Hyper Wiener index of zigzag polyhex nanotorus

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Abstract

The hyper Wiener index of a connected graph G is defined as $WW(G) = \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v) + \frac{1}{2}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2$, where $d(u,v)$ is the distance between vertices $u, v \in V(G)$. In this paper we find an exact expression for hyper Wiener index of $HC_6[p,q]$, the zigzag polyhex nanotori.

1 Introduction

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it must not depend on the labeling or the pictorial representation of a graph. Many topological indices have been defined and several of them have found applications as means to model chemical, pharmaceutical and other properties of molecules [23]. The topological indices were widely used in obtaining physico-chemical properties, such as the boiling point, molar refraction, critical pressure, viscosity, chromatographic retention, etc., of chemical compounds. In fact it is of interest to have a theoretical tool, say an equation, that can help one in obtaining a desired parameter by structure-related calculations.

For a connected graph G, the set of vertices and edges of will be denoted by $V(G)$ and $E(G)$, respectively. The topological distance between a pair of vertices u and v of G, denoted by $d(u,v)$, is the the number of edges on the shortest path, joining u and v. The Wiener and hyper Wiener indices are the most studied topological indices, both for algebraic aspects and

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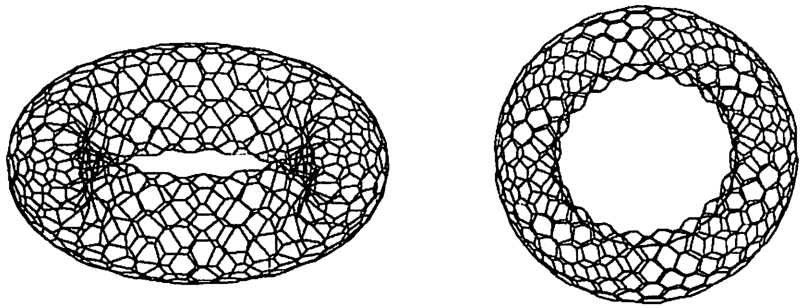

Figure 1: $HC_6[20,40]$:Side view; Top view. (The picture is taken form [6])

applications. The Wiener index of G is the half sum of distances between all vertices of the graph G:

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

The Wiener index is oldest topological indices. In 1947 chemist Harold Wiener [24] developed the most widely known topological descriptor, the Wiener index, and used in to determine physical properties of types of alkanes known as paraffins. Numerous of its chemical applications were reported and its mathematical properties are well understood (see for example [24], [10], [11]).

Randić in [22] introduced an extension of the Wiener index for trees, and this has come to be known as the hyper-Wiener index. Klein et al. [20] generalized this extension to cyclic structures as

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

(see also [4], [12], [19], [21]).

In a series of papers, Diudea and coauthors [5]-[9], [18] studied the structure and topological indices of some chemical graphs related to nanostructures. In particular, the Wiener indices of some nanotubes are computed.

In [1]-[3], [26]-[27] Ashrafi and coauthors computed some topological indices of nanotubes. Also in [13]-[14], [16]-[17] we computed some other topological indices of nanotubes. In this paper we find an exact expressions for hyper Wiener index of the polyhex nanotorus (see Figure 1). For this purpose we choose a coordinate label for vertices of $HC_6[p,q]$ as shown in Figure 2. Throughout this paper $G := HC_6[p,q]$, denotes an arbitrary zig-zag polyhex nanotori in terms of the circumference p and the length q.

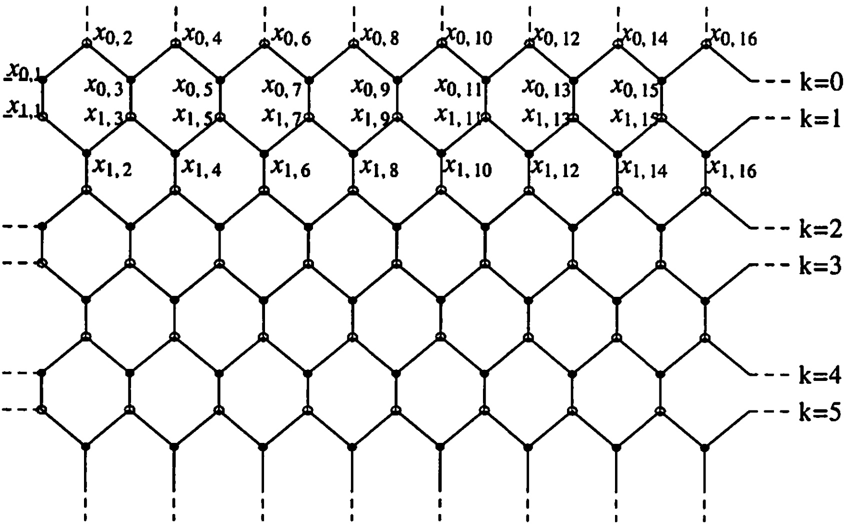

Figure 2: A zig-zag polyhex nanotorus lattice with $p = 16$ and $q = 6$.

We notice that p and q must be even. In Figure 3 the distances from x_{01} to all vertices are given. Note that the graph is bipartite, or equivalently, the vertices can be colored with white and black so that adjacent vertices have different color (see [15, Theorem 2.4]). Since the graph is symmetric respect to the line joining $x_{0,\frac{p}{2}+1}$ to $x_{1,\frac{p}{2}+1}$, one half of the numbers are shown in Figure 3. In [14] we have included a MATHEMATICA [25] program to produce the graph of $HC_6[p,q]$. With this program we are able to compute the hyper Wiener index of the graph, using the definitions.

2 Hyper Wiener index of polyhex nanotorus

In this section we derive an exact formula for the hyper Wiener index of $G := HC_6[p,q]$. For a vertex $u \in V(G)$ we define

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

$$d'(u) = \sum_{v \in V(G)} (d(u,v))^2$$

$$dd(u) = \sum_{u \in V(G)} [d(u) + d'(u)].$$

(If it is necessary we show these quantities by $d_G(u)$, $d'_G(u)$ and $dd_G(u)$.)

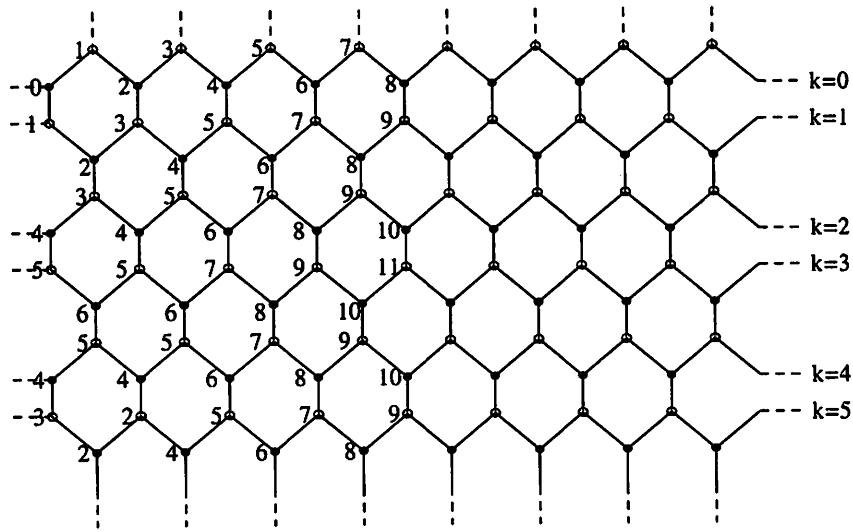

Figure 3: Distances from x_{01} to each vertex of $HC_6[6,16]$.

Then

$$\begin{aligned} WW(G) &= \frac{1}{4}\sum_{u\in V(G)} d(u) + \frac{1}{4}\sum_{u\in V(G)} d'(u) \\ &= \frac{1}{4}\sum_{u\in V(G)} dd(u). \end{aligned}$$

Now for $u, v \in V(G)$ we define $dd(u,v)$ (or $dd_G(u,v)$), the hyper distance between u and v, to be

$$dd(u,v) = d(u,v) + (d(u,v))^2.$$

In the following lemma we give a formula for the hyper distances of one white (black) vertex of level 0 of the graph G to all vertices on the level $k < \frac{q}{2}$.

Lemma 1 In the graph G we have

$$\begin{aligned} ww_k &:= \sum_{x\in \text{ level } k<\frac{q}{2}} dd(x_{02}, x) \\ &= \sum_{x\in \text{ level } k<\frac{q}{2}} dd(x_{04}, x) \\ &\ \ \vdots \end{aligned}$$

$$= \begin{cases} \frac{1}{6}p + \frac{5}{3}k + 5k^2 + kp + k^2p + \\ \qquad \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3 & \text{if } 0 \le k < \frac{p}{2} \\ p(2k+1)^2 & \text{if } \frac{p}{2} \le k \end{cases}$$

and

$$\begin{aligned} bb_k &:= \sum_{x \in \text{ level } k < \frac{p}{2}} dd(x_{01}, x) \\ &= \sum_{x \in \text{ level } k < \frac{p}{2}} dd(x_{03}, x) \\ &\vdots \\ &= \begin{cases} \frac{1}{6}p - \frac{1}{3}k - 3k^2 + kp + kp^2 + \\ \qquad \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3 & \text{if } 0 \le k < \frac{p}{2} \\ 4k^2p & \text{if } \frac{p}{2} \le k. \end{cases} \end{aligned}$$

PROOF: We compute b_k. It is suffices to consider x_{01}. For other black vertices, the argument is similar. At first note that the lattice is symmetric (with respect to the line joining x_{01} to x_{11}). We distinguish three cases:

Case 1: $k \ge \frac{p}{2}$ and k is even. In this case for all $1 \le j \le \frac{p}{2} + 1$, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k-1 & \text{if } j \text{ is even} \\ 2k & \text{if } j \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain $\frac{p}{2}$ vertices having distance $2k-1$ from x_{01}, and $\frac{p}{2}$ vertices having $2k$ distance from x_{01}. So

$$\begin{aligned} \sum_{u \in \text{ level } k} [d(x_{01}, u) + (d(x_{01}, u))^2] = & \sum_{j \text{ is even}} [d(x_{01}, x_{ji}) + (d(x_{01}, x_{ji}))^2] + \\ & \sum_{j \text{ is odd}} [d(x_{01}, x_{ji}) + (d(x_{01}, x_{ji}))^2] \\ = & \frac{p}{2}[(2k-1) + (2k-1)^2] + \frac{p}{2}[(2k) + (2k)^2] \\ = & 8k^2\frac{p}{2}. \end{aligned}$$

Case 2: $k \ge \frac{p}{2}$ and k is odd. In this case for all $1 \le j \le \frac{p}{2} + 1$, we have

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } j \text{ is even} \\ 2k-1 & \text{if } j \text{ is odd.} \end{cases}$$

Now by considering these vertices and their symmetric vertices we obtain p vertices having distance $2k-1$ from x_{01}, and p vertices having $2k$ distance from x_{01}. So

$$\sum_{u \in \text{ level } k} [d(x_{01},u) + (d(x_{01},u))^2] = \sum_{j \text{ is even}} [d(x_{01},x_{ji}) + (d(x_{01},x_{ji}))^2] + \sum_{j \text{ is odd}} [d(x_{01},x_{ji}) + (d(x_{01},x_{ji}))^2]$$
$$= \frac{p}{2}[(2k) + (2k)^2] + \frac{p}{2}[(2k-1)] + (2k-1)^2]$$
$$= 8k^2\frac{p}{2}.$$

Case 3: $k \leq p-1$. For all j's, such that $p+1 \leq j$ and $j > k+1$,we have

$$d(x_{01}, x_{kj}) = k + j - 1.$$

Thus the summation of the distances between x_{01} and x_{kj} (for all j's such that $p+1 \leq j$ and $j > k+1$) and their symmetric vertices is

$$\begin{aligned} S_1 &= 2\sum_{j=k+2}^{\frac{p}{2}} [(k+j-1) + (k+j-1)^2] + \\ &\quad [(k+\frac{p}{2}+1-1) + (k+\frac{p}{2}+1-1)^2] \\ &= \frac{1}{6}p - \frac{7}{3}k + kp - 7k^2 + k^2p + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 - \frac{14}{3}k^3. \end{aligned}$$

Also if $1 \leq j \leq k+1$, then

$$d(x_{01}, x_{kj}) = \begin{cases} 2k & \text{if } \ k-j \text{ is odd} \\ 2k-1 & \text{if } \ k-j \text{ is even.} \end{cases}$$

Therefore the summation of the distances between x_{01} and x_{kj} (for all j such that $1 \leq j \leq k+1$) and their symmetric vertices is

$$S_2 = (k+1)(2k + (2k)^2) + k(2k - 1 + (2k-1)^2) = 2k(2k + 4k^2 + 1).$$

Hence

$$\begin{aligned} bb_k &= S_1 + S_2 \\ &= \frac{1}{6}p - \frac{7}{3}k + kp - 7k^2 + k^2p + \frac{1}{4}p^2 + \\ &\quad \frac{1}{2}kp^2 + \frac{1}{12}p^3 - \frac{14}{3}k^3 + 2k(2k + 4k^2 + 1) \\ &= \frac{1}{6}p - \frac{1}{3}k - 3k^2 + kp + kp^2 + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3. \end{aligned}$$

The proof for ww_k is similar. □

Lemma 2 For one white or black vertex x_{0j} of level 0 we have

$$bb_{\frac{q}{2}} := \sum_{x \in \text{ level } \frac{q}{2}} dd(x_{0j}, x) = \begin{cases} -\frac{4}{3}p - \frac{10}{3}(\frac{q}{2}) - 2(\frac{q}{2})p - 8(\frac{q}{2})^2 + \\ \quad (\frac{q}{2})p^2 + \frac{1}{3}p^3 + \frac{4}{3}(\frac{q}{2})^3 & \text{if} \quad \frac{q}{2} < \frac{p}{2} \\ 4(\frac{q}{2})^2 p & \text{if} \quad \frac{p}{2} \le \frac{q}{2}. \end{cases}$$

PROOF: Since G is symmetric (with respect to the line joining x_{01} to x_{11}), it is sufficient to porve the assertion for x_{01} and x_{02}. For x_{01}, the proof is exactly the proof of Lemma 1. We consider the tori that can be built up from two halves collapsing at level 0. In the top part x_{02} is such as a black vertex so by the proof of Lemma 1, we obtain that $b_{\frac{q}{2}}$. □

Corollary 3 For each $u \in V(G)$ we have

$$D := dd(u) = bb_0 + bb_1 + \cdots + bb_{\frac{q}{2}} + ww_1 + \cdots + ww_{\frac{q}{2}-1}.$$

PROOF: At first note that the lattice is symmetric (with respect to the leve k). So it is suffices to consider x_{01} and x_{02}. For other black (white) vertices the argument is similar. Now we begin with x_{01}. Let

$$B_1 = \{k \mid 0 \le k < \frac{q}{2}\} \quad \text{and} \quad B_2 = \{k \mid \frac{q}{2} < k \le q-1\}.$$

We have

$$dd(x_{01}) = \sum_{v \in V(G)} dd(x_{01}, v) = \sum_{v \in B_1} dd(x_{01}, v) + bb_{\frac{q}{2}} + \sum_{v \in B_2} dd(x_{01}, v).$$

But

$$\begin{aligned} \sum_{v \in B_1} dd(x_{01}, v) &= \sum_{v \in \text{ level } 0} dd(x_{01}, v) + \sum_{v \in \text{ level } 1} dd(x_{01}, v) + \cdots + \\ &\qquad \sum_{v \in \text{ level } \frac{q}{2}-1} dd(x_{01}, v) \\ &= bb_o + bb_1 + \cdots + bb_{\frac{q}{2}-1}. \end{aligned}$$

For computing the last sum we consider the tori that can be built up from two halves collapsing at level 0. The top part is formed of the lines of B_2

that x_{01} is such as a black vertex. So by a changing index and using the proof of the Lemma 1, we can obtain that

$$\begin{aligned}\sum_{v\,\in\,B_2} dd(x_{01},v) &= \sum_{v\,\in\,level\ q-1} dd(x_{01},v) + \sum_{v\,\in\,level\ q-2} dd(x_{01},v) + \cdots + \\ &\qquad \sum_{v\,\in\,level\ \frac{q}{2}+1} dd(x_{01},v) \\ &= ww_1 + ww_1 + \cdots + ww_{\frac{q}{2}-1}\end{aligned}$$

which completes the proof. □

Theorem 1 The hyper Wiener index, $WW(G)$, of $G := HC_6[p,q]$ nanotori is given by

$$\begin{cases} \frac{1}{192}pq^2\Big[-16+16p-20q+4p^3+6p^2q+ \\ \qquad 4pq^2+12p^2+5q^3+4q^2+12pq\Big] & \text{if } q \leq p \\ \frac{1}{192}p^2q\Big[3p^3+4p^2-12p-6+16q^3+24q^2+8q\Big] & \text{if } p < q. \end{cases}$$

PROOF: We have

$$WW(G) = \frac{1}{4}\sum_{u\in V(G)} dd(u) = \frac{1}{4}\sum_{u\in V(G)} D = \frac{1}{4}D \mid V(G) \mid = \frac{1}{4}D\ pq.$$

First suppose that $q \leq p-2$. In this case $\frac{q}{2} < \frac{p}{2}$, so by Corollary 3 and Lemma 1 we have

$$\begin{aligned} D =& bb_0 + bb_1 + \cdots + bb_{\frac{q}{2}} + ww_1 + \cdots + ww_{\frac{q}{2}-1} \\ =& \sum_{k=0}^{\frac{q}{2}}\left(\frac{1}{6}p - \frac{1}{3}k - 3k^2 + kp + kp^2 + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) + \\ & \sum_{k=1}^{\frac{q}{2}-1}\left(\frac{1}{6}p + \frac{5}{3}k + 5k^2 + kp + k^2p + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) \\ =& \frac{q}{48}(-16+16p-20q+4p^3+6p^2q+4pq^2+12p^2+5q^3+4q^2+12pq). \end{aligned}$$

Hence in this case

$$WW(G) = \frac{1}{192}pq^2(-16+16p-20q+4p^3+6p^2q+4pq^2+12p^2+5q^3+4q^2+12pq).$$

Now suppose that $p \le q-2$. In this case $\frac{p}{2}-1 < \frac{q}{2}-1$, so by Corollary 3 and Lemma 1 we have

$$\begin{aligned}
D &= bb_0 + bb_1 + \cdots + bb_{\frac{q}{2}} + ww_1 + \cdots + ww_{\frac{q}{2}-1} \\
&= bb_0 + bb_1 + \cdots + bb_{\frac{p}{2}-1} + bb_{\frac{p}{2}} + \cdots + bb_{\frac{q}{2}} + \\
&\qquad ww_1 + \cdots + ww_{\frac{p}{2}-1} + ww_{\frac{p}{2}} + \cdots + ww_{\frac{q}{2}-1} \\
&= \sum_{k=0}^{\frac{p}{2}-1} \left(\frac{1}{6}p - \frac{1}{3}k - 3k^2 + kp + kp^2 + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) + \\
&\qquad \sum_{k=\frac{p}{2}}^{\frac{q}{2}} 4k^p + \\
&\qquad \sum_{k=1}^{\frac{p}{2}-1} \left(\frac{1}{6}p + \frac{5}{3}k + 5k^2 + kp + k^2p + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) + \\
&\qquad \sum_{k=\frac{p}{2}}^{\frac{q}{2}-1} (p(2k+1)^2) \\
&= \frac{p}{48}p[3p^3 + 4p^2 - 12p - 16 + 16q^3 + 24q^2 + 8q].
\end{aligned}$$

Hence

$$\begin{aligned}
WW(G) &= \frac{pq}{4}\frac{p}{48}p(3p^3 + 4p^2 - 12p - 16 + 16q^3 + 24q^2 + 8q) \\
&= \frac{1}{192}p^2q(3p^3 + 4p^2 - 12p - 16 + 16q^3 + 24q^2 + 8q).
\end{aligned}$$

Finally if $p = q$, then $\frac{p}{2} - 1 = \frac{q}{2} - 1$ so by Corollary 3 and Lemma 1, for each $u \in V(G)$ we have

$$\begin{aligned}
D &= bb_0 + bb_1 + \cdots + bb_{\frac{q}{2}} + ww_1 + \cdots + ww_{\frac{q}{2}-1} \\
&= bb_0 + bb_1 + \cdots + bb_{\frac{p}{2}-1} + bb_{\frac{p}{2}} + ww_1 + \cdots + ww_{\frac{p}{2}-1} \\
&= \sum_{k=0}^{\frac{p}{2}-1} \left(\frac{1}{6}p - \frac{1}{3}k - 3k^2 + kp + kp^2 + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) + \\
&\quad p^3 + \sum_{k=1}^{\frac{p}{2}-1} \left(\frac{1}{6}p + \frac{5}{3}k + 5k^2 + kp + k^2p + \frac{1}{4}p^2 + \frac{1}{2}kp^2 + \frac{1}{12}p^3 + \frac{10}{3}k^3\right) \\
&= \frac{p(p-2)(19p^2 + 30p + 8)}{48}.
\end{aligned}$$

Hence

$$WW(G) = \frac{pp}{4}\frac{p(p-2)(19p^2+30p+8)}{48} = \frac{1}{192}p^3(19p^3 + 28p^2 - 4p - 16).$$

Note that this case is exactly the case 1, when $p = q$. □

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