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3-Dimensional Distance Matrix of a $TC_4C_8(R)$ Nanotorus

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Abstract

A 3-dimensional matrix method for computing the number of vertices with a given distance d from a fixed vertex b in a $TC_4C_8(R)$ nanotorus is presented. As a special case, the Wiener and hyper-Wiener indices of this molecular graph are computed.

1. Introduction

Nanostructured materials have received a lot of attention because of their novel properties, which differ from those of the bulk materials. One-dimensional materials are an important category of nanostructured materials and have been widely researched yielding various special structures like nanotubes and nanotorus. The materials of these nano–materials can be prepared from carbon.

Let G be a graph. A topological index Top(G) is a number related to the graph G invariant under all elements of Aut(G), where Aut(G) denotes the set of all automorphisms of the graph G. The Wiener index is one of the most studied topological indices, both from a theoretical point of view and applications [1]. It is equal to the sum of distances between all pairs of vertices of the respective graph, see for details [2,3]. The hyper–Wiener index of acyclic graphs was introduced by Milan Randić in 1993. Then Klein et al. [4], generalized Randić's definition for all connected graphs, as a generalization of the Wiener index. It is defined as $WW(G) = 1/2W(G) + 1/2\sum_{\{u,v\}\subseteq V(G)}d(u,v)^2$, where $d^2(u, v) = d(u,v)^2$ and d(u,v) is the length of a minimal path connecting u and v.

The present authors [5–13] studied the distance matrix of the armchair and zig-zag polyhex nanotubes, $TUC_4C_8(R/S)$ nanotubes, polyhex nanotorus and $TC_4C_8(R/S)$

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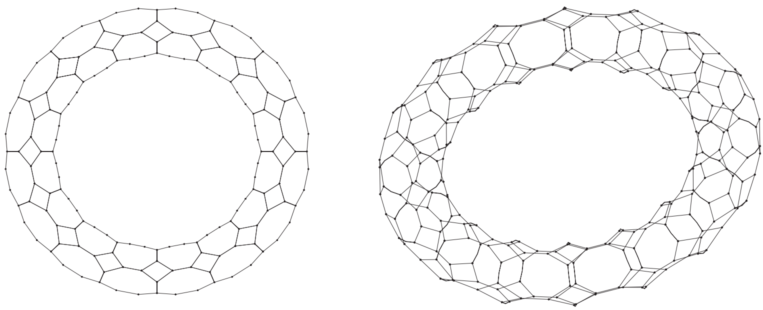
nanotori. As a special case, the Wiener index of these molecular graphs was calculated. In this paper, we consider the molecular graph of $TC_4C_8(R)$ nanotorus and compute the number of its vertices with a given distance d from a fixed vertex b. Using our calculations, one can compute too many distance based topological indices of an $TC_4C_8(R)$ nanotorus. As special cases, the Wiener and hyper-Wiener indices of these nano-materials are concluded. Our motivation for this study come from the pioneering work of Diudea [14–17]. We encourage the reader to consult papers [18–21] for background materials, as well as basic computational techniques.

For a permutation σ on n objects, the corresponding permutation matrix is an $n \times n$ matrix P_σ given by $P_\sigma = [x_{ij}]$, $x_{ij} = 1$ if $i = \sigma(j)$ and 0 otherwise. It is easy to see that $P_\sigma P_\tau = P_{\sigma\tau}$, for any two permutations σ and τ on n objects, and permutational matrices are orthogonal. Our notation is standard and taken from the standard book of graph theory. Throughout this paper T = T[m,n] denotes an arbitrary $TC_4C_8(R)$ nanotorus in terms of the number of rhombs in a fixed row (m) and column (n), see Figure 1.



(b)

Figure 1: An $TC_4C_8(R)$ tori (a) Top view (b) Side view.

2. Main Results and Discussion

It is clear that the molecular graph T has exactly 4mn vertices and 6mn edges. Choose a base vertex b from the 2–dimensional lattice of T and assume that x_{ij} is the sum of all distances between b and vertices of the $(i,j)^{th}$ rhomb of T, Figure 2. Define $X_{m,n} = [x_{ij}]_{m\times n}$. Suppose $\mathbf{N}_i^{(m)}$ denotes the number of entries of $X_{m,m}$ equal to i. Notice that $x_{1,1} = 3$, when m = 1; and $x_{1,1} = 4$, otherwise. In [8], the present authors proved an algorithm for computing the matrix $X_{m,n}$. In this work, we will find a closed formula for $\mathbf{N}_i^{(m)}$. As an immediate consequence of this formula, the Wiener and hyper-Wiener indices of T are calculated.

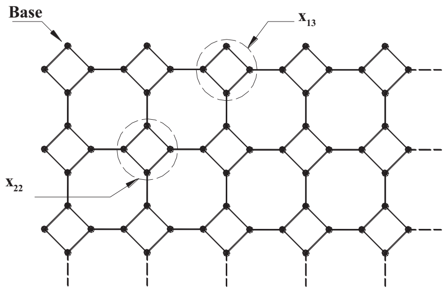


Figure 2. 2–Dimensional Lattice of $TUC_4C_8(R)$ Nanotube.

It is an easy fact that $|V(T)| = 4mn$ and $|E(T)| = 6mn$. Suppose r_{ij} denotes the $(i,j)^{th}$ rhomb in the 2-dimensional representation of T, Figure 2. In Figure 2, if we choose the down vertex of r_{11} as base then the corresponding matrix is denoted by $F_{m,n}$. We also define the matrices $G_{m,n}$ and $H_{m,n}$, when the left side and right side vertices of r_{11} are considered as the base vertex, respectively. From Figure 2, one can see that $F_{m,n}$ is obtained from $X_{m,n}$ by a permutation on vertices of T. So, these matrices constructed from the same set of entries. On the other hand, all entries of $X_{m,n}$ are functions of m and n. If we change the base vertex b by left (right) side vertex of r_{11}, then one half (2mn) of entries of $X_{m,n}$ are again entries of $G_{m,n}$ ($H_{m,n}$) and for remaining 2mn vertices, it is enough to interchange m and n in $X_{n,m}$.

We first assume that m = n. From our calculations given in [8], one can see that when m is odd,

$$N_i^{(m)} = \begin{cases} 1 & i = 0 \\ 3i - \left\lceil \frac{i+1}{3} \right\rceil & 1 \le i \le \frac{3m-1}{2} \\ 8(2m - i) & \frac{3m+1}{2} \le i \le 2m - 1 \end{cases} \tag{1}$$

and when m is even, we have:

$$N_i^{(m)} = \begin{cases} 1 & i = 0 \\ 3i - \left\lceil \frac{i+1}{3} \right\rceil & 1 \le i \le \frac{3m}{2} \\ 4m - 3 & i = \frac{3m}{2} \\ 8(2m - i) & \frac{3m}{2} + 1 \le i \le 2m \\ 2 & i = 2m \end{cases} \tag{2}$$

The most important part of our problem is the cases that m < n and m > n. For these cases we first introduce two 3-dimensional matrices $L = [L_{i,j,k}]$ and $M = [M_{i,j,k}]$. To define, we just determine the non-zero entries of these matrices as follows:

$$L_{1,1,1} = L_{1,1,2} = L_{2,1,1} = L_{2,1,3} = 2;\ L_{2,1,2} = 4 \tag{3}$$

If j is odd then we define:

$$L_{1,j,k} = L_{1,j-1,k} \text{ and } L_{1,j,1/2(3j-1)} = L_{1,j,1/2(3j+1)} = 2,\ k \le 3/2(j-1) \tag{4}$$

and when j is even,

$$L_{1,j,k} = L_{1,j-1,k} \text{ and } L_{1,j,3/2j-1} = 4,\ L_{1,j,3/2j} = 2,\ k \le 3/2(j-1) \tag{5}$$

The equations (3–5) define the entries of the first level of 3–dimensional matrix L. To define the second level, again two cases that j is odd and even are considered. Suppose j is odd. Then we define:

$$L_{2,j,k} = L_{2,j-1,k} \text{ and } L_{2,j,1/2(3j-1)} = L_{2,j,1/2(3j+1)} = 6,\ k \le 3/2(j-1) \tag{6}$$

and for even j,

$$L_{2,j,k} = L_{2,j-1,k},\ L_{2,j,3/2j} = L_{2,j,3/2j+1} = 4 \text{ and } L_{2,j,3/2j+2} = 2,\ k \le 3/2j-1 \tag{7}$$

The equations (3,6,7) complete our definition for the second level of L. We are now ready to define the matrix L completely. When i is odd or even, $L_{i,j,k}$ is defined as follows:

$$L_{i,j,k} = \begin{cases} L_{i-2,j,k} & k < \frac{i+1}{2} \\ L_{i-2,j,k} + 2L_{1,j,k-\frac{i-1}{2}} & k \ge \frac{i+1}{2} \end{cases} \text{ and } L_{i,j,k} = \begin{cases} L_{i-2,j,k} & k < \frac{i}{2} \\ L_{i-2,j,k} + L_{2,j,k-\frac{i}{2}+1} & k \ge \frac{i}{2} \end{cases}$$

These equations together with equations (3–7) defined completely the matrix L.

Next, we describe our second 3-dimensional matrix M. To do this, define two ordinary matrices $M^1 = [M^1_{i,j}]$ and $M^2 = [M^2_{i,j}]$ as follows:

$$M^1_{1,1} = 3, M^1_{1,2} = M^1_{2,1} = 1, M^1_{2,2} = 4, M^1_{2,3} = 3, \tag{8}$$

$$M^2_{1,1} = 1, M^2_{1,2} = M^2_{2,1} = 3, M^2_{2,2} = 4, M^2_{2,3} = 1 \tag{9}$$

$$M^1_{i,j} = \begin{cases} M^1_{i-2,j} & 2 \nmid i \,\&\, j \le \frac{i-1}{2} \\ M^1_{i-2,j} + 2M^1_{1,j-\frac{i-1}{2}} & 2 \nmid i \,\&\, j > \frac{i-1}{2} \\ M^1_{i-2,j} & 2 \mid i \,\&\, j < \frac{i}{2} \\ M^1_{i-2,j} + M^1_{1,j-\frac{i}{2}+1} & 2 \mid i \,\&\, j \ge \frac{i}{2} \end{cases} \tag{10}$$

$$M^2_{i,j} = \begin{cases} M^2_{i-2,j} & 2 \nmid i \,\&\, j \le \frac{i-1}{2} \\ M^2_{i-2,j} + 2M^2_{1,j-\frac{i-1}{2}} & 2 \nmid i \,\&\, j > \frac{i-1}{2} \\ M^2_{i-2,j} & 2 \mid i \,\&\, j < \frac{i}{2} \\ M^2_{i-2,j} + M^2_{1,j-\frac{i}{2}+1} & 2 \mid i \,\&\, j \ge \frac{i}{2} \end{cases} \tag{11}$$

We now apply equations (9–11) to define 3–dimensional matrix M. To do this, we use the matrix M^1 and M^2 defined above. It is enough to define all non-zero entries of the matrix M. Define $M_{i,1,k} = M^1_{i,k}$ and

$$M_{i,j,k} = \begin{cases} M_{i,j-1,k} & 2 \nmid j \,\&\, k \le \frac{3}{2}(j-1) \\ M_{i,j-1,k} + M^1_{i,k-\frac{3}{2}(j-1)} & 2 \nmid j \,\&\, \frac{3}{2}(j-1) \\ M_{i,j-1,k} & 2 \mid j \,\&\, k \le \frac{3}{2}j - 1 - \left(i - 2\left[\frac{i}{2}\right]\right) \\ M_{i,j-1,k} + M^2_{i,k-\frac{3}{2}j-1-\left(i-2\left[\frac{i}{2}\right]\right)} & 2 \mid i \,\&\, k > \frac{3}{2}j - 1 - \left(i - 2\left[\frac{i}{2}\right]\right) \end{cases} \tag{12}$$

We are now ready to state our main result as follows:

Theorem. Suppose $\mathbf{N_i^{(m,n)}}$ denotes the number of entries of $X_{m,n}$ equal to i. Then

$$N_i^{(m,n)} = \begin{cases} N_i^{(m)} & m < n \ \& \ 2 \nmid m \ \& \ i \le \frac{3m-1}{2} \\ N_i^{(m)} + L_{m,n-m,i-\frac{3m-1}{2}} & m < n \ \& \ 2 \nmid m \ \& \ \frac{3m-1}{2} < i \le \frac{m-1}{2} + \left\lceil \frac{3n}{2} \right\rceil \\ N_i^{(m)} & m < n \ \& \ 2|m \ \& \ i < \frac{3m}{2} \\ N_i^{(m)} + L_{m,n-m,i-\frac{3m}{2}+1} & m < n \ \& \ 2|m \ \& \ \frac{3m}{2} \le i \le \frac{m}{2} + \left\lceil \frac{3n}{2} \right\rceil \\ N_i^{(n)} & m > n \ \& \ 2 \nmid m \ \& \ i \le \frac{3n-1}{2} \\ N_i^{(n)} + M_{n,m-n,i-\frac{3n-1}{2}} & m > n \ \& \ 2 \nmid m \ \& \ \frac{3n-1}{2} < i \le \frac{n-1}{2} + \left\lceil \frac{3m}{2} \right\rceil \\ N_i^{(n)} & m > n \ \& \ 2|m \ \& \ i < \frac{3n}{2} \\ N_i^{(n)} + M_{n,m-n,i-\frac{3n}{2}+1} & m > n \ \& \ 2|m \ \& \ \frac{3n}{2} \le i \le \frac{n}{2} + \left\lceil \frac{3m}{2} \right\rceil \end{cases}$$

Corollary. If m = n then $W(T) = 2/3m^3(14m^2 - k_1)$ and $WW(T) = m^3/3(37m^3+28m^2 + k_2m - 2k_1)$, where $k_1 = \begin{cases} 2 & 2|m \\ 5 & 2 \nmid m \end{cases}$ and $k_2 = \begin{cases} 2 & 2|m \\ -19 & 2 \nmid m \end{cases}$.

Set O ={(5,5), (6,6), (8,8), (5,8), (6,8), (8,5), (8,6)}. In the end of this paper, the number of vertices of a given distance are computed, for all elements of the set O.

Table 1. The Values of $N_i^{(m,n)}$, when (m,n) $\in$ O.

		i	**0**	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**
m	**n**																		
5	**5**		1	3	5	8	11	13	16	19	16	8	0	0	0	0	0	0	0
6	**6**		1	3	5	8	11	13	16	19	21	21	16	8	2	0	0	0	0
8	**8**		1	3	5	8	11	13	16	19	21	24	27	29	29	24	16	8	2
8	**5**	N_i	1	3	5	8	11	13	16	19	19	16	13	13	13	8	2	0	0
5	**8**		1	3	5	8	11	13	16	19	18	16	14	14	10	8	4	0	0
6	**8**		1	3	5	8	11	13	16	19	21	23	22	18	14	10	6	2	0
8	**6**		1	3	5	8	11	13	16	19	21	22	21	19	16	11	5	1	0

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