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On the Distance-Based Topological Indices of Polyhex Nanotori

Majid Arezoomand[a] and Bijan Taeri[b,•]

[a]Islamic Azad University, Majlesi Branch, Isfahan, Iran

[b]Department of Mathematical Sciences, Isfahan University of Technology, Isfahan 86154-83111, Iran

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Abstract

In this paper we compute some distance-based topological indices of polyhex nanotori using a mathematical model given by Cotfas (An alternate mathematical model for single-wall carbon nanotubes, J. Geom. Phys. **55** (2005) 123-134).

1. Introduction

A topological index is a real number related to a graph of a molecule, which is structural. It does not depend on the labeling or pictorial representation of the graph. In recent years, there has been considerable interest in the general problem of determining topological indices of nanotubes and nanotori[1-6]. It has been established, for example, that the Wiener and hyper-Wiener indices of polyhex nanotubes and tori are computable from the molecular graph of these structures. Accordingly, some of the interest has been focused on computing topological indices of these nanostructures. Let *G* be an undirected connected graph without loops or multiple edges, with the vertex set *V(G)* and the edge set *E(G)*. The distance between two vertices *x* and *y* is denoted by *d(x,y)*. The Wiener index[7] *W(G)* of *G*, which is the oldest topological index, is a distance-based topological index and is defined as the sum of distances between all vertices of the graph:

$$W(G)=\sum_{\{u,v\}\subseteq V(G)} d(u,v).$$

•Corresponding Author (Email: b.taeri@cc.iut.ac.ir).

There are some other distance-based topological indices. The Hyper Wiener index[8] *WW(G)* of *G* is defined as

$$WW(G) = \frac{1}{2}W(G) + \frac{1}{4}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2 \ .$$

The diameter *d* of a graph is the largest topological distance between any two vertices, i.e. the largest *d(u,v)* value in the distance matrix. Balaban and co-authors introduced the reverse Wiener index. They showed that starting from the distance matrix and subtracting from *d* each *d(u,v)* value, one obtains a new symmetrical matrix which, like the distance matrix, has zeroes on the main diagonal and, in addition, at least one pair of zeroes of the main diagonal corresponding to the diameter in the distance matrix. They obtained a general formula for reverse Wiener index of a graph *G* with *N* vertices and the diameter *d* as[9]

$$\Lambda(G) = \frac{1}{2}N(N-1)d - W(G) \ .$$

Let *u* and *v* be two adjacent vertices of the graph *G* and *e=uv* be the edge between them. The Balaban index of a molecular graph *G* is introduced by Balaban[10] as one of less degenerated topological indices. It calculate the average distance sum connectivity index according to the equation

$$J(G) = \frac{m}{\mu+1}\sum_{uv\in E(G)}[d(u)d(v)]^{-0.5}$$

where *m* is the number of edges in *G* and μ=*m*+*n*-*1* (*n* is the number of vertices of *G*) is the cyclomatic number of *G* and $d(u) = \sum_{v\in V(G)} d(u,v)$ is the distance sum of a vertex *u* of *G*.

In this paper, we introduce a new method to find distance-based topological indices of polyhex nanotorus. Our method is based on a mathematical model, given by Cotfas[11] for the honeycomb lattice. Let us recall briefly this model. Consider a honeycomb lattice as shown in Figure 1. Single wall nanotori may be described as a long rolled-up graphite sheet bent around to the form of torus. Let $e_0 = (2/\sqrt{6},0)$, $e_1 = (-1/\sqrt{6},1/\sqrt{2})$ and $e_2 = (-1/\sqrt{6},-1/\sqrt{2})$. Then there is a bijection

$$\psi : \ell \to L; \ \ (v_0, v_1, v_2) \mapsto v_0e_0 + v_1e_1 + v_2e_2$$

from the set $\ell = \{(v_0, v_1, v_2) \in Z^3 \mid v_0 + v_1 + v_2 \in \{0,1\}\}$ to the set L of all vertices of a honeycomb lattice (see Ref. [11]).

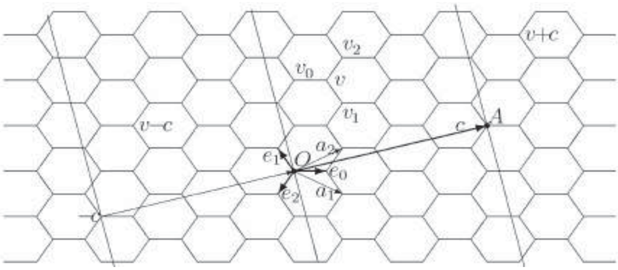

Figure 1. Honeycomb lattice and vectors e_0, e_1 and e_2.

2. Results and discussion

Throughout the paper $T := HC_6[p; q]$ denotes an arbitrary armchair polyhex nanotorus in terms of the circumference p and the length q. We notice that p and q must be even. We assume that a_{ij} denotes the (i,j)-entry of the two-dimensional lattice of T as shown in Figure 2.

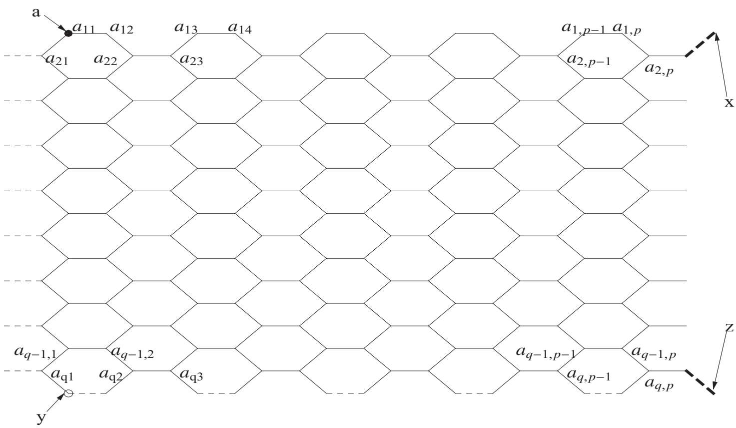

Figure 2. Two dimensional lattice for T=HC_6[10, 16].

We put the origin O at a_{11} and consider the vectors e_0, e_1 and e_2 as shown in Figures 1, 3. Let $a=a_{11}$, $b=a_{12}$, $c=a_{21}$ and $d=a_{22}$. It is easy to see that every point of T can be constructed by a translation of these points in two directions $w=-e_1+e_2$ and $v=2e_0-e_1-e_2$. In fact, from definitions of the vertices $a, b, c, d,$ the vectors v and w, and the geometry of the lattice, it is easy to see that the lattice points of T is the disjoint union of the sets A, B, C and D, where

$A = \{a+(i-1)/2w+(j-1)/2v \mid i,j \text{ are odd}\}$, $B = \{b+(i-1)/2w+(j/2-1)v \mid i \text{ is odd and } j \text{ is even}\}$

$C = \{c+(i/2-1)w+(j-1)/2v \mid i \text{ is even and j is odd}\}$, $D = \{d+(i/2-1)w+(j/2-1)v \mid i,j \text{ are even}\}$.

The points of *T* and their types are shown in Figure 3. By considering the coordinates of points *a,b,c,d* and the vectors *v,w* we can see that the following fundamental relation holds.

$$a_{ij}=\begin{cases} a_{ij}^0 & \text{if } i,j \text{ both even or both odd} \\ a_{ij}^1 & \text{otherwise} \end{cases} \quad (1)$$

where $a_{ij}^0=(j-1,\frac{2-i-j}{2},\frac{i-j}{2})$ and $a_{ij}^1=(j-1,\frac{3-i-j}{2},\frac{1+i-j}{2})$.

The mapping $f:\ell\times\ell\rightarrow\{0,1,2,3,\ldots\}$, $f(x,y)=\sum_{i=0}^{2}|x_i-y_i|$ is a distance function on ℓ and *f(x,y)* is the length of a shortest path between vertices *x* and *y* of the honeycomb lattice regarded as a graph[9]. Now we need to compute *d(a,a$_{ij}$)*, where a_{ij} is a point of T, 1≤i≤q, 1≤j≤p. According to the construction of the lattice we divide the lattice into four equal parts (these parts contain *a, x, y, z*, respectively, see Figure 2). If a_{ij} is in the first part, then $d(a,a_{ij})=f(a,a_{ij})$; if a_{ij} is in the second part, then $d(a,a_{ij})=f(x,a_{ij})$; if a_{ij} is in the third part, then $d(a,a_{ij})=f(y,a_{ij})$; and finally if a_{ij} is in the forth part, then $d(a,a_{ij})=f(z,a_{ij})$;. Therefore after rolling up the lattice and constructing the nanotorus *T*, the length of a shortest path between a and all vertices of *T* is given by

$$d(a,a_{ij})=\begin{cases} f(a,a_{ij}) & \text{if} \quad 1\le i\le q/2+1,\ 1\le j\le p/2+1 \\ f(x,a_{ij}) & \text{if} \quad 1\le i\le q/2+1,\ p/2+1\le j\le p \\ f(y,a_{ij}) & \text{if} \quad q/2+1\le i\le q,\ 1\le j\le p/2+1 \\ f(z,a_{ij}) & \text{if} \quad q/2+1\le i\le q,\ p/2+2\le j\le p \end{cases} \quad (2)$$

where *x=(p, -p/2, -p/2)*, *y=(0, -q/2, q/2)* and *z=(p, -(q+p)/2, (q-p)/2)*. We keep this notation throughout the paper. Using (2) we can compute some distance-based topological index of nanotori.

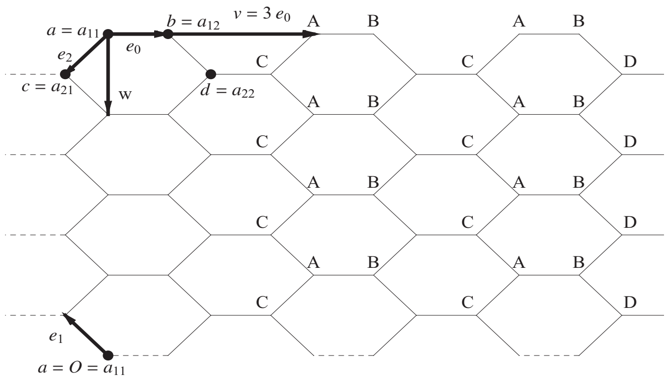

Figure 3. The points of types A, B, C, D.

Theorem 1. (See Refs. [1] and [4]) The Wiener index of T is given by

$$W(T)=\begin{cases}\dfrac{pq^2}{24}(6p^2+q^2-4) & \text{if } q<p\\ \dfrac{p^3}{24}(7p^2-4) & \text{if } q=p\\ \dfrac{p^2q}{24}(3q^2+3pq+p^2-4) & \text{if } p<q.\end{cases}$$

Proof: For $1\le i\le q/2+1$, $1\le j\le p/2+1$ we have

$$d(a,a_{ij})=\begin{cases}i+j-2 & i>j\\ 2i-2 & i=j\\ 2j-2 & i<j\end{cases} \qquad (3)$$

when *i,j* are both even or both odd, and otherwise

$$d(a,a_{ij})=\begin{cases}i+j-2 & 1+i>j\\ 2i-1 & 1+i=j\\ 2j-3 & 1+i<j\end{cases} \qquad (4)$$

and for $1\le i\le q/2+1$, $q/2+2\le j\le q$, we have

$$d(a,a_{ij})=\begin{cases}p+i-j & j>p-i+2\\ 2i-2 & j=p-i+2\\ 2p-2j+2 & j<p-i+2\end{cases} \qquad (5)$$

when i,j are both even or both odd, and otherwise

$$d(a,a_{ij})=\begin{cases}p+i-j & j>p-i+3\\ 2i-3 & j=p-i+3\\ 2p-2j+3 & j<p-i+3\end{cases} \qquad (6)$$

It is clear that $W(T)=\frac{pq}{2}d(a)$, where $d(a)=\sum_{x\in V(T)}d(a,x)$. Now if we put $d_i(a)=\sum_{x\text{ in }i\text{th row}}d(a,x)$, since for $2\le i\le q/2$, $d(a,a_{ij})=d(a,a_{q-i+2,j})$ we have

$$W(T)=\frac{pq}{2}\left(d_1(a)+d_{q/2+1}(a)+2\sum_{i=2}^{q/2}d_i(a)\right).$$

By considering the relations (3), (4), (5) and (6) and separate cases (even or odd) for *i, p* and *q* one can easily compute the wiener index (see Ref. [12] for details). Also using the relations (3), (4), (5) and (6) we can write a simple MATHEMATICA program for computing this topological index as follows. At the end of this program W is equal to the Wiener index of the given polyhex nanotorus.

```
Clear[a];
p=10; q=16; (*for example*)
A=Table[a[i,j],{i,1,q},{j,1,p}];
```

```
For[i=1,i ≤ q/2 +1,
      For[j=1,j≤ p/2 +1,
              If[(OddQ[i] && OddQ[j]) || (EvenQ[i] && EvenQ[j]),
                a[i,j]= Which[i>j,i+j-2,   i==j, 2i-2,  i<j,2j-2],
                   a[i,j]= Which[1+i>j,i+j-2,  1+i==j, 2i-1, 1+i<j,2j-3]
                  ];
        j++ ];
       i++];
For[i=1,i ≤ q/2 +1,
      For[j= p/2 +2,j≤p,
              If[(OddQ[i] && OddQ[j]) || (EvenQ[i] && EvenQ[j]),
                a[i,j]= Which[j>p-i+2,p+i-j,   j==p-i+2, 2i-2, j<p-i+2,2p-2j+2],
                   a[i,j]= Which[j>p-i+3,p+i-j,  j==p-i+3, 2i-3, j<p-i+3,2p-2j+3]
                  ];
         j++ ];
        i++];
For[k=q/2+2,k ≤ q,
       A[[k]]=A[[q-k+2]];
     k++];
A;
A//MatrixForm
W=p*q/2*Sum[Sum[A[[i,j]],{i,1,q}],{j,1,p}];
```

Now by considering relation (3) and the geometry of nanotori we can compute the reverse Wiener index of polyhex nanotori as follows:

Theorem 2. The reverse Wiener index of the nanotorus T is

$$\Lambda(T)=\begin{cases}\frac{pq}{24}(-12p+4q+6p^2q-q^3) & \text{if } q<p\\ \frac{p^3}{24}(-8+5p^2) & \text{if } p=q\\ \frac{pq}{24}(-p^3-6q+3p^2q-2p+3pq^2) & \text{if } p<q\end{cases}$$

Proof: Since we have $\Lambda(G)=\frac{1}{2}N(N-1)d-W(G)$, it is enough to calculate the diameter of the graph. By the geometry of polyhex nanotori we have

$$d=\begin{cases} d(a,a_{q/2+1,p/2+1}) & \text{if } q<p,\ p/2+1,\ q/2+1 \text{ both odd or both even}\\ d(a,a_{q/2,p/2+1}) & \text{if } q<p, \text{ one of } p/2+1,\ q/2+1 \text{ odd and other even}\\ d(a,a_{q/2+1,p/2+1}) & \text{if } q=p\\ d(a,a_{q/2+1,p/2+1}) & \text{if } p<q\end{cases}$$

and so by relation (3) we get that

$$d=\begin{cases} p & q\le p\\ (p+q)/2 & p<q\end{cases}$$

and this completes the proof.

Theorem 3. (See Ref. [2]) The Balaban index of the armchair polyhex nanotorus is given by

$$J(T)=\begin{cases} \dfrac{54p^2q}{(pq+4)(6p^2+q^2-4)} & \text{if } q<p \\ \dfrac{54p^3}{(p^2+4)(7p^2-4)} & \text{if } q=p \\ \dfrac{54pq^2}{(pq+4)(3q^2+3pq+p^2-4)} & \text{if } p<q. \end{cases}$$

Proof: Again we consider *d(a)* as defined in Theorem 1. Then we claim that $J(T)=\dfrac{m^2}{(\mu+1)d(a)}$,

where $m=|E(T)|=3pq/2$, $|V(T)|=pq$ and so $\mu=3pq/2-pq+1=pq/2+1$. To prove the claim, we note that from the geometry of nanotori, for every *u* in vertex set of *T*, we have $d(u)=d(a)$ and so

$$J(T)=\frac{m}{\mu+1}\sum_{uv\in E(T)}(d(u)d(v))^{-0.5}=\frac{m}{\mu+1}\sum_{uv\in E(T)}d(u)^{-1}=\frac{m}{\mu+1}\frac{|E(T)|}{d(a)}=\frac{m^2}{(\mu+1)d(a)}.$$

But since $d(a)=2W(T)/(pq)$, by replacing *m*, μ and *d(a)* we can get the desired formula for *J(T)*.

If we delete the last line of the MATHEMATICA program for calculating the Wiener index of nanotori, and replace the below lines the output of the program will be the Balaban index of nanotori.

```
m=3*p*q/2;
n=p*q/2+2;
J=m^2/(n* Sum[Sum[A[[i,j]],{i,1,q}],{j,1,p}])
```

By a similar argument, we can compute the hyper-Wiener index of the polyhex nanotori as follows.

Theorem 4. (See Ref. [4]) The hyper-Wiener index of the chemical graph of polyhex nanotorus *T* is

$$WW(T)=\begin{cases} \dfrac{pq^2}{192}(8p+16p^3+3q(-4+q^2)+4(-4+6p^2+q^2)) & \text{if } q<p \\ \dfrac{p^3}{192}(-16-4p+28p^2+19p^3) & \text{if } q=p \\ \dfrac{p^2q}{192}(5p^3+4p^2(1+q)+2p(-10+6q+3q^2)+4(-4+4q+3q^2+q^3)) & \text{if } p<q \end{cases}$$

Proof: From the geometry of nanotori, it is easy to see that for every $u, v \in V(T)$,

$$\{d(u,x) \mid x\in V(T)\}=\{d(v,x) \mid x\in V(T)\}$$

Thus if we put $d^2(a)=\sum_{x\in V(T)}d(a,x)^2$ and $d_i^2(a)=\sum_{x \text{ in ith row}}d(a,x)^2$, then we have

$$\sum_{\{u,v\}\subseteq V(T)}d(u,v)^2=pq\left(d_1^2(a)+d_{q/2+1}^2(a)+2\sum_{i=2}^{q/2}d_i^2(a)\right)$$

Now by relations (3), (4), (5) and (6) and considering separate cases for p, q and i we can get the above formula for the hyper-Wiener index of nanotori. Finally if we add the below line to the MATHEMATICA program, for computing the Wiener index, we get the hyper-Wiener index of nanotori

```
1/2*W+1/4*p*q*Sum[Sum[A[[i,j]]^2,{i,1,q}],{j,1,p}]
```

3. Conclusion

A method has been developed which is usually very useful for calculating the distance based topological indices of C_6 nanotubes and nanotorus. As a consequence of calculating the distances between vertices of zigzag polyhex nanotorus, the Wiener, revers Wiener, hyper-Weiner and Balaban index of such nanotorous were computed.

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