}^{q/2} d_y(k) \\ &= \sum_{k=0}^{q/2-1}\Big(4p^2 + 4kp + 2(k^2+k)\Big) + \sum_{k=0}^{q/2}\Big(4p^2 + 4kp + 2(k^2-k)\Big) \\ &= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q \end{aligned}$$

The last results which obtained for vertex x_{0p} can be used for all of the vertices of graphs. Therefore

$$W(G) = \sum_{\{i,j\}\subseteq V(G)} d(i,j) \quad = \quad pq \sum_{i\in V(G)} d(i, x_{0p}) = \frac{pq^2}{3}(24p^2 + 6qp + q^2 - 4).$$

p	q	$W(G)$	p	q	$W(G)$
2	2	320	5	4	19520
2	4	1664	5	8	96000
2	8	10496	8	2	17408
3	2	1008	8	8	337920
3	4	4800	8	10	568320
3	8	26880	10	4	141440
4	2	2304	10	10	1032000
4	4	10496	10	12	1584000
4	8	54272	12	10	1708800
5	2	4400	12	12	2568960

Table 1: Wiener index of short $C_4C_8(S)$ Nanotorus.

Now suppose $q > p$. Thus

$$\begin{aligned}\sum_{i\in V(G)} d(x_{0p}, i) &= \sum_{k=0}^{p} d_x(k) + \sum_{k=1}^{p} d_y(k) + \sum_{k=p+1}^{q/2-1} d_x(k) + \sum_{k=p+1}^{q/2} d_y(k)\\ &= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q + \sum_{k=p+1}^{q/2-1}\Big(4p^2 + 4kp + 2(k^2+k)\Big) + \sum_{k=p+1}^{q/2}\Big(4p^2 + 4kp + 2(k^2-k)\Big)\\ &= \frac{4p^3}{3} + 2p^2q + (2q^2 - \frac{4}{3})p.\end{aligned}$$

So in this case $W(G)$ computed as follow:

$$W(G) = \sum_{\{i,j\}\subseteq V(G)} d(i,j) = pq \sum_{i\in V(G)} d(i, x_{0p}) = \frac{4p^2q}{3}(2p^2 + 3qp + 3q^2 - 2).$$

This completes the proof. □

In the following table the numerical data for Wiener index of $C_4C_8(S)$ Nanotorus of various dimensions are given.

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