MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **63** (2010) 217-238

ISSN 0340 - 6253

PI index of toroidal polyhexes *

Saihua Liu, Heping Zhang†

School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P. R. China.

E-mail addresses: zhanghp@lzu.edu.cn, liush2005@lzu.cn.

(Received January 9, 2009)

Abstract

Padmakar-Ivan (PI) index of a graph G is defined as $PI(G) = \sum_{e=uv \in E}(n_u(e) + n_v(e))$, where $n_u(e)$ (resp. $n_v(e)$) is the number of edges of G lying closer to u (resp. v) than to v (resp. u). In this paper, we obtain a formula of the PI index of toroidal polyhexes without torsion.

1 Introduction

Topological indices reflect important information about the chemical structure of molecules. The first well-known topological index in chemistry is the Wiener index proposed by H. Wiener [15] in the study of paraffin boiling points. The Wiener index of a tree T can be expressed as

$$W(T) = \sum_{e=uv \in E} n'_u(e) \cdot n'_v(e),$$

where $n'_u(e)$ (resp. $n'_v(e)$) denotes the number of vertices of T lying nearer to u (resp. v) than to v (resp. u). Then, I. Gutman [4] generalized the above formula of the Wiener index on trees to arbitrary graphs with cycles and named it the Szeged index. Note that the Wiener index and Szeged index coincide on trees.

*This work is supported by NSFC (grant no. 10831001).

†Corresponding author.

The Wiener-Szeged-Like Padmakar-Ivan (PI) index proposed by P.V. Khadikar et al. [10] is a modification of the Szeged index. The PI index of a graph G is defined as

$$PI(G) = \sum_{e=uv\in E} (n_u(e) + n_v(e)),$$

where $n_u(e)$ (resp. $n_v(e)$) is the number of edges of G lying closer to u (resp. v) than to v (resp. u). In the QSPR/QSAR studies, PI index promises to be a useful descriptor and a combination of PI index and Szeged index could give good results [6, 8, 9, 10].

Let $G = (V, E)$ be a graph with vertex set V and edge set E. The distance between two vertices u and v of G, denoted by $d(u, v)$, is the length of a shortest $u, v-$ path. For an edge $e = xy$ and a vertex z of G, the distance between e and z in G, denoted by $d(e, z)$, is defined as $d(e, z) = \min\{d(x, z), d(y, z)\}$. Given an edge $e = uv$, let N_e be the set of all the edges which have equidistance to both ends of e; that is, $N_e = \{e' \in E|\ d(e', u) = d(e', v)\}$. It is trivial that $e \in N_e$. We use $|N_e|$ for the number of the edges in N_e. Then $PI(G)$ can be also expressed as

$$PI(G) = \sum_{e\in E}(|E| - |N_e|).$$

Up to now, the PI index has been computed for a class of molecular graphs, such as benzenoid systems [14], hexagonal chains [7], polyhex nanotubes [1] and so on [2, 3, 11]. Especially, P.V. Khadikar et al. [14] described a method for computing PI index of benzenoid systems using orthogonal cuts.

Generally, S. Klavžar [13] introduced PI-partitions to simplify the computation of the PI index of a class of graphs, which include the partial Hamming graphs. Later, M.H. Khalifeha et al. [5] obtained a general formula for the PI index of Cartesian product of graphs.

For the toroidal polyhex $H(p, q)$, the edges can be decomposed into three edge classes under automorphisms [16]. In this paper, we count the edges in N_e for one edge e of each of the three edge classes by dividing $H(p, q)$ into several subgraphs and computing the distances in the subgraphs independently. Then we obtain a formula for $PI(H(p, q))$.

2 Preliminaries

A toroidal polyhex $H(p, q, t)$ can be drawn in the plane regular hexagonal lattice L using the representation of the torus by a $p \times q$-parallelogram Q with the usual torus boundary identification with torsion t: each side of Q connects the centers of two hexagons and is perpendicular to an edge-direction of L, where both top and bottom sides pass through p vertical edges and two lateral sides pass through q edges. In order to form a toroidal polyhex

$H(p,q,t)$, first identify two lateral sides of Q to form a tube, and then identify the top side of the tube with its bottom side after rotating it through t hexagons.

For example, the toroidal polyhex $H(4,3,0)$ arising from a 4×3-parallelogram of the hexagonal lattice is shown in Figure 1, where the two gray half-hexagons are glued into one.

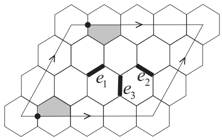


Figure 1. $H(4,3,0)$ with a left-slant edge e_1, a right-slant edge e_2 and a vertical edge e_3.

We use $H(p,q)$ shortly for toroidal polyhexes without torsion in the following. Let Q be a $p \times q$-parallelogram to represent $H(p,q)$ by the usual torus boundary identification without torsion. We define a set of symbols first for convenience: A *right (resp. left) slant edge* is an edge directed from left (resp. right) to right (resp. left) when it goes from the top down in Q (illustrated in Figure 1). Denote the left slant edge set, right slant edge set and vertical edge set by M_1, M_2 and M_3, respectively. Then M_1, M_2 and M_3 form a decomposition of the edge set of $H(p,q)$. *A* right (resp. left)-down-directed path, RDP (resp. LDP) for short, is a path consisting of right (resp. left) slant edges and vertical edges alternatively in Q. The paths P_i $(i = 0,1,2\cdots)$ in Figure 2 are all RDPs. And in a path, we call an edge a *step*. Let P be a path and a,b be two vertices on P. Then aPb denotes the sub-path from a to b on P and $|P|$ is the length of P.

Let $B(m,n)$ be the graph obtained from the $p \times q$ parallelogram with two vertices x,y as shown in Figure 2 by adding new edges $e = uv$, ux and vy.

Lemma 2.1. *For graph $B(m,n)$ with the given edge $e = uv$, we have*

$$|N_e| = \theta(m+n-1) \cdot \min\{m,n\} + 1,$$

where $\theta(X) = \frac{3}{2} + \frac{(-1)^X}{2}$.

Proof. Denote the RDPs illustrated in bold in Figure 2 by $P_1, P_2, \cdots P_t$. Note that $t = m+n$ and all the vertices on P_i are nearer to u than to v when $i \leqslant \lfloor \frac{m+n}{2} \rfloor$ and they are nearer to v than to u when $i \geqslant \lceil \frac{m+n}{2} \rceil$. Moreover, the vertices on P_i adjacent to P_{i-1} are one step nearer (resp. further) to u (resp. v) than those adjacent to P_{i+1}. Two cases are distinguished:

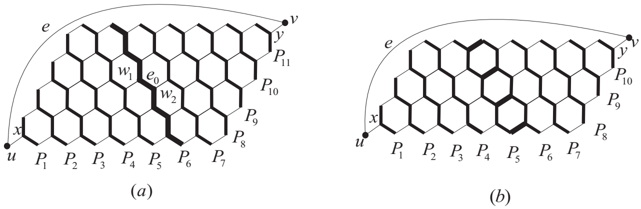


Figure 2. Benzenoid parallelograms: (a), $m+n$ is odd, and (b), $m+n$ is even.

Case 1. $m+n$ is odd (see Figure 2 (a)).

Let $e_0 = w_1w_2$ be any edge on $P_{\lceil \frac{m+n}{2} \rceil}$ such that w_1 and w_2 are adjacent to $P_{\lceil \frac{m+n}{2} \rceil -1}$ and to $P_{\lceil \frac{m+n}{2} \rceil +1}$, respectively. Then $d(u, e_0) = d(u, w_1) = d(v, w_2) = d(v, e_0)$. Obviously, all the vertices on P_i are nearer to u than to v when $i \leqslant \lfloor \frac{m+n}{2} \rfloor$ and nearer to v than to u when $i \geqslant \lceil \frac{m+n}{2} \rceil$. Then all the edges of $P_{\lceil \frac{m+n}{2} \rceil}$ but no other edges belong to N_e. Thus $|N_e| = 2$ $\min\{m, n\} + 1$ since $P_{\lceil \frac{m+n}{2} \rceil}$ passes through $\min\{m, n\}$ hexagons and the length of $P_{\lceil \frac{m+n}{2} \rceil}$ is $2 \min\{m, n\} + 1$.

Case 2. $m+n$ is even (see Figure 2 (b)).

In this case, no edges other than those between $P_{\frac{m+n}{2}}$ and $P_{\frac{m+n}{2}+1}$ (the edges in bold) belong to N_e. Thus $|N_e| = \min\{m, n\} + 1$.

In all, $|N_e| = \theta(m+n-1) \cdot \min\{m, n\} + 1$, where $\theta(X) = \frac{3}{2} + \frac{(-1)^X}{2}$. □

Note that in $B(m, n)$, if the two edges ux, vy are substituted by two paths with the same length, the same conclusion as in Lemma 2.1 can be obtained.

Let $T_{vuu'}(k)$ be the graph obtained from the benzenoid triangularity with k hexagons on each of the three sides by adding new edges uc_0, $u'c$ and uv, where c_0, c and $v(= c_0')$ are three vertices on the benzenoid triangularity as shown in Figure 3.

$T_{vu'u}(k)$ is the graph obtained from $T_{vuu'}(k)$ by deleting $e = uv$ and adding a new edge vu'. In fact, $T_{vu'u}(k)$, $T_{vuu'}(k)$ are the same graph and vu, vu' are the same edge in the sense of isomorphism.

Lemma 2.2. *For graph $T_{vuu'}(k)$ with the given edge $e = uv$, we have*

$$|N_e| = k + 1.$$

If the edge uc_0 in $T_{vuu'}(k)$ is substituted by an odd path P with length $2t_1 + 1$ and the vertex $v(= c_0')$ is substituted by an even vc_0 path P' with length $2t_2$ (see Figure 3 (b)), then

$$|N_e| = \begin{cases} k - (t_1 - t_2) + 1, & \text{if } t_1 \geqslant t_2 \text{ and } k \geqslant |t_1 - t_2|, \\ k - (t_2 - t_1) + 2, & \text{if } t_2 \geqslant t_1 \text{ and } k \geqslant |t_1 - t_2|, \\ 1, & \text{if } |t_2 - t_1| > k, \end{cases}$$

where the only edge of N_e lies on P or on P' when $|t_2 - t_1| > k$.

Proof. Let $P_0, P_1, P_2, \cdots P_k$ be the LDPs in $T_{vuu'}(k)$ and c_i, c_i' be the end vertices of P_i for each i $(0 \leqslant i \leqslant k)$. Denote the vertex between c_i and c_{i+1} (resp. c_i' and c_{i+1}') on the boundary of $T_{vuu'}(k)$ by b_i (resp. b_i') for $1 \leqslant i \leqslant k$ (see Figure 3).

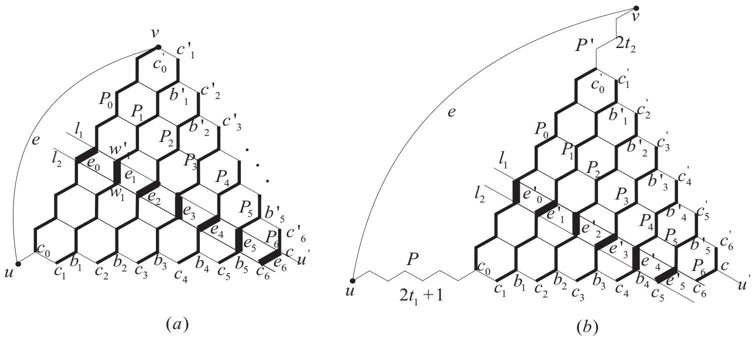


Figure 3. (a), $T_{vuu'}(k)$ with $t_1 = t_2 = 0$; (b), $T_{vuu'}(k)$ with $t_1 = 3$, $t_2 = 2$.

Let $e_i = w_i w_i'$ be the middlemost edge of the odd path $uc_0c_1b_1 \cdots c_iP_ic_i'c_{i-1}' \cdots c_1'c_0'v$ for $0 \leqslant i \leqslant k$. Since $d(u, c_i) = d(v, c_i') + 1$ and $|P_i| \geqslant 2$ for all i, $e_i \in P_i$. Note that $w_iP_ic_ib_{i-1}c_{i-1} \cdots c_0u$ is a shortest $w_i, u-$ path avoiding v and $w_i'P_ic_i'b_{i-1}'c_{i-1}' \cdots c_0'$ is a shortest $w_i', v-$ path avoiding u and $d(w_i, u) = d(w_i', v)$. Then $e_i \in N_e$.

Moreover, e_{k-i} is the $(i+1)$th edge on P_{k-i} from the c_i end and the $(i+2)$th edge from c_i' end, which means that e_i is the $(k-i+1)$th edge on P_i from the c_i end and the $(k-i+2)$th edge from the c_i' end. All these edges lie between two parallel lines l_1, l_2 (see Figure 3) and all the vertices below (resp. above) l_2 (resp. l_1) containing those on l_2 (resp. l_1) are closer to u (resp. v) than to v (resp. u). Hence, no edges other than $e_0, e_1, \ldots, e_k$ belong to N_e. Thus $|N_e| = k + 1$.

We now consider the situation that the edge uc_0 is substituted by an odd path P of length $(2t_1 + 1)$ and the vertex v (c_0') is substituted by an even path P' with length $2t_2$ (see Figure 3 (b)).

Similarly, let e_i' be the middlemost edge of $P_i' = uPc_0 \cdots c_iP_ic_i'c_{i-1}' \cdots c_0'P'v$ for $0 \leqslant i \leqslant k$. Then e_i' is the edge after moving toward u from e_i by $t_1 - t_2$ steps on P_i' if $t_1 \geqslant t_2$ and moving toward v by $t_2 - t_1$ steps if $t_2 > t_1$.

Then e_i' is the $(k-i+1-(t_1-t_2))$th edge on P_i from the c_i end and the $(k-i+2-(t_2-t_1))$th edge from the c_i' end when e_i' lies on P_i.

But if e_i' lies out of P_i, either the sub-path from e_i' to v or the sub-path from e_i' to u on $uPc_0 \cdots c_iP_ic_i' \cdots c_1'P'v$ is no longer a shortest path. Thus $e_i' \notin N_e$ at this moment.

First suppose that $k \geqslant |t_1 - t_2|$. If $t_1 \geqslant t_2$, e'_i lies out of P_i when $k-(t_1-t_2)+1 \le i \le k$ (that is, $k-i+1-(t_1-t_2) \leqslant 0$), which means that (t_1-t_2) e'_is lie out of P_i. Then e'_i belongs to N_e if and only if $0 \leqslant i \leqslant k-(t_1-t_2)$ and they are all the edges between l_1 and l_2 illustrated in Figure 3 (b). As above, no other edges belong to N_e. Thus $|N_e| = k+1-(t_1-t_2)$.

If $t_2 = t_1+1$, no e'_i $(0 \leqslant i \leqslant k)$ lies out of P_i. And $|N_e| = k+1 = k-(t_2-t_1)+2$.

If $t_2 > t_1+1$, e'_i lies out of P_i when $k-(t_2-t_1)+2 \le i \le k$, that is, (t_2-t_1-1) e'_is lie out of P_i. Then $|N_e| = k+2-(t_2-t_1)$ in this case.

Then suppose that $|t_2-t_1| > k$. We have $|N_e| = 1$, where the only edge of N_e lies on P when $t_1 - t_2 > k$ and on P' otherwise. □

Let $T'_{vuu'}(k)$ be the graph (shown in Figure 4) obtained from $T_{vuu'}(k)$ by adding the edge vu', replacing the two edges uc_0 and $u'c$ by two odd paths P, P' with lengths $2t_1+1$ and $2t_2+1$, respectively, replacing v by a path with length $2t_3$, and identifying vertices u, u' and edges e, e', respectively.

Lemma 2.3. *For graph $T'_{vuu'}(k)$ with the edge $e = e' = uv$, we have*

(1) *if $t_3 = 0$,*

$$|N_e| = \begin{cases} 2k-(t_1+t_2)-\lfloor\frac{4}{3}(k-t_1-t_2-1)\rfloor, & \text{if } k > t_1+t_2, \\ 2k-t_1-t_2+2, & \text{if } t_1, t_2 < k \leqslant t_1+t_2, \\ k+2-t_i, & \text{if } t_i \leqslant k \leqslant t_j,\ i \neq j,\ i,j \in 1,2, \\ 2, & \text{if } k \leqslant t_1, t_2; \end{cases}$$

(2) *if $t_1 = t_2 = 0$,*

$$|N_e| = \begin{cases} \lceil\frac{2}{3}(k-t_3+2)\rceil, & \text{if } k \geqslant t_3, \\ 1, & \text{otherwise.} \end{cases}$$

Proof. (1) Suppose that $t_3 = 0$.

In order to avoid confusion, let $N(e)$ (resp. $N(e')$) be the set of edges with equidistance to the ends of e (resp. e') in $T_{vuu'}(k)$ (resp. $T_{vu'u}(k)$) and N_e be the set of edges with equidistance to the ends of $e = e'$ in $T'_{vuu'}(k)$. $|N(e)|$ and $|N(e')|$ can be computed according to Lemma 2.2. Our aim is to count $|N_e|$.

There exists a line l (illustrated in Figure 4 (a) and (b)) bisecting the path $uPc_0 \ldots cP'u'$ such that the vertices on the same bank of l with u (resp. u') are nearer to u (resp. u') than to u' (resp. u). Then the edges of $N(e)$ on the same side of l with u (containing those on l) and those of $N(e')$ on the same side with u' make up N_e. We need only count the edges in these two sections. Set $\overline{N(e)} = N(e) \setminus N_e$ and $\overline{N(e')} = N(e') \setminus N_e$ (the edges of $\overline{N(e)}$ and $\overline{N(e')}$ are the edges signed with short segments in Figure 4). We consider four cases:

Case 1. $k > t_1, t_2$.

Then $k > |t_1 - t_2|$ and l passes through the path $c_0c_1b_1c_2 \cdots c_kc$. Since $uPc_0c_1 \cdots c_kcP'u'$ is an even path, l passes through some vertex, say w_0, of $c_0c_1b_1c_2 \cdots c_kc$. By Lemma 2.2, the edges of $N(e)$ and $N(e')$ rank along two lines l', l'', respectively (see Figure 4). Let c_i, c_j be the initial points of l' and l'' on $c_0c_1b_1c_2 \cdots c_kc$, respectively.

First suppose that l' and l'' intersect at a point on l, say w (that is, $i \geqslant j$). Let the geometric length of each edge of the hexagons be a unit length. Since the length of the diagonals of regular hexagons is twice the unit length, the length of line segment wc_i, denoted by $|wc_i|$, equals the length of the path $c_ib_{i-1}c_{i-1} \cdots w_0$. Similarly, $|wc_j|$ equals the length of $c_jb_jc_{j+1} \cdots w_0$. Then we have $|wc_i| = |wc_j| = i - j$ by symmetry.

Observe that starting at c_i, there are 2 edges of $\overline{N(e)}$ along every line segment with length 3 on l' besides the initial one. Thus $|\overline{N(e)}| = \lfloor \frac{2}{3}|wc_i| \rfloor + 1$. Similarly, $|\overline{N(e')}| = |\overline{N(e)}| = \lfloor \frac{2}{3}|wc_j| \rfloor + 1$.

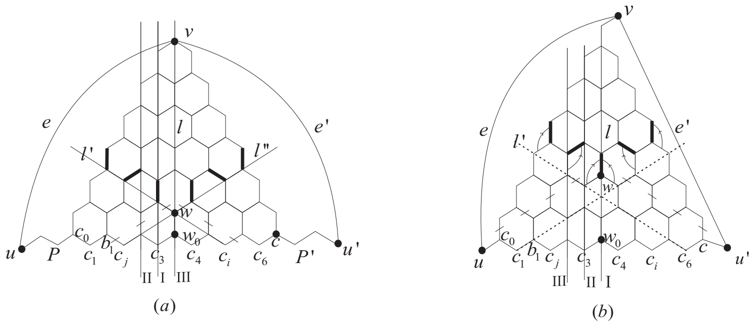


Figure 4. (a), $T'_{vuu'}(k)$ with $t_3 = 0$ and $t_1 = t_2 = 1$; (b), $T'_{vuu'}(k)$ with $t_3 = 1$ and $t_1 = t_2 = 0$.

With respect to the co-positions of l and the nearest edges of N_e to l, there are three kinds of positions marked I, II, III, respectively, in which l can be located (symmetrically, see the co-positions of them on the left side of l in Figure 4 (a)). The nearest edges of N_e to l parallel l but not in l when it is in position III for example. At this moment, $|wc_i| = i - j \equiv 0 \pmod 3$.

If l is in position I, $|wc_i| = i - j \equiv 1 \pmod 3$. Since the edge of N_e on l counts twice in $(N(e) \setminus \overline{N(e)}) \cup (N(e') \setminus \overline{N(e')})$, one more edge should be subtracted. Then

$$|N_e| = |N(e)| + |N(e')| - 2(\lfloor \frac{2}{3}|wc_i| \rfloor + 1) - 1 = |N(e)| + |N(e')| - (\lfloor \frac{4}{3}|wc_i| \rfloor + 2).$$

If l is in position II, that is, $|wc_i| = i - j \equiv 2 \pmod 3$, then

$$|N_e| = |N(e)| + |N(e')| - 2(\lfloor \frac{2}{3}|wc_i| \rfloor + 1) = |N(e)| + |N(e')| - (\lfloor \frac{4}{3}|wc_i| \rfloor + 2).$$

If l is in the third position (i.e., $|wc_i| = i - j \equiv 0 \pmod 3$), then

$$|N_e| \;=\; |N(e)| + |N(e')| - 2(\lfloor \frac{2}{3}|wc_i| \rfloor + 1) = |N(e)| + |N(e')| - (\lfloor \frac{4}{3}|wc_i| \rfloor + 2).$$

By the proof of Lemma 2.2, we know that $i = k - t_1$, $|N(e)| = k + 1 - t_1$. Symmetrically, we have $j = t_2 + 1$ and $|N'(e)| = k + 1 - t_2$. Thus $|wc_i| = i - j = k - t_1 - t_2 - 1$. Since we assume that $i - j \geqslant 0$, we have $k - t_1 - t_2 - 1 \geqslant 0$, that is, $k > t_1 + t_2$. Then

$$|N_e| \;=\; |N(e)| + |N'(e)| - (\lfloor \frac{4}{3}|wc_i| \rfloor + 2) = 2k - (t_1 + t_2) - \lfloor \frac{4}{3}(k - t_1 - t_2 - 1) \rfloor.$$

Particularly, $i - j = k - 1$ and $|N_e| = 2k - \lfloor \frac{4}{3}(k-1) \rfloor$ when $t_1 = t_2 = 0$.

Suppose that l' dose not intersect l'', which means that $k - t_1 < t_2 + 1$ (i.e. $k \leqslant t_1 + t_2$). Then $|N_e| = |N(e)| + |N(e')| = 2k + 2 - t_1 - t_2$ at this moment.

Case 2. $t_2 \leqslant k \leqslant t_1$.

Then $k \leqslant t_1 + t_2$ and l' dose not intersect l''. Thus $N(e') \subseteq N_e$ and N_e contains the only edge of $N(e)$ that lies on P. Hence, $|N_e| = |N(e')| + 1 = k + 2 - t_2$.

Case 3. $t_1 \leqslant k \leqslant t_2$.

Symmetrically, we have $|N_e| = |N(e)| + 1 = k + 2 - t_1$.

Case 4. $k \leqslant t_1, t_2$.

$|N_e| = 2$ and the only two edges lie on P and P', respectively.

(2) Suppose that $t_1 = t_2 = 0$ (see Figure 4 (b)).

Let $T_0'(k)$ be the graph $T_{vuu'}'(k)$ with $t_1 = t_2 = t_3 = 0$. Denote the set of equidistance edges to the two ends of e in $T_0'(k)$ by N_e'. Then $|N_e'| = 2k - \lfloor \frac{4}{3}(k-1) \rfloor$ by (1). Since $t_1 = t_2 = 0$, l passes through v in $T_0'(k)$. Let $T_{t_3}'(k)$ be obtained from $T_0'(k)$ by replacing v by a path P'' with length $2t_3$ ($t_3 > 0$) and N_e be the set of equidistance edges to the two ends of e in $T_{t_3}'(k)$. We need to compute $|N_e|$.

Since $T_{t_3}'(k)$ is obtained from $T_0'(k)$ by replacing v by P'', each edge of N_e' on the left side of l should move upward t_3 steps along the LDP, to which it belongs, to become a member of N_e, except that it moves to the other side of l. The symmetric operation is done for the right side. Since then, we should count the number of edges of N_e' that move to the other side of l, i.e., those no longer belong to N_e. Set $m = |N_e'| - |N_e|$. Then $|N_e| = 2k - \lfloor \frac{4}{3}(k-1) \rfloor - m$.

Note that each edge of N_e' goes half a step nearer to l in the horizontal direction when it moves one step upward on the LDP (or RDP) containing it. If l is in position I with respect to N_e', the nearest edges of N_e' (on l) need 1 step to move to the other side of l and the second nearest ones need 4 steps and so on. There will be $2\lfloor \frac{t_3-1}{3} \rfloor + 1$ edges on the two sides moving to the other side of l. They do not belong to N_e and should be subtracted. Similarly, $2\lfloor \frac{t_3-2}{3} \rfloor + 2$ and $2\lfloor \frac{t_3}{3} \rfloor$ edges move to the other side of l when l is in positions II and III with respect to N'_e, respectively. In the following, we use I, II, III shortly for the meaning that l is in the three positions with respect to N'_e, respectively.

Case 1. $t_3 \equiv 0 \pmod 3$.

I: Observe that the obtained nearest two edges of N_e to l on both sides coincide on l after the moving of the edges of N'_e, which implies that we should eliminate one more edge. Hence, $m = 2\lfloor \frac{t_3-1}{3} \rfloor + 1 + 1 = \frac{2t_3}{3}$. II: $m = 2\lfloor \frac{t_3-2}{3} \rfloor + 2 = \frac{2t_3}{3}$. III: $m = 2\lfloor \frac{t_3}{3} \rfloor = \frac{2t_3}{3}$.

Case 2. $t_3 \equiv 1 \pmod 3$.

I: $m = 2\lfloor \frac{t_3-1}{3} \rfloor + 1 = \frac{2t_3}{3} + \frac{1}{3}$. II: $m = 2\lfloor \frac{t_3-2}{3} \rfloor + 2 + 1 = \frac{2t_3}{3} + \frac{1}{3}$, where one more edge is eliminated for the same reason as in Case 1. III: $m = 2\lfloor \frac{t_3}{3} \rfloor = \frac{2t_3}{3} - \frac{2}{3}$.

Case 3. $t_3 \equiv 2 \pmod 3$.

I: $m = 2\lfloor \frac{t_3-1}{3} \rfloor + 1 = \frac{2t_3}{3} - \frac{1}{3}$. II: $m = 2\lfloor \frac{t_3-2}{3} \rfloor + 2 = \frac{2t_3}{3} + \frac{2}{3}$. III: $m = 2\lfloor \frac{t_3}{3} \rfloor + 1 = \frac{2t_3}{3} - \frac{1}{3}$, where one more edge is eliminated.

Then we compute $|N_e|$ in the nine cases with respect to the values of t_3 and the positions of l in $T'_0(k)$. By (1), when $k - 1 - t_1 - t_2 = k - 1 \equiv 1, 2, 0 \pmod 3$, l is in I, II, III, respectively. The values of $|N_e|$ of the nine cases are computed in the following tabular:

	I ($k-1 \equiv 1 \pmod 3$)	II ($k-1 \equiv 2 \pmod 3$)	III ($k-1 \equiv 0 \pmod 3$)
$t_3 \equiv 0 (\mathrm{mod} 3)$	$\frac{2}{3}(k - t_3 + 2) + \frac{1}{3}$	$\frac{2}{3}(k - t_3 + 2) + \frac{2}{3}$	$\frac{2}{3}(k - t_3 + 2)$
$t_3 \equiv 1 (\mathrm{mod} 3)$	$\frac{2}{3}(k - t_3 + 2)$	$\frac{2}{3}(k - t_3 + 2) + \frac{1}{3}$	$\frac{2}{3}(k - t_3 + 2) + \frac{2}{3}$
$t_3 \equiv 2 (\mathrm{mod} 3)$	$\frac{2}{3}(k - t_3 + 2) + \frac{2}{3}$	$\frac{2}{3}(k - t_3 + 2)$	$\frac{2}{3}(k - t_3 + 2) + \frac{1}{3}$

For example, when $t_3 \equiv 1 \pmod 3$ and l is in position I ($k - 1 \equiv 1 \pmod 3$), $|N_e| = 2k - \lfloor \frac{4}{3}(k-1) \rfloor - m = 2k - \lfloor \frac{4}{3}(k-1) \rfloor - (\frac{2t_3}{3} + \frac{1}{3}) = \frac{2k}{3} - \frac{2t_3}{3} + 2 = \frac{2}{3}(k - t_3 + 2)$.

We can summarize the nine cases in the tabular to the formula $|N_e| = \lceil \frac{2}{3}(k - t_3 + 2) \rceil$.

If $k < t_3$, then $|N_e| = 1$ and the only edge of N_e lies on P''. □

3 A formula for PI index of H(p, q)

Ye and Zhang [16] showed that, for any two edges $e = u_1u_2, e' = v_1v_2 \in M_i$ $(i = 1, 2, 3)$, there is an automorphism φ of $H(p, q)$ mapping e to e'. Since automorphisms preserve distances, it can be seen that $n_{u_1}(e) + n_{u_2}(e) = n_{\varphi(u_1)}(e') + n_{\varphi(u_2)}(e')$, where $\{\varphi(u_1), \varphi(u_2)\} = \{v_1, v_2\}$. Thus $|N_e| = |N_{e'}|$. Hence, we need only compute $|N_e|$ for one edge e in each of M_1, M_2 and M_3 in $H(p, q)$. Moreover, $|M_1| = |M_2| = |M_3| = pq$.

Lemma 3.1. *$PI(H(1, 1)) = 0$.*

Proof. $H(1, 1)$ can be drawn in another way as in Figure 5 (b). Hence, $PI(H(1, 1)) = 0$.

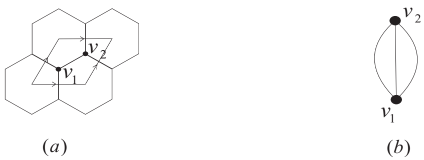


Figure 5. (a), $H(1,1)$; (b), a graph isomorphic to $H(1,1)$.

□

Lemma 3.2.

$$PI(H(p,1)) = PI(H(1,p)) = \begin{cases} 9p(p-1), & \textit{if } p \textit{ is odd;} \\ 9p^2 - 10p, & \textit{otherwise.} \end{cases}$$

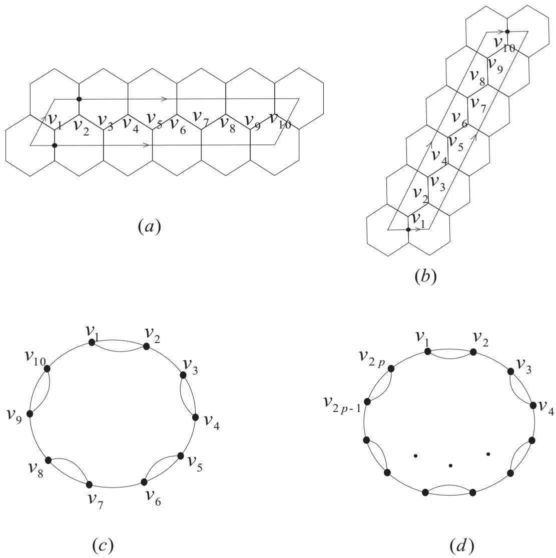


Figure 6. (a), $H(5,1)$; (b), $H(1,5)$; (c), a graph isomorphic to $H(5,1) \cong H(1,5)$; (d), a graph isomorphic to $H(p,1) \cong H(1,p)$.

Proof. It can be seen, from Figure 6, that $H(p,1) \cong H(1,p)$ is isomorphic to the graph of Figure 6 (d).

Case 1. p is odd.

$|N_e| = 3$ for each edge e of $H(p,1) \cong H(1,p)$. For example, $N_{e=v_1v_2}$ consists of the 2 multiple edges of v_1v_2 and edge $v_{p+1}v_{p+2}$ since $d(v_2, v_{p+1}) = d(v_{p+2}, v_1) = p-1$. Thus

$$PI(H(p,1)) = PI(H(1,p)) = \sum_{e \in E}(|E| - |N_e|) = 3p(3p-3) = 9p(p-1).$$

Case 2. p is even.

$$|N_e| = \begin{cases} 4, & \text{if } e = v_{2k+1}v_{2(k+1)} \text{ for } k = 0, 1, \ldots, p-1; \\ 2, & \text{if } e = v_{2k}v_{2k+1} \text{ for } k = 1, \ldots, p-1 \text{ or } e = v_{2p}v_1. \end{cases}$$

Thus

$$PI(H(p,1)) = PI(H(1,p)) = \sum_{e \in E}(|E| - |N_e|) = 2p(3p-4) + p(3p-2) = 9p^2 - 10p.$$

□

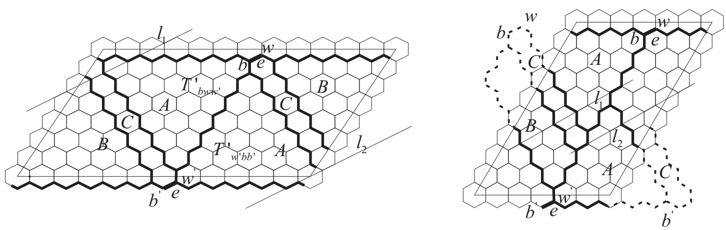
Then we assume that $p, q \geqslant 2$ in the following.

Lemma 3.3. *Let e be a left slant edge of $H(p,q)$. Then*

$$|N_e| = \begin{cases} \theta(p) \cdot q + 4q - 2, & \text{if } p \geqslant 2q-1; \\ \theta(p)(p-1-q) + 8q - 2p - 2(\lfloor \frac{4}{3}(2q-p-2) \rfloor & \\ + \lfloor \frac{2}{3}(2q-p-2) \rfloor) - 8, & \text{if } q < p < 2q-1; \\ q + 2\lceil \frac{2}{3}(q+1) \rceil - 2, & \text{if } p = q; \\ \theta(q)(q-p-1) + 8p - 2q - 2(\lfloor \frac{4}{3}(2p-q-2) \rfloor & \\ + \lfloor \frac{2}{3}(2p-q-2) \rfloor) - 8, & \text{if } p < q < 2p-1; \\ \theta(q) \cdot p + 4p - 2, & \text{otherwise.} \end{cases}$$

Proof. Let $e = wb$ $(= w'b')$ be the left slant edge lying in the middle of the first row of the $p \times q$-parallelogram used to present $H(p,q)$ by usual torus boundary identification (see Figure 7). We divide $H(p,q)$ into three subgraphs A, B and C, where A is the union of $T'_{bw'w}$ (T_b for short) and $T'_{w'bb'}$ ($T_{w'}$ for short) defined in Lemma 2.3, C consists of the parallel edges of e in the same columns with wb and $w'b'$ outside A, and B is $B(m,n)$, defined in Lemma 2.1, containing the leaving edges. The division is illustrated in Figure 7.

Note that $A \cup B \cup C$ covers all the edges of $H(p,q)$ and $e = A \cap B \cap C$. Then the equidistance edges of e in each of the three subgraphs make up of N_e in $H(p,q)$.



(*a*) (*b*)

Figure 7. Division of the edges of $H(p,q)$ into three parts A, B, C.

If $H \subseteq H(p,q)$, set $N_e[H] = N_e \bigcap E(H)$. Then $|N_e[A]| = |N_e[T_b]| + |N_e[T_{w'}]| - |N_e[T_b] \cap N_e[T_{w'}]|$. Observe that in both of A and B, the distance between any vertex and e is equal to their distance in $H(p,q)$. Hence, we can compute $|N_e[A]|$ and $|N_e[B]|$ according to Lemmas 2.1, 2.2 and 2.3.

As $e \in N_e[A] \cap N_e[B] \cap N_e[C]$, we count e in $N_e[C]$.

To compute $|N_e[C]|$, note that only the parallel edges in the same column with $b'w'$ below l_1 and the parallel edges of bw above l_2 belong to $N_e[C]$ when $p \geqslant q$, where l_1 and l_2 are the bisecting lines of T_b and $T_{w'}$, respectively, defined in the proof Lemma 2.3. Moreover, each LDP of $T_b \cup T_{w'}$ between l_1 and l_2 contains an edge of $N_e[A]$ as well as an edge of $N_e[C]$. Hence, $|N_e[C]|$ equals the number of edges of $N_e[A]$ below l_1 and above l_2 when $p \geqslant q$, which is $2|N(e') \setminus \overline{N(e')}| - 1$ by the proof of Lemma 2.3. Similarly, $|N_e[C]|$ equals the number of edges of $N_e[A]$ above l_1 or below l_2 when $q > p$. That is $2|N(e) \setminus \overline{N(e)}| - 1$. See Figure 8 (b) and (d) respectively. To compute $|N_e|$, five cases are distinguished.

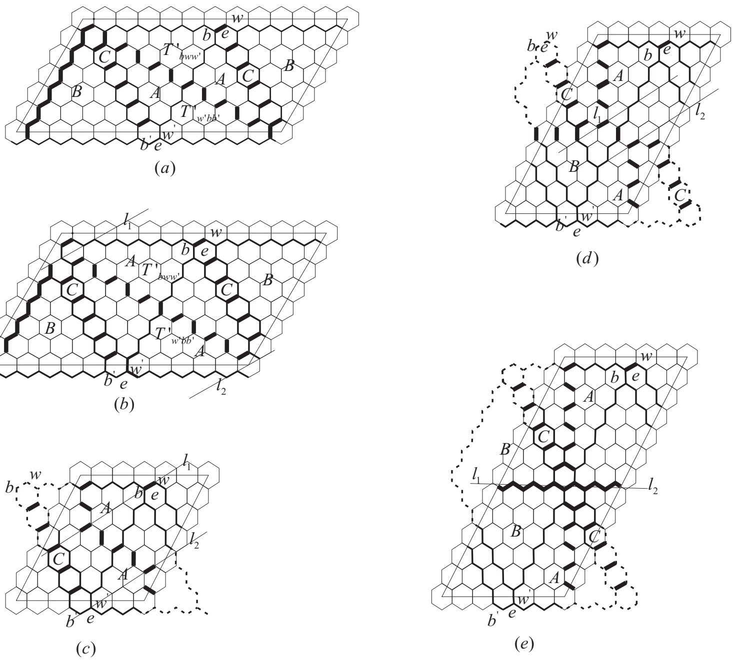


Figure 8. Illustration for the proof of Lemma 3.3: N_e consists of all the edges in bold.

Case 1. $p \geqslant 2q - 1$ (see Figure 8 (a)).

By Lemma 2.3 (1), since $t_3 = t_2 = 0$ and $t_1 = p - q - 1 \geqslant q > k = q - 1$, $|N_e[T_b]| =$

$|N_e[T_{w'}]| = k + 2 - t_1 = q - 1 + 2 = q + 1$. Thus

$$|N_e[A]| = |N_e[T_b]| + |N_e[T_{w'}]| - 2 = 2q$$

for $N_e[T_b]$ and $N_e[T_{w'}]$ have two edges in common on their common boundary.

$|N_e[C]|$ equals the number of edges of $N_e[A]$ below l_1 and above l_2. Since $t_1 \geqslant k$, all the edges of $N_e[A]$ except the one in the first row lying between l_1 and l_2. Thus

$$|N_e[C]| = |N_e[A]| - 1 = 2q - 1.$$

For B, note in this case that $N_e[B]$ and the edge of $N_e[A]$ lying in the same (the first) row with e form a column of right slant edges when p is odd or form a column of LDP otherwise. Then

$$|N_e[B] \cup N_e[A]| = \theta(p) \cdot q + |N_e[A]| - 1 = \theta(p) \cdot q + 2q - 1.$$

Hence,

$$|N_e| = |N_e[B] \cup N_e[A]| + |N_e[C]| = \theta(p) \cdot q + 4q - 2.$$

Case 2. $q < p < 2q - 1$ (see Figure 8 (b)).

Using Lemma 2.3 (1), $t_3 = 0$, $k = q - 1$, $t_1 + t_2 = p - q$ in T_b and $T_{w'}$. Then

$$\begin{aligned} |N_e[T_b]| &= |N_e[T_{w'}]| = 2(q-1) - (p-q) - \lfloor \frac{4}{3}(2q-p-2) \rfloor \\ &= 3q - p - 2 - \lfloor \frac{4}{3}(2q-p-2) \rfloor. \end{aligned}$$

Still, $|N_e[T_b] \cap N_e[T_{w'}]| = 2$. Hence,

$$|N_e[A]| = 2(3q - p - 2 - \lfloor \frac{4}{3}(2q-p-2) \rfloor) - 2.$$

By the proof of Lemma 2.3, $|N(e') \setminus \overline{N(e')}| = (k + 1 - t_2) - (\lfloor \frac{2}{3}(2q-p-2) \rfloor + 1) = q - \lfloor \frac{2}{3}(2q-p-2) \rfloor - 1$. Then

$$|N_e[C]| = 2(q - \lfloor \frac{2}{3}(2q-p-2) \rfloor - 1) - 1.$$

At last, by Lemma 2.1, we have

$$|N_e[B]| = \theta(p) \cdot (p - 1 - q) + 1$$

for $\min\{m, n\} = \min\{p - q - 1, q\} = p - q - 1$ and $m + n - 1 = p - 2 \equiv p \pmod 2$.

Then

$$\begin{aligned} |N_e| &= |N_e[A]| + |N_e[B]| + |N_e[C]| \\ &= \theta(p)(p - 1 - q) + 8q - 2p - 2(\lfloor \frac{4}{3}(2q-p-2) \rfloor + \lfloor \frac{2}{3}(2q-p-2) \rfloor) - 8. \end{aligned}$$

Case 3. $p = q$ (see Figure 8 (c)).

In this case, B consists of only the edge e. Hence $|N_e[B]| = 0$ since we count e in $N_e[C]$.

By Lemma 2.3 and $|N_e[T_b] \cap N_e[T_{w'}]| = 2$,

$$|N_e[A]| = 2\lceil \frac{2}{3}(q+1) \rceil - 2.$$

$|N_e[C]| = q$ for the edges of $N_e[T_b]$ above l_1 and those of $N_e[T_{w'}]$ below l_2 form a whole column of edges parallel e. Thus

$$|N_e| = q + 2\lceil \frac{2}{3}(q+1) \rceil - 2.$$

Case 4. $p < q < 2p - 1$ (see Figure 8 (d)). The calculation is symmetric to that of Case 2.

As in Case 2, by Lemma 2.3 (1), since $t_3 = 0, k = p - 1$ and $t_1 + t_2 = q - p < k$ in T_b and $T_{w'}$,

$$|N_e[A]| = 2(3p - q - 2 - \lfloor \frac{4}{3}(2p - q - 2) \rfloor) - 2.$$

Since $q > p$, only the edges of C above l_1 or below l_2 belong to N_e. By the proof of Lemma 2.3 and $|N_e[C]| = 2|N(e) \setminus \overline{N(e)}| - 1$,

$$|N_e[C]| = 2(p - \lfloor \frac{2}{3}(2p - q - 2) \rfloor - 1) - 1.$$

By Lemma 2.1,

$$|N_e[B]| = \theta(q) \cdot (q - p - 1) + 1.$$

The summation of $|N_e[A]|$, $|N_e[B]|$ and $|N_e[C]|$ comes up to the expression in the Lemma.

Case 5. $q \geqslant 2p - 1$ (see Figure 8 (e)).

By Lemma 2.3,

$$|N_e[A]| = 2(p - 1 + 2) - 2 = 2p$$

since $|N_e[T_b] \cap N_e[T_{w'}]| = 2$.

As before, each edge of $N_e[A]$ corresponds to an edge of $N_e[C]$ except the one on the LDP from b to w'. Then we have

$$|N_e[C]| = 2p - 1.$$

Analogy to Case 1, $N_e[B]$ together with the edge of $N_e[A]$ on the LDP from b to w' form a row of vertical edges when q is odd or form a row of edges consisting of left slant edges and right slant edges alternatively otherwise. Then

$$\begin{aligned} |N_e[B] \cup N_e[A]| &= \theta(q) \cdot p + |N_e[A]| - 1 \\ &= \theta(q) \cdot p + 2p - 1. \end{aligned}$$

Finally, $|N_e| = |N_e[B] \cup N_e[A]| + 2p - 1 = \theta(q) \cdot p + 4p - 2$ in this case. □

Figure 8 (a) gives an example in which the edges in bold are all the edges of N_e and the number is 34, which coincides with $\theta(q) \cdot p + 4p - 2 = 2 \times 6 + 4 \times 6 - 2 = 34$. We will do the jobs for right slant edges and vertical edges in a similar way. So the calculations will be done with less explanations.

Lemma 3.4. *For any right slant edge e of $H(p, q)$,*

$$|N_e| = \begin{cases} \theta(p-1) \cdot q + q, & \textit{if } p \geqslant 2q - 1; \\ \theta(p-1)(p-q) + q + 2\lceil \frac{2}{3}(2q - p + 1) \rceil - 2, & \textit{if } q < p < 2q - 1; \\ q + 2\lceil \frac{2}{3}(q+1) \rceil - 2, & \textit{if } p = q; \\ \theta(q)(q-p) + 6p - q - 2\lfloor \frac{4}{3}(2p - q - 2) \rfloor - 6, & \textit{if } p < q < 2p - 1; \\ \theta(q) \cdot p + 4p - 2, & \textit{otherwise.} \end{cases}$$

Proof. As in the case of left slant edges, we choose the right slant edge $e = wb$ $(= w'b')$ in the middle of the first row of the $p \times q$-parallelogram. We still divide the edge set of $H(p, q)$ into three subgraphs: A is the union of $T'_{bw'w}$ (T_b for short) and $T'_{w'bb'}$ ($T_{w'}$ for short); C contains the parallel edges of wb and $w'b$ in the same columns with them outside A; And B is $B(m, n)$ containing the leaving edges. l_1, l_2 are the bisecting lines of T_b and $T_{w'}$, respectively. The division is illustrated in Figure 9. Similarly, we distinguish five cases.

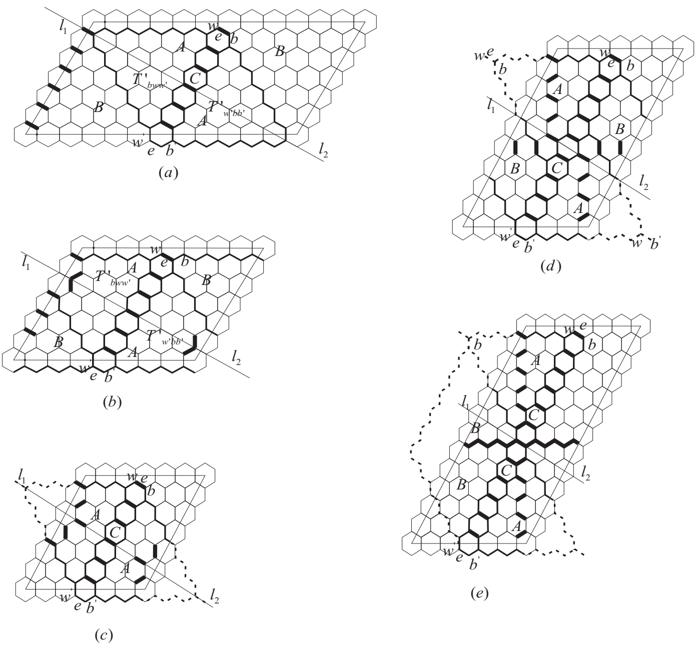


Figure 9. Illustration for the proof of Lemma 3.4: N_e consists of all the edges in bold.

Case 1. $p \geqslant 2q-1$ (see Figure 9 (a)).

By Lemma 2.3, $t_1 = t_2 = 0$, $t_3 > k$. Thus $|N_e[A]| = 1$.

However, $N_e[A] \cup N_e[B]$ is a column of right slant edges when $p-1$ is odd (illustrated in Figure 9 (a)) or a column of LDP otherwise. Thus

$$|N_e[A] \cup N_e[B]| \quad = \quad \theta(p-1) \cdot q.$$

For C, note that all the edges of C below l_1 or above l_2 belong to $N_e[C]$. Since l_1, l_2 also bisect the LDPs from w to w' and from b to b', respectively, they coincide. Thus

$$|N_e[C]| \quad = \quad q.$$

At last,

$$|N_e| = \theta(p-1) \cdot q + q.$$

Case 2. $q < p < 2q-1$ (see Figure 9 (b)).

Using Lemma 2.3, since $k = q-1, t_1 = t_2 = 0, t_3 = p-q$ when $q < p < 2q-1$,

$$|N_e[A]| \quad = \quad 2\lceil \frac{2}{3}(2q-p+1) \rceil - 1$$

for $N_e[T_b]$ and $N_e[T_{w'}]$ have an edge in common on the first row.

As above,

$$|N_e[C]| \quad = \quad q.$$

Using Lemma 2.1, since min$\{m,n\}$ =min$\{p-q, q\} = p-q$ and $m+n-1 = p-1$,

$$|N_e[B]| \quad = \quad \theta(p-1) \cdot (p-q) + 1.$$

Since $|N_e[A] \cap N_e[B]| = 2$, we have

$$|N_e| \quad = \quad \theta(p-1)(p-q) + q + 2\lceil \frac{2}{3}(2q-p+1) \rceil - 2.$$

Case 3. $p = q$ (see Figure 9 (c)).

As the Case 3 in Lemma 3.3, $|N_e[B]| = 0$ and

$$|N_e[A]| \quad = \quad 2\lceil \frac{2}{3}(q+1) \rceil - 2.$$

Moreover, $|N_e[C]| = q$. Thus

$$|N_e| = q + 2\lceil \frac{2}{3}(q+1) \rceil - 2.$$

Case 4. $p < q < 2p - 1$ (see Figure 9 (d)).

By Lemma 2.3 (1), since $t_3 = 0, k = p - 1$ and $t_1 + t_2 = q - p$ in T_b and $T_{w'}$,

$$\begin{aligned} |N_e[A]| &= 2(2(p-1) - (q-p) - \lfloor \frac{4}{3}(p - 1 - (q-p) - 1) \rfloor) - 1 \\ &= 2(3p - q - 2 - \lfloor \frac{4}{3}(2p - q - 2) \rfloor) - 1. \end{aligned}$$

Since only the edges of C above l_1 or below l_2 belong to N_e and l_1, l_2 coincide,

$$|N_e[C]| = q.$$

At last,

$$|N_e[B]| = \theta(q)(q - p) + 1.$$

Since $|N_e[A] \cap N_e[B]| = 2$,

$$|N_e| = \theta(q)(q-p) + 6p - q - 2\lfloor \frac{4}{3}(2p - q - 2) \rfloor - 6.$$

Case 5. $q \geqslant 2p - 1$ (see Figure 9 (e)).

Since $t_2 \geqslant k + t_1$, by Lemma 2.3, $|N_e[T_b]| = p + 1$. Thus

$$|N_e[A]| = 2p + 1$$

for $|N_e[T_b] \cap N_e[T_{w'}]| = 1$.

Each edge of $N_e[A]$ corresponds to an edge of $N_e[C]$ except the two edges on the two LDPs from w to w' and from b to b', respectively. Then

$$|N_e[C]| = |N_e[A]| - 2 = 2p - 1.$$

However, $N_e[B]$ and the two edges of $N_e[A]$ on the two LDPs from b to b' and from w to w', respectively, form a whole row of vertical edges when q is odd. And they form a whole row of edges consisting of left and right slant edges alternatively when q is even. Thus

$$\begin{aligned} |N_e| &= |N_e[B] \cup N_e[A]| + 2p - 1 \\ &= \theta(q) \cdot p + |N_e[A]| - 2 + 2p - 1 \\ &= \theta(q) \cdot p + 4p - 2. \end{aligned}$$

□

Lemma 3.5. *For any vertical edge e of $H(p, q)$,*

$$|N_e| = \begin{cases} \theta(p) \cdot q + 4q - 2, & \text{if } p \geqslant 2q - 1; \\ \theta(p)(p-q) + 6q - p - 2\lfloor \frac{4}{3}(2q - p - 2) \rfloor - 6, & \text{if } q < p < 2q - 1; \\ q + 2\lceil \frac{2}{3}(q+1) \rceil - 2, & \text{if } p = q; \\ \theta(q-1)(q-p) + p + 2\lceil \frac{2}{3}(2p - q + 1) \rceil - 2, & \text{if } p < q < 2p - 1; \\ \theta(q-1) \cdot p + p, & \text{otherwise.} \end{cases}$$

Proof. Choose a vertical edge, say $e = wb = w'b'$, in $H(p,q)$ as in Figure 10. Similarly, we divide the edges of $H(p,q)$ into three parts: A is the union of $T'_{wbb'} = T_w$ and $T'_{b'ww'} = T_{b'}$; C consists of all the parallel edges of wb in the same row with it; B is $B(m,n)$ containing the leaving edges.

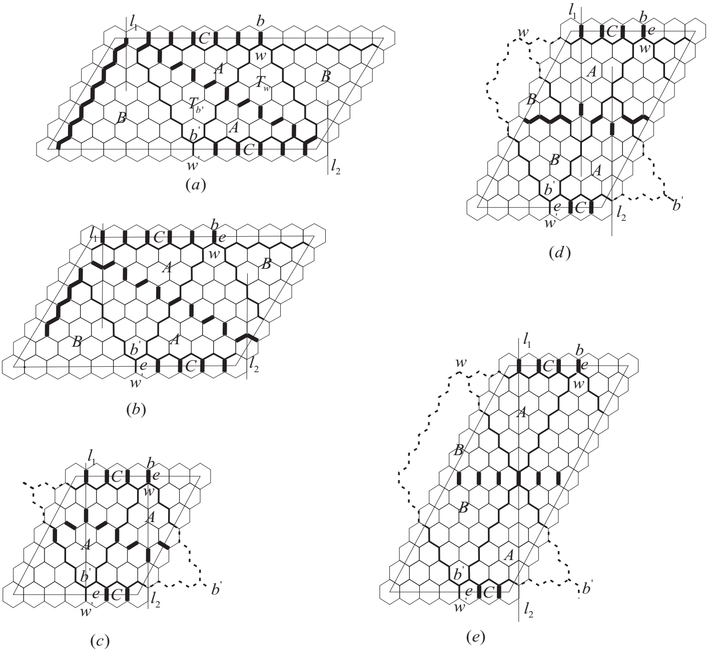


Figure 10. Illustration for the proof of Lemma 3.5: N_e consists of all the edges in bold.

Case 1. $p \geqslant 2q-1$ (see Figure 10 (a)).

$$|N_e[A]| \quad = \quad 2(q+1) - 1 = 2q + 1$$

for $|N_e[T_{b'}] \cap N_e[T_w]| = 1$.

For C, only the parallel edges of bw on the right hand of l_1 (the bisector line of $T_{b'}$) and the parallel edges of $b'w'$ on the left hand of l_2 (the bisector line of T_w) belong to $N_e[C]$. As before, each edge of $N_e[C]$ corresponds to an edge of $N_e[A]$ between l_1 and l_2. Since $p \geqslant 2q-1$,

$$|N_e[C]| \quad = \quad |N_e[A]| - 2 = 2q - 1.$$

Now, the whole column of right slant edges containing $N_e[B]$ belong to N_e when p is odd. And the edges of the whole column of LDP containing $N_e[B]$ belong to N_e when p is even, where they contain two of $N_e[A]$ and one of C that has not been counted in $N_e[C]$. Then

$$\begin{aligned} |N_e| &= (|N_e[B] \cup N_e[A]| + 1) + 2q - 1 \\ &= (\theta(p) \cdot q + |N_e[A]| - 2) + 2q - 1 \\ &= \theta(p) \cdot q + 4q - 2. \end{aligned}$$

Case 2. $q < p < 2q - 1$ (see Figure 10 (b)).

$$|N_e[A]| = 2(3q - p - 2 - \lfloor \frac{4}{3}(2q - p - 2) \rfloor) - 1$$

for $|N_e[T_{b'}] \cap N_e[T_w]| = 1$.

Using Lemma 2.1, $\min\{m, n\} = \min\{p - q, q - 1\} = p - q$ and $m + n - 1 = p - 2 \equiv p \pmod 2$. Then

$$|N_e[B]| = \theta(p) \cdot (p - q) + 1.$$

Note that l_1 and l_2 coincide under the identifying of the top and bottom side of the $p \times q$-parallelogram. Hence the parallel edges of bw on the right hand of l_1 and the parallel edges of $b'w'$ on the left hand of l_2 form a whole row of vertical edges. Thus

$$|N_e[C]| = p.$$

In fact, $|N_e[C]| = p$ for the following three cases by the same reason.

Since $|N_e[A] \cap N_e[B]| = 2$,

$$\begin{aligned} |N_e| &= |N_e[A]| + |N_e[B]| + |N_e[C]| - 2 \\ &= \theta(p)(p - q) + 6q - p - 2\lfloor \frac{4}{3}(2q - p - 2) \rfloor - 6. \end{aligned}$$

Case 3. $p = q$ (see Figure 10 (c)).

As before, $|N_e[B]| = 0$ and

$$|N_e[A]| = 2\lceil \frac{2}{3}(q + 1) \rceil - 2.$$

Thus

$$|N_e| = q + 2\lceil \frac{2}{3}(q + 1) \rceil - 2$$

for $|N_e[C]| = q$.

Case 4. $p < q < 2p - 1$ (see Figure 10 (d)).

As before, using Lemma 2.3 (2), since $t_1 = t_2 = 0, t_3 = q - p$ and $k = p - 1$,

$$|N_e[A]| = 2\lceil \frac{2}{3}(2p - q + 1) \rceil - 1.$$

And by Lemma 2.1,

$$|N_e[B]| \;=\; \theta(q-1)\cdot(q-p)+1.$$

Since $|N_e[A]\cap N_e[B]| = 2$ and $|N_e[C]| = p$,

$$|N_e| \;=\; \theta(q-1)(q-p)+p+2\lceil\frac{2}{3}(2p-q+1)\rceil-2.$$

Case 5. $q \geqslant 2p-1$ (see Figure 10 (e)).

$$|N_e[A]| \;=\; 1$$

for $t_3 \geqslant p > k = p-1$ in Lemma 2.3. And the only edge of $N_e[A]$ lies on the LDP from w to w'.

However, the only edge of $N_e[A]$ together with $N_e[B]$ forms a row of vertical edges when $(q-1)$ is odd and they form a row of edges consisting of left slant edges and right slant edges alternatively when $(q-1)$ is even. Thus

$$|N_e[A]\cup N_e[B]| \;=\; \theta(q-1)\cdot p.$$

Finally, $|N_e| = \theta(q-1)\cdot p + p$ since $|N_e[C]| = p$. □

Theorem 3.6. *The PI index of the toroidal polyhex $H(p,q)$ $(p,q \geqslant 2)$ can be expressed as:*

$$PI(H(p,q)) = \begin{cases} 9p^2q^2 - pq[\theta(p)\cdot q + 12q - 4], & \text{if } p \geqslant 2q-1;\\ 9p^2q^2 - pq[\theta(p)\cdot(p-q-1) + 12q- & \\ 4\lfloor\frac{4}{3}(2q-p-2)\rfloor - 2\lfloor\frac{2}{3}(2q-p-2)\rfloor & \\ +2\lceil\frac{2}{3}(2q-p+1)\rceil - 16], & \text{if } q < p < 2q-1;\\ 9p^2q^2 - 3pq(q+2\lceil\frac{2}{3}(q+1)\rceil - 2), & \text{if } p = q;\\ 9p^2q^2 - pq[\theta(q)\cdot(q-p-1) + 12p- & \\ 4\lfloor\frac{4}{3}(2p-q-2)\rfloor - 2\lfloor\frac{2}{3}(2p-q-2)\rfloor + & \\ 2\lceil\frac{2}{3}(2p-q+1)\rceil - 16], & \text{if } p < q < 2p-1;\\ 9p^2q^2 - pq[\theta(q)\cdot p + 12p - 4], & \text{otherwise,} \end{cases}$$

where $\theta(X) = \frac{3}{2} + \frac{(-1)^X}{2}$.

Proof. The calculation of $PI(H(p,q))$ can be obtained following the above three Lemmas.

$$\begin{aligned} PI(H(p,q)) &= \sum_{e\in E}(|E|-|N_e|) \\ &= \sum_{i=1}^{3}|M_i|\cdot(|E|-|N_{e_i}|) \\ &= |E|^2 - \sum_{i=1}^{3}|M_i|\cdot|N_{e_i}|, \end{aligned}$$

where $e_i \in M_i$ for $i = 1, 2, 3$.

Since $|M_1| = |M_2| = |M_3| = pq$, $|E| = 3pq$ and $\theta(X) + \theta(X-1) = 3$, the PI index of $H(p, q)$ is then obtained by substituting $|N_{e_i}|$ $(i = 1, 2, 3)$ into the above equation. $\square$

Remark: The formula of $PI(H(p, q))$ obtained in this paper is highly symmetric with respect to the above five cases. The symmetric property reflected from the formula consists with the structure property of toroidal polyhexes [12].

Besides providing the formula for $PI(H(p, q))$, one of the main aims of the paper is to present a way for computing the PI index of all the toroidal polyhexes with torsion $t \neq 0$.

References

[1] A. R. Ashrafi, A. Loghman, PI index of zig-zag polyhex nanotubes, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 447–452.

[2] A. R. Ashrafi, F. Rezaei, PI index of polyhex nanotori, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 243–250.

[3] H. Deng, The PI index of $TUVC_6[2p; q]$, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 461–476.

[4] I. Gutman, A formula for the Wiener number of trees and its extension to graphs containing cycles, *Graph Theory Notes N. Y.* **27** (1994) 9–15.

[5] M. H. Khalifeha, H. Yousefi-Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, *Discr. Appl. Math.* **156** (2008) 1780–1789.

[6] P. V. Khadikar, On a novel structural descriptor PI, *Nat. Acad. Sci. Lett.* **23** (2000) 113–118.

[7] P. V. Khadikar, P. P. Kale, N. V. Deshpande, S. Karmarkar, V. K. Agrawal, Novel PI indices of hexagonal chains, *J. Math. Chem.* **29** (2001) 143–150.

[8] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, PI index of polyacenes and its use in developing QSPR, *Nat. Acad. Sci. Lett.* **23** (2000) 124–128.

[9] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, Relationships and relative correlation potential of the Wiener, Szeged and PI Indices, *Nat. Acad. Sci. Lett.* **23** (2000) 165–170.

[10] P. V. Khadikar, S. Karmarkar, V. K. Agrawal, A novel PI index and its applications to QSPR/QSAR studies, *J. Chem. Inf. Comput. Sci.* **41** (2001) 934–949.

[11] P. V. Khadikar, S. Karmarkar, R. G. Varma, The estimation of PI index of polyacenes, *Acta Chim. Slov.* **49** (2002) 755–771.

[12] E. C. Kirby, R. B. Mallion, P. Pollak, Toroidal polyhexes, *J. Chem. Soc. Faraday Trans.* **89** (1993) 1945–1953.

[13] S. Klavžar, On the PI index: PI-partitions and cartesian product graphs, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 573–586.

[14] P. E. John, P. V. Khadikar, J. Singhc, A method of computing the PI index of benzenoid hydrocarbons using orthogonal cuts, *J. Math. Chem.* **42** (2007) 37–45.

[15] H. Wiener, Structural determination of paraffin boiling points, *J. Am. Chem. Soc.* **69** (1947) 17–20.

[16] D. Ye, H. Zhang, 2-Extendability of toroidal polyhexes and klein-bottle polyhexes, *Discr. Appl. Math.* **157** (2009) 292–299.