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Computing the Wiener Index of a $TUC_4C_8(S)$ Nanotorus

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Abstract

The Wiener index is a graphical invariant that has found extensive application in chemistry. It is defined as $W(G) = 1/2\sum_{\{x,y\}\subseteq V(G)}d(x,y)$, where V(G) is the set of all vertices of G and for $x,y \in V(G)$, d(x,y) denotes the length of a minimal path between x and y. In this paper an algorithm for computing the distance matrix of a $TUC_4C_8(R)$ nanotorus T = T[m,n] is given. Using this matrix, the following expression for the Wiener index of T is obtained,

$$W(T) = \begin{cases} \frac{nm^2}{6}(6n^2+3nm+m^2-4) & n\le m \\ \frac{mn^2}{6}(6m^2+3mn+n^2-4) & m<n \end{cases}.$$

1. Introduction

Let G = (V,E) be a connected, simple, undirected graph of order n; for each pair u; v of vertices of G, the distance d(u,v) is defined to be the number of edges in a shortest path from u to v. In 1947 Harold Wiener[1] introduced the quantity W(G) as the sum of distances between all pairs of vertices in the molecular graph G of an alkane, with the evident aim to provide a measure of the compactness of the respective hydrocarbon molecule. About 1948, Wiener published a whole series of papers showing that there are excellent correlations between W = W(G) and a variety of physico−chemical properties of organic compounds. Next Hosoya[2] named such graph invariants, topological index. In fact, topological indices are numerical descriptors that are derived

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from molecular graphs of chemical compounds. Such indices based on the distances in a graph are widely used for establishing relationships between the structure of molecules and their physico-chemical properties. We encourage the reader to consult the special issues of MATCH Communication in Mathematics and in Computer Chemistry[3], Discrete Applied Mathematics[4] and Refs. [5–7], for information on results on the Wiener index, the chemical meaning of the index and its history.

In a series of papers, Diudea and co-authors[8-13] studied the structure and topological indices of some chemical graphs related to nanostructures. In particular, the Wiener indices of some nanotubes are computed. The present authors[14,15] computed the Wiener index of polyhex and $TUC_4C_8(R)$ nanotori. We Proved that:

Theorem 1 ([14]). Suppose T = T[p,q] is a polyhex nanotorus. Then we have:

$$W(T) = \begin{cases} \frac{pq^2}{24}(6p^2 + q^2 - 4) & q < p \\ \frac{p^2q}{24}(3q^2 + 3pq + p^2 - 4) & q \geq p \end{cases}.$$

Theorem 2 ([15]). Suppose T = T[p,q] is a $TUC_4C_8(R)$ nanotorus. Then we have:

$$W(T) = \begin{cases} (2m/3)\left(m^2 - 1\right) + mn\left(m + 3n\right) - k_1 & \text{if} \quad m < n \\ (2n/3)\left(n^2 - 1\right) + mn\left(3m + n\right) - k_2 & \text{if} \quad m > n \\ (n/3)\left(14n^2 - k_3\right) & \text{if} \quad m = n \end{cases},$$

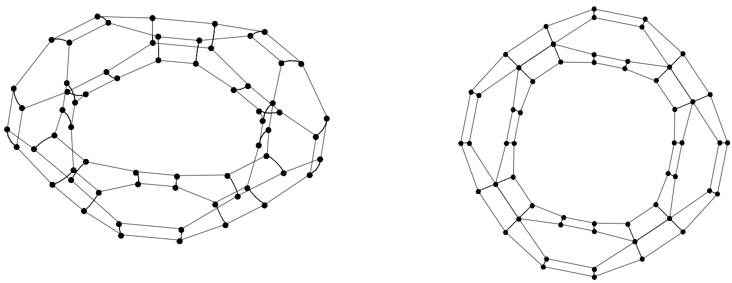
in which $k_1 = \begin{cases} 0 & \text{if} \quad 2|n \ \& \ 2|m \\ n-m & \text{if} \quad 2|n \ \& \ 2\nmid m \\ m & \text{if} \quad 2\nmid n \ \& \ 2|m \\ n & \text{if} \quad 2\nmid n \ \& \ 2\nmid m \end{cases}$, $k_2 = \begin{cases} 0 & \text{if} \quad 2|m \\ m & \text{if} \quad 2\nmid m \end{cases}$, $k_3 = \begin{cases} 2 & \text{if} \quad 2|n \\ 5 & \text{if} \quad 2\nmid n \end{cases}$, and, "|" denotes the divisibility relation.

In Refs. [16–19] another topological index of nanotorus, PI index, are also computed. We encourage the reader to consult these papers for background material as well as basic computational techniques.

The goal of this paper is to continue this program to compute the Wiener index of a $TUC_4C_8(S)$ nanotorus. To do this, we assume that T = T[m,n] denotes an arbitrary $TUC_4C_8(S)$ nanotorus in terms of its circumference (m) and its length (n), see Figure 1. The main result of this paper is as follows:

Theorem. The Wiener index of a $TUC_4C_8(S)$ nanotorus, Figure 1, is as follows:

$$W(T) = \begin{cases} \frac{nm^2}{6}(6m^2+3nm+n^2-4) & n \leq m \\ \frac{mn^2}{6}(6n^2+3mn+m^2-4) & m < n \end{cases}$$



(a) (b)

Figure 1. An $TUC_4C_8(S)$ Torus (a) Side view (b) Top view.

Throughout this paper our notation is standard and taken mainly from [20,21].

2. Main Result

In this section we derive an exact formula for the Wiener index of a $T(m,n) = TUC_4C_8(S)$ nanotorus, in which m and n are two times of the number octagons in every row and column, respectively, Figure 2.

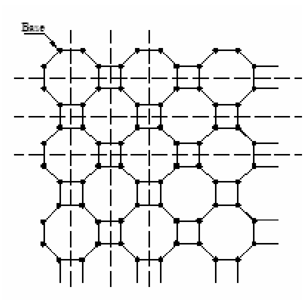


Figure 2. Fragment of $TUC_4C_8(S)$ Nanotorus with m = n =3.

To compute the Wiener index of T = T[m,n], we first calculate the molecular symmetry group of T. Let D_{2n} be the dihedral group of order 2n, $n \geq 3$. This group can be presented by $D_{2n} = \langle x , y \mid x^n = y^2 = 1, y^{-1}xy = x^{-1}\rangle$.

Lemma 1. *The rotation group of T[m,n] is isomorphic to D_n.*

Proof. Suppose $V_1, V_2, \ldots, V_{n/2}$ are octagons of the first column of 2-dimensional lattice of T and $\sigma = (1,2,\ldots,n/2)$. Then σ determines a permutation of the molecular symmetry group G of T. Moreover, the reflection about the horizontal plane will be another element φ of the group G. Now it is easy to see that the group G is generated by σ and φ. This group satisfies the relations $\sigma^n = e$, $\varphi^2 = e$ and $\sigma^{-1}\varphi\sigma = \sigma^{-1}$ and so it is a dihedral group of order n, as desired. ■

From now on, we suppose $X_{m,n} = [x_{i,j}]$ in which $x_{i,j}$ is the sum of distances between vertices of $(i,j)^{th}$ oblique edge of the 2-dimensional lattice of T from the base vertex b, Figure 2. Obviously, $x_{1,1} = 1$. Since $S_b = \sum_{i,j} x_{i,j}$, we must find an algorithm for computing $X_{m,n}$.

Lemma 2. *If $m > n/2$ then $x_{i,j} = x_{m-i+1,j} + 2$.*

Proof. The proof is straightforward. ■

In the following theorem we compute the Wiener index of T[n,n].

Theorem. *If T = T[m,n] is a $TUC_4C_8(S)$ nanotorus then the Wiener index of T is as follows:*

$$W(T) = \begin{cases} \frac{nm^2}{6}(6m^2+3nm+n^2-4) & n \leq m \\ \frac{mn^2}{6}(6n^2+3mn+m^2-4) & m < n \end{cases}.$$

Proof. We first notice that the graph T = T[m,n] has exactly 2mn vertices. To compute the Wiener index of this graph, we first consider a base vertex b for the 2-dimensional lattice of T, Figure 2, and compute $S_b = \sum_{x \in V(G)} d(x,b)$. It is clear that the value of S_b is independent from the base vertex b. Therefore $W(T) = mnS_b$ and so it is enough to compute S_b. To do this, we define a matrix $X_{m,n} = [x_{i,j}]$ in which $x_{i,j}$ is the sum of distances between vertices of $(i,j)^{th}$ oblique edge of the 2-dimensional lattice of T from the base vertex b. Obviously, $x_{1,1} = 1$. Since $S_b = \sum_{i,j} x_{i,j}$, we must find an algorithm for computing $X_{m,n}$. We first consider the case that m = n. Obviously, the 2−dimensional lattice of T[n−2,n−2] is a part of the 2−dimensional lattice of T[n,n]. So we can proceed with induction on n. Suppose $X_{n,n} = [x_{i,j}]$ and $X_{n-2,n-2} = [a_{i,j}]$. To calculate the values of the matrix $X_{n,n}$ in the $(n/2)^{th}$ and $(1+n/2)^{th}$ rows, as well as $(1+n/2)^{th}$ and $(2+n/2)^{th}$ column of the matrix $X_{n,n}$, we use the 2-dimensional lattice of T. We have:

$$x_{\frac{n}{2}+1,j} = \begin{cases} 2(n+j)-3 & j \le \frac{n}{2}+1 \\ 2(2n-j)+1 & j > \frac{n}{2}+1 \end{cases} ; \qquad x_{\frac{n}{2},j} = x_{\frac{n}{2}+1,j} - 2,$$

$$x_{i,\frac{n}{2}+1} = \begin{cases} 2(n+i)-3 & i \le \frac{n}{2}+1 \\ 2(2n-i)+1 & i > \frac{n}{2}+1 \end{cases} ; \qquad x_{i,\frac{n}{2}+2} = x_{i,\frac{n}{2}+1} - 2.$$

For other entries of $X_{n,n}$, we have:

$$x_{i,j} = \begin{cases} a_{i,j} & i \le \frac{n}{2}-1 \ , \ j \le \frac{n}{2} \\ a_{i-2,j} & i > \frac{n}{2}+1 \ , \ j \le \frac{n}{2} \end{cases} ; \quad x_{i,j} = \begin{cases} a_{i,j-2} & i \le \frac{n}{2}-1 \ , \ j > \frac{n}{2}+2 \\ a_{i-2,j-2} & i > \frac{n}{2}+1 \ , \ j > \frac{n}{2}+2 \end{cases} .$$

Therefore, $X_{n,n}$ and $X_{n-2,n-2}$ are essentially different only in the two rows and columns, as above. If V is the (n/2)−th row of the matrix $X_{n,n}$ then by symmetries of a nanotorus and above equations, V + [2 2 … 2] is the (n/2+1)−th row of this matrix, as well as if W is the $(1+n/2)^{th}$ column of $X_{n,n}$ then W − $[2\ 2\ \ldots\ 2]^t$ is its $(1+n/2)^{th}$ column. Thus we can find a recurrence relation for definition of $X_{n,n}$. By solving this simple equation, we have $W(T[n,n]) = n^3/3(5n^2-2)$.

We now assume that n ≠ m, say n < m. In this case by computing $X_{m,m}$ as above, and omitting some of the columns of this matrix, we can calculate $X_{m,n}$. In other words, $X_{m,n}$ contains the first and last (n/2+1) and (n/2−1) columns of the matrix $X_{m,m}$. Suppose $X_{m,m} = [a_{ij}]$ and $X_{m,n} = [x_{ij}]$ then we have:

$$x_{i,j} = \begin{cases} a_{i,j} & j \le \frac{n}{2}+1 \\ a_{i,m-n+j} & j > \frac{n}{2}+1 \end{cases} .$$

Suppose S_I is the sum of omitted entries. Then using a simple calculation one can see that $S_I = (m–n)/12(7m^2 + 4mn + n^2 – 4)$. Therefore, $W(T[m,n]) = W(T[m,m]) – mnS_I = (m^2n/6)(6m^2 + 3nm + n^2 – 4)$.

We now assume that $m < n$, $X_{n,n} = [a_{ij}]$ and $X_{m,n} = [x_{ij}]$. Then $X_{m,n}$ can be constructed from $X_{n,n}$ by considering the first and last m/2–th rows and so,

$$x_{i,j} = \begin{cases} a_{i,j} & i \le \dfrac{m}{2} \\ a_{n-m+i,j} & i > \dfrac{m}{2} \end{cases}.$$

If S_{II} denotes the sum of omitted entries then a simple calculation shows that $S_{II} = (m – n)/12(7m^2 + 4mn + n^2 – 4)$. Therefore, $W(T[m,n]) = W(T[n,n]) – mnS_{II} = (m^2n/6)(6m2 + 3nm + n^2 – 4)$. This Completes the proof. ■

We now present another method to compute the matrix $X_{n,n} = [x_{ij}]$, n is even. Define two $n/2 \times n$ matrices $A = [a_{ij}]$ and $B = [b_{ij}]$, $a_{11} = 1$, as follows:

$$a_{1,j} = \begin{cases} 4j-5 & 2 \le j \le (n/2)+1 \\ 4(n-j)+5 & j > (n/2)+1 \end{cases};\ a_{i,j} = a_{i-1,j} + 2\ \ \forall i > 1$$

$$b_{\frac{n}{2},j} = \begin{cases} 2(n+j)-5 & j \le \dfrac{n}{2}+1 \\ 2(2n-j)-1 & j > \dfrac{n}{2}+1 \end{cases};\ b_{i,j} = b_{i+1,j} - 4\ \ \forall i < n$$

Using similar argument as Theorem, we can prove in the first n/2 rows of the matrix $X_{n,n}$, $x_{ij} = \mathrm{Max}\{a_{ij}, b_{ij}\}$. Moreover, if $i > n/2$ then $x_{i,j} = x_{n-i+1,j} + 2$. In what follows, we calculate $X_{18,18}$ from $X_{16,16}$ by our theorem, as follows:

$$X_{16,16} = \begin{bmatrix}
1 & 3 & 7 & 11 & 15 & 19 & 23 & 27 & 31 & 29 & 25 & 21 & 17 & 13 & 9 & 5 \\
5 & 7 & 9 & 13 & 17 & 21 & 25 & 29 & 33 & 31 & 27 & 23 & 19 & 15 & 11 & 7 \\
9 & 11 & 13 & 15 & 19 & 23 & 27 & 31 & 35 & 33 & 29 & 25 & 21 & 17 & 13 & 11 \\
13 & 15 & 17 & 19 & 21 & 25 & 29 & 33 & 37 & 35 & 31 & 27 & 23 & 19 & 17 & 15 \\
17 & 19 & 21 & 23 & 25 & 27 & 31 & 35 & 39 & 37 & 33 & 29 & 25 & 23 & 21 & 19 \\
21 & 23 & 25 & 27 & 29 & 31 & 33 & 37 & 41 & 39 & 35 & 31 & 29 & 27 & 25 & 23 \\
25 & 27 & 29 & 31 & 33 & 35 & 37 & 39 & 43 & 41 & 37 & 35 & 33 & 31 & 29 & 27 \\
29 & 31 & 33 & 35 & 37 & 39 & 41 & 43 & 45 & 43 & 41 & 39 & 37 & 35 & 33 & 31 \\
31 & 33 & 35 & 37 & 39 & 41 & 43 & 45 & 47 & 45 & 43 & 41 & 39 & 37 & 35 & 33 \\
27 & 29 & 31 & 33 & 35 & 37 & 39 & 41 & 45 & 43 & 39 & 37 & 35 & 33 & 31 & 29 \\
23 & 25 & 27 & 29 & 31 & 33 & 35 & 39 & 43 & 41 & 37 & 33 & 31 & 29 & 27 & 25 \\
19 & 21 & 23 & 25 & 27 & 29 & 33 & 37 & 41 & 39 & 35 & 31 & 27 & 25 & 23 & 21 \\
15 & 17 & 19 & 21 & 23 & 27 & 31 & 35 & 39 & 37 & 33 & 29 & 25 & 21 & 19 & 17 \\
11 & 13 & 15 & 17 & 21 & 25 & 29 & 33 & 37 & 35 & 31 & 27 & 23 & 19 & 15 & 13 \\
7 & 9 & 11 & 15 & 19 & 23 & 27 & 31 & 35 & 33 & 29 & 25 & 21 & 17 & 13 & 9 \\
3 & 5 & 9 & 13 & 17 & 21 & 25 & 29 & 33 & 31 & 27 & 23 & 19 & 15 & 11 & 7
\end{bmatrix}$$

$$X_{18,18} = \begin{bmatrix}
1 & 3 & 7 & 11 & 15 & 19 & 23 & 27 & 31 & 35 & 33 & 29 & 25 & 21 & 17 & 13 & 9 & 5 \\
5 & 7 & 9 & 13 & 17 & 21 & 25 & 29 & 33 & 37 & 35 & 31 & 27 & 23 & 19 & 15 & 11 & 7 \\
9 & 11 & 13 & 15 & 19 & 23 & 27 & 31 & 35 & 39 & 37 & 33 & 29 & 25 & 21 & 17 & 13 & 11 \\
13 & 15 & 17 & 19 & 21 & 25 & 29 & 33 & 37 & 41 & 39 & 35 & 31 & 27 & 23 & 19 & 17 & 15 \\
17 & 19 & 21 & 23 & 25 & 27 & 31 & 35 & 39 & 43 & 41 & 37 & 33 & 29 & 25 & 23 & 21 & 19 \\
21 & 23 & 25 & 27 & 29 & 31 & 33 & 37 & 41 & 45 & 43 & 39 & 35 & 31 & 29 & 27 & 25 & 23 \\
25 & 27 & 29 & 31 & 33 & 35 & 37 & 39 & 43 & 47 & 45 & 41 & 37 & 35 & 33 & 31 & 29 & 27 \\
29 & 31 & 33 & 35 & 37 & 39 & 41 & 43 & 45 & 49 & 47 & 43 & 41 & 39 & 37 & 35 & 33 & 31 \\
33 & 35 & 37 & 39 & 41 & 43 & 45 & 47 & 49 & 51 & 49 & 47 & 45 & 43 & 41 & 39 & 37 & 35 \\
35 & 37 & 39 & 41 & 43 & 45 & 47 & 49 & 51 & 53 & 51 & 49 & 47 & 45 & 43 & 41 & 39 & 37 \\
31 & 33 & 35 & 37 & 39 & 41 & 43 & 45 & 47 & 51 & 49 & 45 & 43 & 41 & 39 & 37 & 35 & 33 \\
27 & 29 & 31 & 33 & 35 & 37 & 39 & 41 & 45 & 49 & 47 & 43 & 39 & 37 & 35 & 33 & 31 & 29 \\
23 & 25 & 27 & 29 & 31 & 33 & 35 & 39 & 43 & 47 & 45 & 41 & 37 & 33 & 31 & 29 & 27 & 25 \\
19 & 21 & 23 & 25 & 27 & 29 & 33 & 37 & 41 & 45 & 43 & 39 & 35 & 31 & 27 & 25 & 23 & 21 \\
15 & 17 & 19 & 21 & 23 & 27 & 31 & 35 & 39 & 43 & 41 & 37 & 33 & 29 & 25 & 21 & 19 & 17 \\
11 & 13 & 15 & 17 & 21 & 25 & 29 & 33 & 37 & 41 & 39 & 35 & 31 & 27 & 23 & 19 & 15 & 13 \\
7 & 9 & 11 & 15 & 19 & 23 & 27 & 31 & 35 & 39 & 37 & 33 & 29 & 25 & 21 & 17 & 13 & 9 \\
3 & 5 & 9 & 13 & 17 & 21 & 25 & 29 & 33 & 37 & 35 & 31 & 27 & 23 & 19 & 15 & 11 & 7
\end{bmatrix}$$

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