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# HYPER WIENER INDEX $C_4C_8(S)$ NANOTORUS

ABBAS HEYDARI
*Department of Mathematics, Azad University of Arak, Arak 38135-567, I. R. Iran*

The hyper Wiener index of a molecular graph is defined as one half of the sum of the distances and square distances between all (ordered) pairs of vertices of the graph. In this paper we obtain an exact formula for calculation the hyper Wiener index of nanotorus which have square and octagon structure and denoted by $C_4C_8(S)$ nanotorus.

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## 1. Introduction

A topological index is a real number related to a structural graph of a molecule. It does not depend on the labeling 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 [3, 16]. The hyper Wiener index is one of the recently conceived distance-based graph invariants, used as a structure-descriptor for predicting physicochemical properties of organic compounds. This topological index was introduced by Randi'c and has been extensively studied [10, 13].

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 hyper Wiener index of the graph *G* is the half sum of distances and square distances over all its vertex pairs *(i , j)*:

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

Recently computing topological indices of nano structures have been the object of many papers [6-9]. In a series of papers, Ashrafi and coauthors [1, 2] and [14-15] studied the topological indices of some chemical graphs related to nanotorus. The hyper Wiener index of graphs with different structure may be obtained by various methods [4,5] and [11,12]. In this paper we compute this topological index by calculation summation of distance and square distance between a vertex and vertices which placed in a row of the graph. In [1] Ashrafi and coauthor compute the wiener index of $C_4C_8(S)$ nanotorus. To

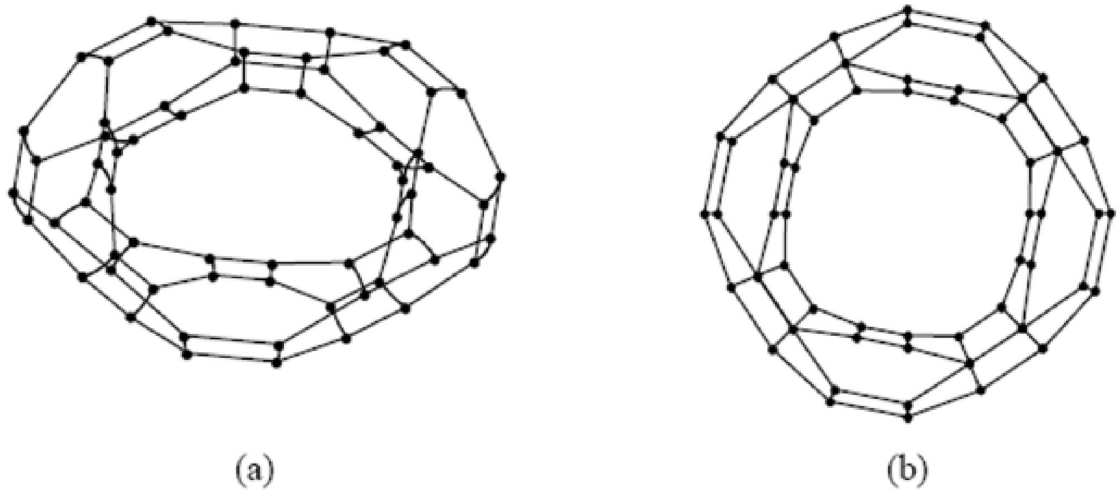


*Fig. 1. AC4C8(S) Nanotorus (a) Side view (b) Top view.*

compute the hyper Wiener index of this graph we need to Wiener index of the graph so we compute the Wiener index of graph by a simple method.

## 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 rows and p columns of vertices ( q and p are positive even integer ). Therefore the graph of nanotorus can be denoted the by T(p, q). To compute WW(G), at first the summation of distance between all of the pair vertices of the graph, $\sum_{\{i,j\}\subseteq V(G)}(d(i,j)$, most be computed.

For this purpose we consider vertices $x_{0p}$ and $y_{0p}$ in the first row of the graph and obtain summation of distances between these two vertices and other vertices of the graph. The obtained results in this computations can be used for calculation summation of distances between each two vertices $x_{tp}$ and $y_{tp}$ (for $t=1,2,\ldots,q-1$) and other vertices of the graph other 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 *k*th row of the graph. Thus

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

Similarly we de_ne dy(k) as follows:

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

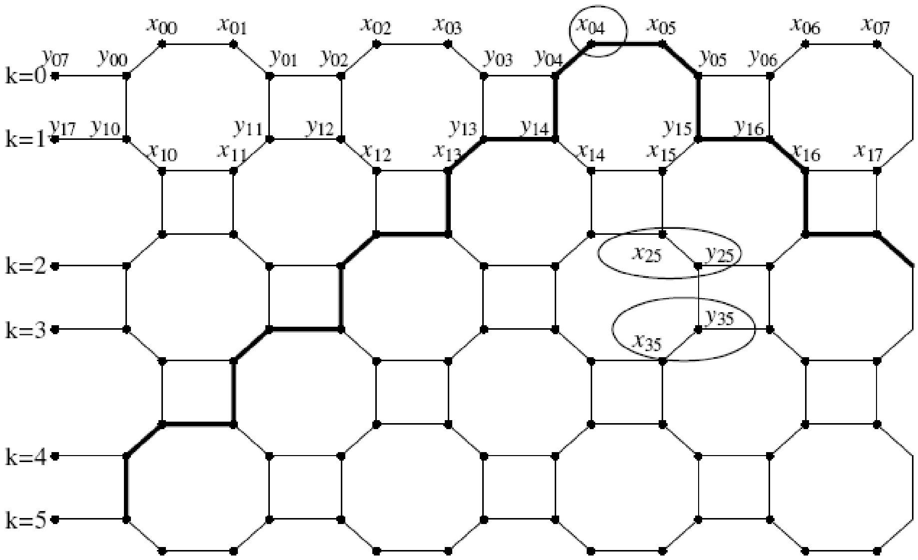


*Fig. 2. A $C_4C_8$ (S) Lattice with p=4 and q=6.*

In Lemma 3 of Ref [6] we compute $d_x(k)$ and $d_y(k)$ as follows:

Lemma 1. Let $0 \le k < \frac{q}{2}$, then

$$d_x(k) = \begin{cases} p^2 + 2kp + 2(k^2 + k) & if \quad 2k \le p \\ \frac{p^2}{2} + 4kp + p & if \quad 2k > p. \end{cases}$$

and

$$d_y(k) = \begin{cases} p^2 + 2kp + 2(k^2 - k) & if \quad 2k \le p \\ \frac{p^2}{2} + 4kp - p & if \quad 2k > p. \end{cases}$$

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 is equal to Wiener index of this graph. Let $q \le p$ , by usingof Lemma 1 we have

$$\sum_{\{i,j\} \subseteq V(G)} (d(i,j) = pq \sum_{k=0}^{\frac{q}{2}-1} d_x(k) + \sum_{k=1}^{\frac{q}{2}} d_y(k)$$

$$= \sum_{k=0}^{\frac{q}{2}-1} (4p^2 + 4kp + 2(k^2 + k)) + \sum_{k=1}^{\frac{q}{2}} (4p^2 + 4kp + 2(k^2 - k))$$

$$= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q.$$

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

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

Now suppose q>p. Thus

$$\sum_{i\in V(G)} d(i,x_{0p}) = \sum_{k=0}^{p} d_x(k) + \sum_{k=1}^{p} d_y(k) + \sum_{k=p+1}^{\frac{q}{2}-1} d_x(k) + \sum_{k=p+1}^{\frac{q}{2}} d_y(k)$$

$$= \frac{q^3}{6} + pq^2 + (4p^2 - \frac{2}{3})q + \sum_{k=p+1}^{\frac{q}{2}-1}(4p^2 + 4kp + 2(k^2+k)) + \sum_{k=p+1}^{\frac{q}{2}}(4p^2 + 4kp + 2(k^2-k))$$

$$= \frac{4p^3}{3} + 2qp^2 + (2p^2 - \frac{4}{3})p.$$

So in this case the Wiener index of the graph ,*W(G)*, computed as follows:

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

In continue of this section we compute the summation of square distance between all of the pairs vertices, $\sum_{\{i,j\}\subseteq V(G)} d^2(i,j)$ ,of the graph $C_4C_8(S)$ nanotorus. At first we compute the summation of square distances between a vertex of graph and vertices of graph placed in *k* rows which placed bellow of this vertex (see figure 2). Then by suitable summation we can obtain summation of distances between a vertex and all of the vertices of the graph.

Let $x_{kt}$ and $y_{kt}$ be vertices in the *k*th row and *t*th column of the graph for $1 \le k < q$ and $1 \le t < p$. Put

$$X_{kt} = d^2(x_{0p}, x_{kt}) + d^2(x_{0p}, y_{kt}) - d^2(x_{0p}, x_{k-1,t}) - d^2(x_{0p}, y_{k-1,t}).$$

In the following Lemma we compute $X_{kt}$ in two cases which the vertices are considered below the black edges and the vertices are placed on or above the black edges ( see figure 2 ).

Lemma 2 Let $1 \le k < \frac{q}{2}$ and $1 \le t < p$ and $r = | p - t |$. If $p - k + 1 \le t < p + k$, then $X_{kt} = 8(2k + r) - 4$. If $t > p$ and $t < p$ -k+1 then

$$X_{kt} = \begin{cases} 4(2r+k) & if \quad t < p \\ 4(2r+k) - 4 & if \quad t \ge p. \end{cases}$$

Proof: Let $p - k + 1 \le t < p + k$ . If *k* is an odd integer then $d(x_{0p}, x_{kt}) = 2k+r+1$ and $d(x_{0p}, y_{kt}) = 2k+r$. Also if *k* is even, integer $d(x_{0p}, x_{kt}) = 2k+r$ and $d(x_{0p}, y_{kt}) = 2k+r+1$ Anyway $X_{kt}$ computed as follow:

$$X_{kt} = ((2k + r + 1)^2 + (2k + r)^2) - ((2(k-1) + r + 1)^2 + (2(k-1) + r)^2) = 8(2k + r) - 4.$$

Now Suppose $t > p + k$ or $t < p < k + 1$. For $t \le p$ we have $d(x_{0p}, x_{kt}) = 2r + k+1$ and $d(x_{0p}, y_{kt}) = 2r + k$ if *r* be odd integer. If *r* be even integer then $d(x_{0p}, x_{kt}) = 2r+k$ and $d(x_{0p}, y_{kt})) = 2r+k+1$. Therefore

$$X_{kt} = ((2r + k)^2 + (2k + r)^2) - ((2r + (k-1) + 1)^2 + (2r + k - 1)^2) = 4(2r + k).$$

Now suppose $t > p$. So $d(x_{0p}, y_{kt}) = 2r + k - 1$ and $d(x_{0p}, x_{kt}) = 2k + r$, if *r* be even integer. If *r* be odd we have $d(x_{0p}, y_{kt}) = 2r+k$ and $d(x_{0p}, x_{kt}) = 2k+r-1$. Therefore

$$X_{kt} = ((2r+k)^2 + (2r+k-1)^2) - ((2r+k-1)^2 + (2r+(k-1)-1)^2) = 4(2r+k)-4.$$

This completes the proof.

Now we consider vertex $y_{0p}$ instead $x_{0p}$ and derive Similar results. Put

$$Y_{kt} = d^2(y_{0p}, x_{kt}) + d^2(y_{0p}, y_{kt}) - d^2(y_{0p}, x_{k-1,t}) - d^2(y_{0p}, y_{k-1,t}).$$

By similar argument we can calculate $Y_{kt}$ with consideration two cases for vertices of the graph.

Lemma 3. Let $1 \le k < \frac{q}{2}$ and $1 \le t < p$ and $r = |p-t|$. If $k \ge 2$ and $p-k+1 \le t < p+k-2$ then $Y_{kt} = 8(2k+r)-12$. If $t < p-k+1$ and $t > p+k-2$, then

$$Y_{kt} = \begin{cases} 4(2r+k)-4 & if \quad t < p \\ 4(2r+k) & if \quad t \ge p. \end{cases}$$

Proof: The proof is similar to that of Lemma 2 .

Now let $d_x^2(k)$ denotes the summation of square distances between vertex $x_{0p}$ and all of the vertices placed in $k$th row of the graph. Thus

$$d_x^2(k) = \sum_{t=0}^{p-1} (d(x_{kt}, x_{0p}) + d(y_{kt}, x_{0p}))$$

Similarly we define $d_y^2(k)$ as follows:

$$d_y^2(k) = \sum_{t=0}^{p-1} (d(x_{kt}, y_{0p}) + d(y_{kt}, y_{0p}))$$

In the following Lemma we compute $d_x^2(k)$ and $d_y^2(k)$ for $k$th row of the graph.

Lemma 4. Let $1 \le k < \frac{q}{2}$, then

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

And

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

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

$$\sum_{t=0}^{p-1} d^2(a_{0t}, x_{0p}) = \sum_{t=0}^{p-1} d^2(a_{0t}, y_{0p}) = (1^2 + 2^2 + \ldots + (2p)^2) + (1^2 + 2^2 + \ldots + (2p-1)^2) = \frac{2p}{3}(8p^2+1).$$

So $d_x^2(k) = d_y^2(k) = \frac{2p}{3}(8p^2+1)$. Now suppose that $k \le p$. Then

$$d_x^2(k) = d_x^2(0) + (d_x^2(1) - d_x^2(0)) + (d_x^2(2) - d_x^2(1)) + \ldots + (d_x^2(k) - d_x^2(k-1))$$
$$= d_x^2(0) + \sum_{i=1}^{k} \sum_{t=0}^{p-1} (X_{it} + Y_{it}).$$

By using Lemma 1 and 2, we have

$$d_x^2(k) = \frac{3p}{2}(8p^2+1) + \sum_{i=1}^{k}\Big(\sum_{r=i}^{p-1} 4(2r+i) + \sum_{r=i+1}^{p}(4(2r+i)-4) + \sum_{r=0}^{i}(8(2i+r)-4) + \sum_{r=0}^{i}(8(2i+r)-4)\Big)$$
$$= \frac{2}{3}(12k^3 + (6p+15)k^2 + (12p^2+3)k + 8p^3 + p).$$

Therefore by using similar argument, in proof of Lemma *2*, we have

$$d_y^2(k) = d_y^2(0) + (d_y^2(1) - d_y^2(0)) + (d_y^2(2) - d_y^2(1)) + \ldots + (d_y^2(k) - d_y^2(k-1))$$
$$= d_y^2(0) + \sum_{i=1}^{k}\sum_{t=0}^{p-1}(X_{it} + Y_{it})$$
$$= \frac{3p}{2}(8p^2+1) + \sum_{i=1}^{k}\Big(\sum_{r=i-1}^{p-1} 4(2r+i) + \sum_{r=i}^{p}(4(2r+i)-4)\Big) + \sum_{i=2}^{k}\ \sum_{r=0}^{i-2}(8(2i+r)-12) +$$
$$\sum_{r=1}^{i-1}(8(2i+r)-12))$$
$$= \frac{2}{3}(12k^3 + (6p-15)k^2 + (12p^2+3)k + 8p^3 + p).$$

Now let $k > p$. Then for all of the vertices of the graph we have $p-i+1 \le t \le p+i$. So by using Lemma *1,* we have

$$d_x^2(k) = d_x^2(0) + (d_x^2(1) - d_x^2(0)) + \ldots + (d_x^2(p) - d_x^2(p-1)) + \ldots + (d_x^2(k) - d_x^2(k-1))$$
$$= d_x^2(p) + \sum_{i=p+1}^{k}\Big(\sum_{r=0}^{p}(8(2i+r)-12) + \sum_{r=1}^{p-1}(8(2i+r)-12)\Big)$$
$$= \frac{2}{3}(24pk^2 + 12(p^2-p)k + 2p^3 - 3k^2 + 4p).$$

This completes the proof.

In two pervious Lemmas we compute the summation of square distances between vertices $x_{0p}$ and $y_{0p}$ and vertices of the graph which placed in $k$ rows bellow of those vertices. By using symmetry of graph the obtained results can be used for computation the summation of square distances between vertex $x_{kt}$ (or $y_{kt}$ ) and vertices of graph placed in $k$ rows bellow of $x_{kt}$ ( or $y_{kt}$ ) respectively for $1 \le k < \frac{q}{2}$ and $0 \le t < p$. Also we can use of these results for computation the summation of square distances between vertex $x_{kt}$ (or $y_{kt}$) and vertices of graph placed in $k$ rows above of the vertex $x_{kt}$ (or $y_{kt}$). Now we can compute the hyper Wiener index of the graph.

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

$$WW(G) = \begin{cases} \frac{p^2}{3}\Big(-\frac{89}{5}p^4 + (12q - \frac{153}{2})p^3 + (4q^2 + 16q - 121)p^2 + \\ (8q^3 + 18q^2 - 8q - \frac{189}{2})p + 4q^2(q^2+6q+3) - q - \frac{161}{5}\Big), \quad if \quad q \le p \\ \frac{p^2}{3}\Big(-\frac{178}{5}p^4 + (24q - 151)p^3 + 2(4q^2 + 12q - 121)p^2 + \\ 16q^3 + 24q^2 - 16q - 191)p + 8q^2(2q^2+4q+3) + 10q - \frac{322}{5}\Big), \quad if \quad q > p. \end{cases}$$

Proof: At First we compute the expression $\sum_{\{i,j\}\subseteq V(G)} d^2(i,j)$ as follows:

$$\sum_{j\in V(G)} d^2(x_{kt},j) = \sum_{k=0}^{\frac{q}{2}-2} d_x^2(k) + \sum_{k=1}^{\frac{q}{2}-1} d_y^2(k) - d_x^2(0).$$

The last equation can be used for all of the *4p* vertices which placed in *k*th row of the graph. So

$$\sum_{\{i,j\}\subseteq V(G)} d^2(i,j) = \frac{1}{2}\sum_{i,j\in V(G)} d^2(i,j) = 2p\left(\sum_{k=0}^{\frac{q}{2}-2} d_x^2(k) + \sum_{k=1}^{\frac{q}{2}-1} d_y^2(k) - d_x^2(0)\right).$$

Therefore $W^2 = \sum_{\{i,j\}\subseteq V(G)} d^2(i,j)$ can be computed by using Lemma *3* as follow:

$$W^2 = \begin{cases} \dfrac{pq^2}{6}[3q^3 + 4pq^2 + (24p^2 - 12)q + 16p(4p^2 + 1)] & if \quad q \le p \\ \dfrac{p^2q}{3}[8q^3 + 12pq^2 + 8(p^2 + 1)q + 24p(p^2 - 1)] & if \quad q > p. \end{cases}$$

The proof is completed by replacing $W^2$, (2) and (3) in (1).

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