

# The forcing number of toroidal polyhexes

Hongwei Wang, Dong Ye, and Heping Zhang\*

*School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000,  
People's Republic of China  
E-mail: zhanghp@lzu.edu.cn*

Hongwei Wang

*Department of Mathematics, Linyi Normal University, Linyi, Shandong 276005,  
People's Republic of China*

Received 28 August 2006; accepted 20 September 2006

The forcing number, denoted by  $f(G)$ , of a graph  $G$  with a perfect matching is the minimum number of independent edges that completely determine the perfect matching of  $G$ . In this paper, we consider the forcing number of a toroidal polyhex  $H(p, q, t)$  with a torsion  $t$ , a cubic graph embedded on torus with every face being a hexagon. We obtain that  $f(H(p, q, t)) \geq \min\{p, q\}$ , and equality holds for  $p \leq q$  or  $p > q$  and  $t \in \{0, p - q, p - q + 1, \dots, p - 1\}$ . In general, we show that  $f(H(p, q, t))$  is equal to the side length of a maximum triangle on  $H(p, q, t)$ . Based on this result, we design a linear algorithm to compute the forcing number of  $H(p, q, t)$ .

**KEY WORDS:** toroidal polyhex, forcing number, kekulé structure, perfect matching

## 1. Introduction

The concept of forcing number of benzenoids was first proposed by Harary et al. [4]. The same idea appeared in earlier papers by Randić and Klein [15] and Klein and Randić [5] in terms of “innate degree of freedom” of a Kekulé structure. The benzenoids with forcing number 1 was investigated in [21–24]. The forcing number of Buckminsterfullerene ( $C_{60}$ ) have been given by Vukičević et al. [18].

In this paper we gives a fast computation for the forcing number of a toroidal polyhex, or toroidal fullerene, a cubic bipartite graph on torus such that every face is a hexagon [9], which can be denoted by  $H(p, q, t)$  for a string  $(p, q, t)$  of three integers ( $p \geq 1, q \geq 1, 0 \leq t \leq p - 1$ ). In 1997, the “Crop circles fullerenes” discovered by Liu et al. [13] has been presumably torus-shaped.

\*Corresponding author.

Enumeration of isomers [10], Kekulé structure count [6], spanning tree count [8], and chirality [11] of toroidal polyhexes have been investigated.

Our approach relies on a general research on the forcing number of a bipartite graph with a perfect matching (or Kekulé structure in chemistry). Let  $G$  be a graph with a perfect matching  $M$ . A set  $S \subset M$  is called a *forcing set* of  $M$  if  $S$  is not contained in any other perfect matchings of  $G$ . The *forcing number* of  $M$ , denoted by  $f(G, M)$ , is the minimum size of forcing sets of  $M$ . The *forcing number* of  $G$ , denoted by  $f(G)$ , is the minimum value of the forcing numbers of all perfect matchings of  $G$ .

Recently, the forcing numbers of bipartite graphs [1, 2], in particular, for square grids [14], stop signs [12], torus, and hypercube [1, 7, 16], have been considered. Riddle [16] gave a lower bound of the forcing number of bipartite graphs. Adams et al. [1] proved it is NP-complete to find the smallest forcing set of a bipartite graph with maximum degree 3. Most recently, the global forcing number and anti-forcing number of benzenoids were introduced by Došlić [3], Vukičević and Sedlar [19], and Vukičević and Trinajstić [20], respectively.

By improving Riddle's method which produces a lower bound of the forcing number of bipartite graphs we determine the forcing numbers of toroidal polyhexes  $H(p, q, t)$ . For the degenerated cases:  $H(1, q, 0)$ ,  $H(p, 1, 0)$ , and  $H(p, 1, p-1)$ , their forcing numbers equal one. From now on we suppose that toroidal polyhexes in question always means the non-degenerated cases. We prove that  $f(H(p, q, t)) \geq \min\{p, q\}$ , and equality holds for  $p \leq q$  or  $p > q$  and  $t \in \{0, p-q, p-q+1, \dots, p-1\}$ . Generally, we prove that  $f(H(p, q, t))$  is equal to the side length of a maximum triangle on  $H(p, q, t)$ . Finally, we design a fast algorithm of  $O(n)$  times to compute the forcing number of  $H(p, q, t)$ , where  $n$  is the number of vertices of  $H(p, q, t)$ .

## 2. Preliminaries for toroidal polyhex

A *toroidal polyhex*  $H(p, q, t)$  can be defined as: Let  $P$  be a  $p \times q$  parallelogram section cut from the hexagonal lattice such that every corner lies on the center of a hexagon, two lateral sides pass through  $q$  oblique edges, top and bottom sides pass through  $p$  vertical edges; Identify two lateral sides of  $P$  to form a cylinder, and then identify top and bottom sides with a torsion  $t$  hexagons (see figure 1). The toroidal polyhex  $H(p, q, t)$  is a bipartite graph since the vertices admit a proper 2-coloring: the vertices incident with a downward vertical edge and two upwardly lateral edges are colored by white, and the other vertices black.

We put  $H(p, q, t)$  in an affine coordinate system  $XOY$ : take the bottom side as  $x$ -axis and a lateral side as  $y$ -axis such that  $x$ -axis and  $y$ -axis form an angle with  $60^\circ$ , the origin  $O$  is their intersection and  $P$  lies on non-negative region (see figure 1). We take the distance between a pair of parallel edges in

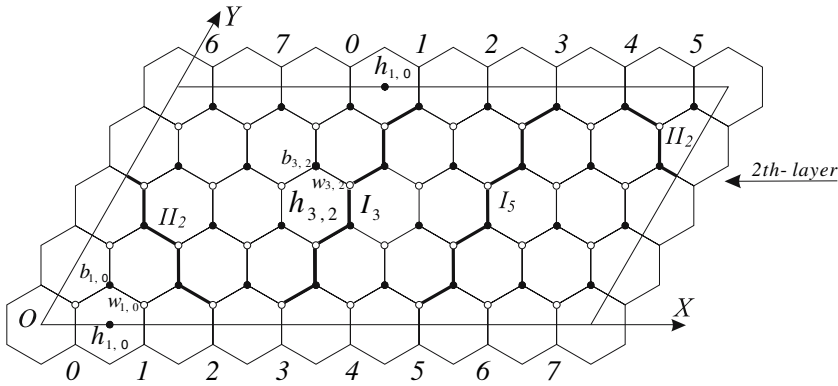


Figure 1. Toroidal polyhex  $H(8, 4, 2)$ ,  $I$ -column ( $I_3$  and  $I_5$ ) and  $II$ -column ( $II_2$ ).

a hexagon as unit length. Each hexagon is labeled by the coordinates  $(x, y)$  of its center, and denoted by  $(x, y)$  or  $h_{x,y}$ , where  $x \in \mathbb{Z}_p := \{0, 1, \dots, p - 1\}$  and  $y \in \mathbb{Z}_q := \{0, 1, \dots, q - 1\}$ . In a hexagon  $h_{x,y}$ , label the ends of the upper one in the two edges vertical to  $y$ -axis by  $b_{x,y}$  and  $w_{x,y}$  with respecting to the vertex colors (see figure 1). Under this labeling, each  $w_{0,y}$  is adjacent to  $b_{0,y}$  and  $w_{x,0}$  is adjacent to  $b_{x+t+1,q-1}$  ( $y \in \mathbb{Z}_q, x \in \mathbb{Z}_p$ ). The  $y$ th layer is defined to be the even cycle  $w_{0,y}b_{1,y}w_{1,y}b_{2,y} \dots w_{p-1,y}b_{0,y}w_{0,y}$  ( $y \in \mathbb{Z}_q$ ).

An automorphism  $\phi$  of a graph is a bijection from the vertex set to itself which satisfies both  $\phi$  and the inverse  $\phi^{-1}$  preserve the adjacency between vertices. A graph is *vertex-transitive* if there exists an automorphism between any two vertices. Let  $\phi_{rl}(v_{x,y}) = v_{x-1,y}$  and  $\phi_{tb}(v_{x,y}) = v_{x,y-1}$  where  $v \in V(H(p, q, t))$ ,  $x - 1, x \in \mathbb{Z}_p$  and  $y - 1, y \in \mathbb{Z}_q$ , then  $\phi_{rl}$  and  $\phi_{tb}$  are two automorphisms of  $H(p, q, t)$  (see [17]).

The path  $w_{x,0}b_{x+1,0}w_{x+1,1}b_{x+1,1} \dots w_{x,q-1}b_{x+1,q-1}$  is called  $I_x$ -column ( $0 \leq x \leq p - 1$ ), simply denoted by  $I_x$ , and the vertices  $w_{x,0}$  and  $b_{x+1,q-1}$  are called the *head* and the *tail* of  $I_x$ , respectively. The  $I_{x_2}$  is called the *successor* of  $I_{x_1}$  if the tail of  $I_{x_1}$  is adjacent to the head of  $I_{x_2}$ , and thereby  $w_{x_2,0}$  is adjacent to  $b_{x_1+1,q-1}$ , further  $x_2 \equiv x_1 - t \pmod{p}$  (see figure 1,  $I_3$  is the successor of  $I_5$ ). Let  $I_{x_1}, I_{x_2}, \dots, I_{x_g}$  be  $g$  different  $I$ -columns such that  $I_{x_{i+1}}$  is the successor of  $I_{x_i}$  for  $i, i + 1 \in \mathbb{Z}_g$ , then these  $g$   $I$ -columns form a cycle, called  $I$ -cycle. According to the automorphism  $\phi_{rl}$ , every  $I$ -column lies in an  $I$ -cycle and every  $I$ -cycle contains the same number of  $I$ -columns. The direction of a  $I$ -cycle is called  $I^+$ -direction if it is from head to tail along every  $I$ -column of this cycle, and the another direction is called  $I^-$ -direction.

The path  $w_{x,0}b_{x,0}w_{x-1,1}b_{x-1,1} \dots w_{x-q+1,q-1}b_{x-q+1,q-1}$  is called  $II_x$ -column ( $0 \leq x \leq p - 1$ ). Similarly, we can define the *head*, *tail*, *successor* of a  $II$ -column and  $II$ -cycle,  $II^+$ -direction,  $II^-$ -direction as these defined for a

$I$ -column. If  $II_{x_2}$  is the successor of  $II_{x_1}$ , then  $w_{x_2,0}$  is adjacent to  $b_{x_1-q+1,q-1}$ , further  $x_2 \equiv x_1 - (q + t) \pmod{p}$ .

**Lemma 2.1.** If a  $I$ -cycle (resp.  $II$ -cycle) of  $H(p, q, t)$  has  $g$   $I$ -columns ( $II$ -columns), then:

- (a)  $H(p, q, t)$  has  $\frac{p}{g}$   $I$ -direction cycles where  $g$  is the smallest positive integer satisfying  $gt \equiv 0 \pmod{p}$  and any consecutive  $\frac{p}{g}$   $I$ -columns:  $I_x, \dots, I_{x+\frac{p}{g}-1}$  lie on distinct  $I$ -cycles.
- (b)  $H(p, q, t)$  has  $\frac{p}{g}$   $II$ -direction cycles where  $g$  is the smallest positive integer satisfying  $g(q + t) \equiv 0 \pmod{p}$  and any consecutive  $\frac{p}{g}$   $II$ -columns:  $II_x, \dots, II_{x+\frac{p}{g}-1}$  lie on distinct  $II$ -cycles.

*Proof.* (a) According to the automorphism  $\phi_{rt}$ , it suffices to consider the  $I$ -cycle consisting of  $I_0, I_{p-t}, \dots, I_{p-(g-1)t}$ . By the definition of  $I$ -cycle, the head of  $I_0$  is adjacent to the tail of  $I_{p-(g-1)t}$ , then  $w_{0,0}b_{p-(g-1)t+1,q-1} \in E(H(p, q, t))$ , then  $p - gt = 0$  and  $p - rt \neq 0$  for  $r < g$ . Hence,  $g$  is the smallest positive integer satisfying  $gt \equiv 0 \pmod{p}$ . If  $t = 0$ , then  $g = 1$ . Hence,  $H(p, q, t)$  has  $p$   $I$ -cycles and the assertion holds. So suppose  $t \neq 0$ , then  $g \geq 2$ . Since  $H(p, q, t)$  has  $p$   $I$ -columns and every  $I$ -column lies on one  $I$ -cycle, every  $I$ -cycle contains  $\frac{p}{g}$   $I$ -columns.

In the following, we will prove any two  $I$ -columns from  $I_0, I_1, \dots, I_{\frac{p}{g}-1}$  do not lie on the same  $I$ -direction cycle. Suppose to the contrary that  $I_0$  and  $I_k$  with  $0 < k < \frac{p}{g}$  lies on the same  $I$ -cycle by the automorphism  $\phi_{rt}$ . Then  $p - rt \equiv k \pmod{p}$  with  $0 < r \leq g - 1$  and further  $rt \equiv k \pmod{p}$ . Therefore, there exists  $\mu \in \mathbb{Z}^+$  such that  $\mu p - rt = k$ , further  $1 \leq \mu p - rt \leq \frac{p}{g} - 1$ . Hence  $2 \leq g \leq \mu p g - rt g \leq p - g$ . According  $gt \equiv 0 \pmod{p}$ , there exists  $\lambda \in \mathbb{Z}^+$  such that  $\lambda p = gt$ . Then  $2 \leq g \leq (\mu g - \lambda r)p \leq p - g$ , which contradicts  $\mu, \lambda, g, r \in \mathbb{Z}^+$ . Therefore,  $I_0, \dots, I_{\frac{p}{g}-1}$  lie on the distinct  $I$ -cycles.

(b) It suffices to consider the  $II$ -cycle consisting of  $II_0, II_{p-q-t}, \dots, II_{(g-1)(p-q-t)}$ . By the definition of  $II$ -cycle, then  $w_{g(p-q-t),0} = w_{0,0}$  and  $w_{r(p-q-t),0} \neq w_{0,0}$  for  $r < g$ . So  $g$  is the smallest positive integer satisfying  $g(p - q - t) \equiv 0 \pmod{p}$ . If  $p - q - t \equiv 0 \pmod{p}$ , then  $g = 1$ . Hence,  $H(p, q, t)$  has  $p$   $II$ -cycles and the assertion holds. So suppose  $p - q - t \not\equiv 0 \pmod{p}$ , then  $g \geq 2$ . Since  $H(p, q, t)$  has  $p$   $II$ -columns and every  $II$ -column lies on one  $II$ -cycle, then  $II$ -direction cycle contains  $\frac{p}{g}$   $II$ -columns.

In the following, we will prove any two  $II$ -columns from  $II_0, II_1, \dots, II_{\frac{p}{g}-1}$  do not lie on the same  $II$ -cycle. Suppose to the contrary that  $II_0$  and  $II_k$  with  $0 < k < \frac{p}{g}$  lies on the same  $II$ -cycle by the automorphism  $\phi_{rt}$ . Then  $p - r(p - q - t) \equiv k \pmod{p}$  with  $0 < r \leq g - 1$ , further  $r(p - q - t) \equiv k \pmod{p}$ . Therefore, there exists  $\mu \in \mathbb{Z}^+$  such that  $r(p - q - t) = k + \mu p$ , further

$1 \leq r(p - q - t) - \mu p \leq \frac{p}{g} - 1$ . On the other hand, since  $g(p - q - t) \equiv 0 \pmod{p}$ , there exists  $\lambda \in \mathbb{Z}^+$  such that  $g(p - q - t) = \lambda p$ . Hence  $2 \leq g \leq r(p - q - t)g - \mu pg = r\lambda p - \mu pg = (r\lambda - \mu g)p \leq p - g$  which contradicts  $\lambda, \mu, r, g \in \mathbb{Z}^+$ . Therefore,  $II_0, \dots, II_{\frac{p}{g}-1}$  lie on the distinct  $II$ -cycles.  $\square$

### 3. The forcing number for bipartite graphs

In this section, we consider only bipartite graphs with a perfect matching. For convenience, a bipartite graph  $G$  has bipartition  $(W, B)$ ,  $W$  is the vertex set colored white and  $B$  black. Let  $\mathcal{M}$  be the set of all perfect matchings of  $G$ . A vertex  $u \in V(G)$  is a *neighbor* of  $v \in V(G)$  if  $u$  is adjacent to  $v$ . All neighbors of  $v$  form its *neighborhood*, denoted by  $N(v)$ , and define  $N[v] = N(v) \cup \{v\}$ . More generally for  $T \subset V(G)$ , the neighborhood of  $T$  is defined as  $N(T) := (\cup_{v \in T} N(v)) \setminus T$  and  $N[T] = N(T) \cup T$ .

Define functions  $\alpha$  and  $\beta$  on  $E(G)$ : for any edge  $e = wb \in E(G)$  with  $w \in W$  and  $b \in B$ ,  $\alpha(e) = w$  and  $\beta(e) = b$ . Given an  $M \in \mathcal{M}$ ,  $S \subset M$  and  $u \in V(G) \setminus V(S)$ , we say  $S$  *forces*  $u$  if  $|N(u) \setminus V(S)| = 1$ . In particular,  $S$  *W-forces* (resp. *B-forces*) an edge  $e$  if  $\alpha(e)$  (resp.  $\beta(e)$ ) is forced by  $S$ . If there exists a sequence of edges  $e_1, e_2, \dots, e_k$  and a sequence of edge sets  $S = S_0, S_1, S_2, \dots, S_k$  such that  $S_i = S_{i-1} \cup \{e_i\}$  and  $S_{i-1}$  *W-forces* (resp. *B-forces*)  $e_i$  ( $i = 1, 2, \dots, k$ ), then we say  $S$  *W-forces* (resp. *B-forces*) the set  $S_k$ .

**Lemma 3.1.** [16].  $S$  *W-forces*  $M$  if and only if  $S$  forces  $M$ .  $\square$

Let  $|M| = n$ . Assign an ordering to the edges in  $M$ :  $e_n > e_{n-1} > \dots > e_1$ . Let  $b_n > b_{n-1} > \dots > b_1$  be the corresponding ordering of the vertices in  $B$ , where  $b_i = \beta(e_i)$  ( $1 \leq i \leq n$ ). For a vertex  $b \in B$ ,  $b$  *leads*  $N(w)$  if  $b$  is the largest vertex among all neighbors of  $w \in W$  in the ordering of  $B$ ;  $b$  is called a *leading vertex* if such a  $w \in W$  exists, and *trailing vertex* otherwise. Let  $S_i = \{e_1, e_2, \dots, e_i\}$  and  $B_i := \beta(S_i) = \{b_1, b_2, \dots, b_i\}$ . Put  $\bar{B}_i := \{b_n, \dots, b_{i+1}\}$ .

**Lemma 3.2.** [16]. If  $S_i$  *W-forces*  $e_{i+1}$ , then  $b_{i+1}$  leads  $N(w_{i+1})$  where  $w_{i+1} = \alpha(e_{i+1})$ .  $\square$

For  $T \subset V(G)$ , the *excess* of  $T$  is defined as  $\epsilon(T) = |N(T)| - |T|$ . The maximum excess of an ordering  $b_n > b_{n-1} > \dots > b_1$  of  $B$  is the maximum value in all  $\epsilon(\bar{B}_i)$  ( $1 \leq i \leq n-1$ ). The *excess of*  $b_i$  is defined to be  $\epsilon(b_i) = \epsilon(\bar{B}_{i-1}) - \epsilon(\bar{B}_i)$ . We call  $b_i$  an *m-excess vertex*, simply *m-ex*, if  $\epsilon(b_i) = m$ . Riddle gave the following lower bound for  $f(G)$ :

**Lemma 3.3.** [16].  $f(G)$  is bounded below by the smallest possible maximum excess for all orderings of  $B$ .  $\square$

According to the definition of leading vertex and trailing vertex, we have the following lemma:

**Lemma 3.4.** Let  $b_n > b_{n-1} > \dots > b_i > \dots > b_1$  be an ordering of  $B$ . Then:

- (a) the following statements are equivalent:
  1.  $b_i$  is a leading vertex;
  2.  $|N(\bar{B}_{i-1})| - |N(\bar{B}_i)| \geq 1$ ;
  3.  $\epsilon(\bar{B}_{i-1}) \geq \epsilon(\bar{B}_i)$ ;
  4.  $\epsilon(b_i) \geq 0$ .
  
- (b) the following statements are equivalent:
  1.  $b_i$  is a trailing vertex;
  2.  $|N(\bar{B}_{i-1})| = |N(\bar{B}_i)|$ ;
  3.  $\epsilon(\bar{B}_{i-1}) = \epsilon(\bar{B}_i) - 1$ ;
  4.  $\epsilon(b_i) = -1$ .

□

**Definition 3.5.** An ordering  $b_n > b_{n-1} > \dots > b_1$  of  $B$  is *canonical* if its smallest leading vertex is larger than the largest trailing vertex; *non-canonical*, otherwise. □

By lemma 3.4, we have:

**Lemma 3.6.** The maximum excess of a canonical ordering of  $B$  is equal to the number of trailing vertices. □

**Lemma 3.7.** Let  $M$  be a perfect matching of  $G$ . If  $S$  is a minimum forcing set of  $M$ , then there exists a canonical ordering of  $B$  such that  $\beta(S)$  is the set of trailing vertices and  $B \setminus \beta(S)$  is the set of leading vertices.

*Proof.* Let  $|M| = n$  and  $S = \{e_1, e_2, \dots, e_k\} \subseteq M$ , the minimum forcing set of  $M$ . By Lemma 3.1, we have  $S$   $W$ -forces  $M$ . Let  $S_0 = S$ . Then there exists edge  $e_{k+j} \in M$  for any  $j \in \{1, \dots, n - k\}$  and edge set  $S_j = S_{j-1} \cup \{e_{k+j}\}$  such that  $S_{j-1}$   $W$ -forces  $e_{k+j}$  ( $j = 1, 2, \dots, n - k$ ) and  $S_{n-k} = M$ . Since  $\beta(e_{k+j}) = b_{k+j}$  ( $1 \leq j \leq n - k$ ) and lemma 3.2,  $b_{k+j}$  ( $1 \leq j \leq n - k$ ) is a leading vertex of the ordering of  $B$ :  $b_n > b_{n-1} > \dots > b_{k+1} > b_k > \dots > b_1$ . Then  $B \setminus \beta(S)$  is the set of leading vertices.

In the following, we want to show that  $b_i \in \beta(S)$  ( $1 \leq i \leq k$ ) is a trailing vertex. If not, suppose  $b_i$  is a leading vertex, then  $b_i$  leads a set  $N(w_j)$ . If  $j > k$ , then  $b_i \geq b_j > b_k$  since  $b_i$  leads  $N(w_j)$  and  $w_j b_j = e_j \in M$ . Therefore,  $i > k$ , a contradiction. So  $j \leq k$ . Since  $N(w_j) \setminus \{b_j\} \subseteq \beta(S \setminus \{e_j\})$ , then  $S \setminus \{e_j\}$   $W$ -forces  $e_j$  and further  $W$ -forces  $M$ . Hence  $|S \setminus \{e_j\}| < |S|$  which contradicts the minimality of  $|S|$ . Hence  $\beta(S)$  is the set of trailing vertices.

Obviously, the ordering  $b_n > b_{n-1} > \dots > b_{k+1} > b_k > \dots > b_1$  is canonical. □

For any perfect matching  $M$  of  $G$ , lemma 3.7 implies there exists a canonical ordering of  $B$  with  $f(G, M)$  trailing vertices.

**Theorem 3.8.**  $f(G)$  is bounded below by the minimum trailing vertex number over all canonical orderings of  $B$ . □

Let  $b_n > b_{n-1} > \dots > b_1$  be an ordering of  $B$  and  $T \subseteq B$ ,  $\bar{T} = B \setminus T$ . A vertex  $b \in \bar{T}$  is called *forced vertex* of  $N[T]$  (also *forced vertex* of  $T$ ) if  $N(b) \subset N[T]$  or  $|N(b) \cap (W \setminus N[T])| = 1$ . An edge  $e \in E(G)$  is *B-forced* by  $N[T]$  (also *B-forced* by  $T$ ) if  $\beta(e) \in \bar{T}$ ,  $\alpha(e) \in W \setminus N[T]$  and  $N(\beta(e)) \cap (W \setminus N[T]) = \{\alpha(e)\}$ . If there exists a sequence of edges  $e_1, e_2, \dots, e_k$  and a sequence of vertex sets  $T_0 (= T), T_1, T_2, \dots, T_k$  such that  $T_i = T_{i-1} \cup \beta(e_i)$  and  $T_{i-1}$  *B-forces*  $e_i$  ( $i = 1, 2, \dots, k$ ), then we say the edge set  $\{e_1, e_2, \dots, e_k\}$  is *B-forced* by  $T$ . Let  $S$  be the maximum *B-forced* edge set of  $T$  and  $V'$ , the set of all forced vertices of  $N[T] \cup \alpha(S) \cup \beta(S)$ . Then  $N[T] \cup \alpha(S) \cup \beta(S) \cup V'$  is called the *forced domain* of  $T$ , denoted by  $D(T)$ . The forced domain of  $b_i$  is defined to be  $D(b_i) = D(N[\bar{B}_{i-1}])$ . A vertex  $b_i$  is called *key vertex* of the ordering if  $D(b_{i+1}) \subsetneq D(b_i)$ .

**Lemma 3.9.** Let  $b_n > b_{n-1} > \dots > b_1$  be a canonical ordering of  $B$  and  $b_{j_1} > b_{j_2} > \dots > b_{j_l}$ , all key vertices of  $B$ . Then the maximum excess of the ordering is no less than  $\sum_{i=1}^l \epsilon(b_{j_i})$ .

*Proof.* Let  $b_{j_i}$  be any key vertex of the ordering of  $B$ . Then  $D(b_{j_{i+1}}) \subsetneq D(b_{j_i})$ . If  $\epsilon(b_{j_i}) \leq 0$ , then  $|N(b_{j_i}) \setminus N(\bar{B}_{j_i})| \leq 1$ . Hence  $N[b_{j_i}] \subset D(N[\bar{B}_{j_i}])$  and  $D(b_{j_{i+1}}) = D(N[\bar{B}_{j_i}]) = D(N[\bar{B}_{j_i}] \cup N[b_{j_i}]) = D(N[\bar{B}_{j_i-1}]) = D(b_{j_i})$ , a contradiction. So  $\epsilon(b_{j_i}) \geq 1$ .

Since  $b_n > b_{n-1} > \dots > b_1$  is a canonical ordering of  $B$ , let  $b_{k+1}$  be the smallest leading vertex and then  $j_l \geq k+1$ . By lemma 3.4,  $\epsilon(b_i) \geq 0$  for  $i \geq k+1$ . Hence  $\epsilon(\bar{B}_k)$  is the maximum excess of the ordering and satisfies

$$\epsilon(\bar{B}_k) = \sum_{i>k} \epsilon(b_i) = \sum_{i=1}^l \epsilon(b_{j_i}) + \sum_{i>k, i \neq j_1, \dots, j_l} \epsilon(b_i) \geq \sum_{i=1}^l \epsilon(b_{j_i}).$$

□

#### 4. The forcing number for toroidal polyhexes

Let  $T \subset B$ . We say  $T$  is *full* in  $y$ th layer (or  $I$ -column)  $L$  if  $V(L) \subset T \cup N(T)$  and  $T$  *touches*  $L$  if  $V(L) \cap N[T] \neq \emptyset$  and  $V(L) \not\subseteq N[T]$ . For any toroidal polyhex  $H(p, q, t)$ , it has at least three perfect matchings:  $M_1 = \{e | e \text{ is vertical in } H(p, q, t)\}$ ,  $M_2 = \{b_{i,j} w_{i,j} | i \in \mathbb{Z}_p, j \in \mathbb{Z}_q\}$ , and  $M_3 = \{w_{i,j} b_{i+1,j} | i \in \mathbb{Z}_p, j \in \mathbb{Z}_q\}$ . Hence  $f(H(p, q, t)) \geq 1$ .

**Theorem 4.1.** Let  $H(p, q, t)$  be a toroidal polyhex. Then  $f(H(p, q, t)) \geq \min\{p, q\}$ .

*Proof.* If  $\min\{p, q\} = 1$ , the assertion holds. So, in the following, we suppose  $\min\{p, q\} \geq 2$ .

Let  $b_{pq} > b_{pq-1} > \dots > b_1$  be any ordering of  $B$ . Then it suffices to prove there exists  $i \in \{1, \dots, pq\}$  satisfying  $\epsilon(\bar{B}_i) \geq \min\{p, q\}$  by lemma 3.3. For any ordering of  $B$ , let  $j$  be the largest one in  $\{1, \dots, pq\}$  such that  $\bar{B}_j$  is full in either a  $y$ th layer or a  $I$ -column. Then we have following cases:

*Case 1:* If  $\bar{B}_j$  is full in a  $y$ th layer but not full in any  $I$ -column. Hence  $\bar{B}_j$  touches every  $I$ -column  $I_k$  ( $0 \leq k \leq p-1$ ). Then  $|N(\bar{B}_j \cap V(I_k))| - |\bar{B}_j \cap V(I_k)| \geq 1$ . Therefore,

$$\epsilon(\bar{B}_j) = |N(\bar{B}_j)| - |\bar{B}_j| = \sum_{k=0}^{p-1} (|N(\bar{B}_j \cap V(I_k))| - |\bar{B}_j \cap V(I_k)|) \geq p$$

since  $(\bar{B}_j \cap V(I_i)) \cap (\bar{B}_j \cap V(I_r)) = \emptyset$  for  $i \neq r$ .

*Case 2:* If  $\bar{B}_j$  is full in a  $I$ -column but not full in any  $y$ th layer. Hence  $\bar{B}_j$  touches every layer  $L_k$  ( $0 \leq k \leq q-1$ ). Then  $|N(\bar{B}_j \cap V(L_k))| - |\bar{B}_j \cap V(L_k)| \geq 1$ . Therefore,

$$\epsilon(\bar{B}_j) = |N(\bar{B}_j)| - |\bar{B}_j| = \sum_{k=0}^{q-1} (|N(\bar{B}_j \cap V(L_k))| - |\bar{B}_j \cap V(L_k)|) \geq q$$

since  $(\bar{B}_j \cap V(L_i)) \cap (\bar{B}_j \cap V(L_r)) = \emptyset$  for  $i \neq r$ .

*Case 3:* If  $\bar{B}_j$  is full in a  $I$ -column and a  $y$ th layer simultaneously. Then  $\bar{B}_{j+1}$  touches every  $I$ -column and every  $y$ th layer. According to cases 1 and 2,  $\epsilon(\bar{B}_{j+1}) \geq \max\{p, q\}$ .

Combining cases 1–3, we have  $f(H(p, q, t)) \geq \epsilon(\bar{B}_i) \geq \min\{p, q\}$  for some  $i \in \{1, \dots, pq\}$  and complete the proof.  $\square$

Theorem 4.1 gives a lower bound for the forcing number of toroidal polyhex and it is sharp for infinitely many toroidal polyhexes, implied by the following theorem.

**Theorem 4.2.**

$$f(H(p, q, t)) = \begin{cases} p, & \text{if } p \leq q, \\ q, & \text{if } p > q \text{ and } t = 0, p-1, \dots, p-q. \end{cases}$$

*Proof.* If  $p \leq q$ . Since  $H(1, 1, 0)$  has only two vertices and three edges, then  $f(H(1, 1, 0)) = 1$ . So suppose  $2 \leq q$  and let  $S = \{b_{j,0}w_{j-1,1} | 0 \leq j \leq p-1\}$ . Then  $S$  forces a perfect matching  $M_1$ . Hence  $f(H(p, q, t), M_1) \leq |S| = q$  for  $1 \leq p \leq q$ . By theorem 4.1, we have  $f(H(p, q, t)) = p$ .



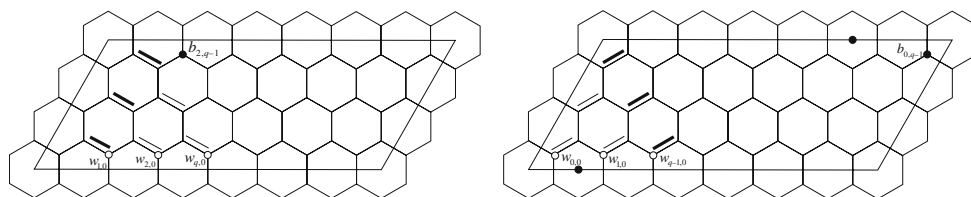


Figure 2. Toroidal polyhex  $H(7, 3, t)$  and illustration for proof of theorem 4.2.

If  $p > q$ . Let  $S = \{b_{1,j}w_{1,j} | 0 \leq j \leq q - 1\}$ . Clearly,  $S$  forces  $E = \{b_{i,j}w_{i,j} | 1 \leq i \leq q, j = q - i\}$ . So  $S$  forces  $M_2$  if and only if  $S \cup E$  forces edge  $b_{2,q-1}w_{2,q-1}$ , equivalently  $w_{1-t,0} \in N(b_{2,q-1}) \cap \{w_{1,0}, \dots, w_{q,0}\}$  (see figure 2 (left)), just  $1 \leq p + 1 - t \leq q$  and further  $p - q + 1 \leq t \leq p$ . Therefore,  $f(H(p, q, t)) \leq |S| = q$  for  $t = 0, p - 1, \dots, p - q + 1$ . For  $t = p - q$ , let  $S = \{w_{i,j}b_{i+1,j} | 0 \leq i \leq q - 1, j = q - 1 - i\}$ . Then  $S$  forces  $M_3$  (see figure 2 (right)). Hence  $f(H(p, q, t)) \leq |S| = q$  for  $t = p - q$ . By theorem 4.1, we have  $f(H(p, q, t)) = q$  for  $p > q$  and  $t = 0, p - 1, \dots, p - q$ .  $\square$

Theorem 4.2 gives the forcing numbers of partial toroidal polyhexes. For the toroidal polyhex  $H(p, q, t)$  with  $p > q \geq 1$  and  $1 \leq t \leq p - q - 1$ , it becomes a little complicated to give its forcing number. Let  $H$  denote a toroidal polyhex  $H(p, q, t)$  for convenience. For a vertex set  $S \subset V(H)$ ,  $H[S]$  is the subgraph induced by  $S$  in  $H$ .

A triangle  $T$  on  $H$  is defined to be an equilateral triangle whose corners lie on the centers of three hexagons  $h_{x_1,y}, h_{x_2,y}$ , and  $h_{x_3,y'}$  such that  $w_{x_1,y}$  and  $w_{x_3,y'}$  are on the same  $I$ -cycle and  $w_{x_2-1,y}$  and  $w_{x_3-1,y'}$  are on the same  $II$ -cycle, the side length of  $T$  is  $|x_2 - x_1|$ , denoted by  $\delta(T)$ . For convenience, we use a hexagon notation to denote its center, then  $T = h_{x_1,y}h_{x_2,y}h_{x_3,y'}$ . A triangle  $T$  is *maximum* on  $H$  if  $\delta(T)$  is largest among all triangles. The triangle  $h_{0,0}h_{k,0}h_{i,j}$  ( $i = p - st$  and  $j = k - sq$  with  $s \geq 0, i \in \mathbb{Z}_p$  and  $j \in \mathbb{Z}_q$ ) is also called *normal* triangle, denoted by  $\Delta_k$ . By the automorphism  $\phi_{tb}$  and  $\phi_{rt}$ , every triangle is isomorphic to a normal triangle. According to the representation of  $H$  in the plane,  $\Delta_k$  consists of  $s$  trapeziums  $P_{i+1} = h_{p-it,0}h_{k-i(q+t),0}h_{k-(i+1)(q+t),0}h_{p-(i+1)t,0}$  with  $0 \leq i \leq s - 1$  and a small triangle  $P_{s+1} = h_{p-st,0}h_{k-s(q+t),0}h_{p-st,k-sq}$ . For example, the  $\Delta_5$  in  $H(11, 3, 3)$  consists of a trapezium  $P_1 = h_{0,0}h_{5,0}h_{10,0}h_{8,0}$  and a triangle  $P_2 = h_{8,0}h_{10,0}h_{8,2}$  (see figure 3). Simply, we also use a triangle to denote the vertex set consisting of all vertices lying in it, for example,  $\Delta_2 = N[b_{1,0}]$ . For a normal triangle  $\Delta_i$ , define  $\bar{\Delta}_i = V(H) - \Delta_i$ .

Let  $T$  be a triangle,  $II_x$  is *adjacent* to  $T$  if  $V(II_x) \cap T = \emptyset$  and  $V(II_x) \cap N(T) \neq \emptyset$ . A vertex  $b \in V(II_x)$  is *II-adjacent* to  $T$  if  $b \in N(T)$  and  $V(II_x)$  is adjacent to  $T$  ( $II_5$  and  $II_{10}$  are adjacent to  $\Delta_5$  and all black vertices on  $II_5$  are *II-adjacent* to  $\Delta_k$  in figure 3), let  $N_{II}(T)$  be the vertex set consisting all *II-adjacent* vertices together with their neighbors in all *II*-columns adjacent to  $T$ . If a normal triangle  $\Delta_i$  satisfies  $|\Delta_i \cap N(b)| \leq 1$  for any  $b \in \bar{\Delta}_i$ , then

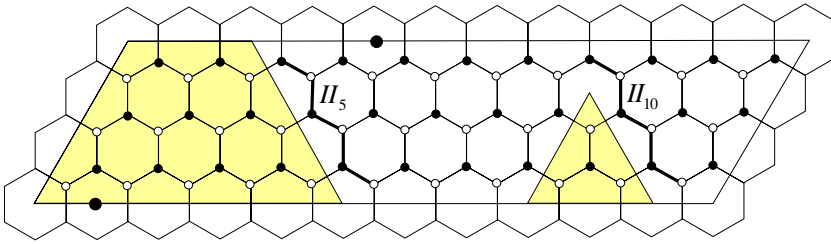


Figure 3. Toroidal polyhex  $H(11, 3, 3)$  and the normal triangle  $\Delta_5$ .

$\Delta_{i+1} = \Delta_i \cup N_{II}(\Delta_i)$ . The process from  $\Delta_i$  to  $\Delta_{i+1}$  is called *triangle extension*. We continue the triangle extension and stop at  $\Delta_k$  which satisfies there exists a vertex  $b \in \bar{\Delta}_k$  such that  $|N(b) \cap \Delta_k| = 2$ , the  $\Delta_k$  is called *characteristic triangle* of  $H$ .

**Lemma 4.3.** Let  $\Delta_k$  be the characteristic triangle of  $H$ . Then for any  $i < k$ , the normal triangle  $\Delta_i$  satisfies  $D(\Delta_i) = \Delta_i$ .

*Proof.* For any  $\Delta_i$  ( $i < k$ ),  $|N(v) \cap \Delta_i| \leq 1$  for any vertex  $b \in \bar{\Delta}_i$  since  $\Delta_k$  is a characteristic triangle. Hence  $\Delta_i$  does not  $B$ -force  $v$ . Immediately, we have  $D(\Delta_i) = \Delta_i$ . □

**Theorem 4.4.** Let  $\Delta_k$  consist of  $s$  trapezia  $P_{i+1}$  ( $0 \leq i \leq s - 1$ ) and one triangle  $P_{s+1}$ . Then  $\Delta_k$  is the characteristic triangle if and only if one of following cases appears:

- (1) there exists  $l$  ( $0 \leq l \leq s$ ) such that  $P_1$  and  $P_{l+1}$  have the same corner  $h_{k,0}$ ;
- (2) there exists  $l$  ( $0 \leq l \leq s$ ) such that  $P_1$  and  $P_{l+1}$  have the same corner  $h_{0,0}$ ;
- (3) the corner  $h_{p-st,k-sq}$  of  $P_{s+1}$  coincides with  $h_{x,0}$  where  $0 \leq x \leq k$ .

*Proof. Sufficiency:* It suffices to prove there exists  $b \in \bar{\Delta}_k$  such that  $|N(b) \cap \Delta_k| = 2$ . If (1) holds, let  $b = b_{k,0} \in \bar{\Delta}_k$ . Since  $w_{k-1,0} \in P_1$  and  $w_{k,0} \in P_{l+1}$ ,  $|N(b_{k,0}) \cap \Delta_k| = 2$ . If (2) holds, let  $b = b_{0,0} \in \bar{\Delta}_k$ . Hence  $|N(b_{0,0}) \cap \Delta_k| = 2$  since  $w_{p-1,0} \in P_{l+1}$ ,  $w_{0,0} \in P_1$ . If (3) holds, then let  $b = b_{x+t+1,q-1} \in \bar{\Delta}_k$  if  $x < k$  and  $b = b_{x+t,q-1} \in \bar{\Delta}_k$  if  $x = k$ . Then the assertion holds since  $w_{x,0} \in P_1$ ,  $w_{x+t,q-1} \in P_{s+1}$  for  $x < k$  and  $w_{x-1,0} \in P_1$ ,  $w_{x+t,q-1} \in P_{s+1}$  for  $x = k$ .

*Necessary:* Since  $\Delta_k$  is the characteristic triangle, there exists  $b \in \bar{\Delta}_k$  such that  $|N(b) \cap \Delta_k| = 2$ . Hence  $b \in N(\Delta_k)$ . For a vertex  $b \in \Delta_k \cap B$ , we have

$N(b) \subset \Delta_k$ . So  $b \in B \cap \bar{\Delta}_k$ , say  $b = b_{i,j}$ . Then  $N(b_{i,j}) = \{w_{i-1,j}, w_{i,j}, w_{x,y}\}$  where  $x = i - 1, y = j + 1$  if  $j \neq q - 1$  and  $x = i - t - 1, y = 0$  if  $j = q - 1$ .

*Case 1:* If  $w_{i-1,j} \in P_{l_1}$  and  $w_{i,j} \in P_{l_2}$ . Then the center  $h_{i,j}$  is a point in the intersection of  $P_{l_1}$  and  $P_{l_2}$ . If  $j \neq 0$ , then the vertex  $b_{i,j-1} \notin \Delta_{k-1}$  satisfies  $|N(b_{i,j-1}) \cap \Delta_{k-1}| = 2$  since  $w_{i-1,j-1}, w_{i,j-1} \in \Delta_{k-1}$ , then  $b_{i,j-1} \in D(\Delta_{k-1})$  which contradicts  $D(\Delta_{k-1}) = \Delta_{k-1}$  by lemma 4.3, so  $j = 0$ . If  $\min\{l_1, l_2\} \neq 1$ , then the vertex  $b_{i+t,q-1} \notin \Delta_{k-1}$  satisfies  $|N(b_{i+t,q-1}) \cap \Delta_{k-1}| = 2$  since  $w_{i+t,q-1}, w_{i+t-1,q-1} \in \Delta_{k-1}$ , then  $b_{i+t,q-1} \in D(\Delta_{k-1})$ , a contradiction. Therefore, we have  $\min\{l_1, l_2\} = 1$  and  $j = 0$ . If  $l_1 = 1$ , then (1) appears. If  $l_2 = 1$ , then (2) appears.

*Case 2:* If  $w_{i-1,j} \in P_{l_1}$  and  $w_{x,y} \in P_{l_2}$  or  $w_{i,j} \in P_{l_1}$  and  $w_{x,y} \in P_{l_2}$ . If  $l_2 \neq 1$  or  $y \neq 0$ , we have  $w_{x,y}b_{i,j} \in E(H[\Delta_k])$  which contradicts  $b_{i,j} \in \bar{\Delta}_k$ , so  $l_2 = 1$  and  $y \neq 0$ , just  $j = q - 1$ . If  $P_{l_1}$  is a trapezium, then  $b_{i-1,q-1} \in P_{l_1}$ . Since  $w_{x,0} \in P_1$ , then  $0 \leq x \leq k$ . If  $x > 0$ , then  $w_{x-1,0}, w_{i-2,q-1} \in \Delta_k$  and further  $|N(b_{i-1,q-1}) \cap \Delta_{k-1}| = 2$ , then  $b_{i-1,q-1} \in D(\Delta_{k-1})$  which contradicts lemma 4.3. So  $x = 0$ , then  $P_{l_1+1}$  and  $P_1$  have the same corner  $h_{0,0}$ , (2) appears. If  $P_{l_1}$  is a triangle, then  $l_1 = s + 1$ , further the corner  $h_{p-st,k-sq} = h_{x+t+1,q-1}$  of  $P_{s+1}$  coincides with  $h_{x,0}$  ( $0 \leq x \leq k$ ), (3) appears.  $\square$

According to the isomorphism  $\phi_{lb}$  and  $\phi_{rl}$  of  $H$ , theorem 4.4 and its proof imply the characteristic triangle is, in fact, a maximum triangle on the toroidal polyhex and every maximum triangle is also isomorphic to the characteristic triangle.

**Lemma 4.5.** Let  $\Delta_k$  be the characteristic triangle of  $H$  and every  $II$ -cycle (resp.  $I$ -cycle) of  $H$  has  $g$  (resp.  $g'$ )  $II$ -columns (resp.  $I$ -columns). Then  $k \geq \frac{p}{g}$  if one of cases (1)–(3) with  $x \neq k$  in theorem 4.4 appears and  $k \geq \frac{p}{g'}$  if case (3) with  $x = k$  in theorem 4.4 appears.

*Proof.* *Case 1:* If  $P_1$  and  $P_{l+1}$  ( $1 \leq l \leq s$ ) have the same corner  $h_{k,0}$ . Then  $k \equiv p - lt \pmod{p}$ . Hence there exists  $\lambda \in \mathbb{Z}^+$  such that  $k = \lambda p - lt$ . Since a  $II$ -cycle contains  $g$   $II$ -columns, by lemma 2.1 we have  $g(q+t) \equiv 0 \pmod{p}$ , further  $g[p-(q+t)] \equiv 0 \pmod{p}$ . So there exists  $\mu \in \mathbb{Z}$  such that  $g[p-(q+t)] = \mu p$ , further  $(g - \mu)p = g(q+t)$ .

Since  $k - sq \geq 1, k \geq sq + 1 > lq$ . Hence

$$\begin{aligned} g(k - lq) &= g[\lambda p - lt - lq] = g[\lambda p - l(q + t)] = g\lambda p - g(q + t)l \\ &= [g(\lambda - l) + \mu l]p. \end{aligned}$$

Then  $g(k - lq) \geq p$  since  $g(k - lq) > 0$ . Therefore,  $k > \frac{p}{g}$ .

*Case 2:* If  $P_1$  and  $P_{l+1}$  ( $1 \leq l \leq s$ ) have the same corner  $h_{0,0}$ . Then  $k - l(q+t) \equiv 0 \pmod{p}$ , further  $l(p - q - t) + k \equiv 0 \pmod{p}$ . Let  $\gamma \in \mathbb{Z}$  satisfy  $l(p - q - t) + k = \gamma p$ . Then  $(l - \gamma)p + k = l(q+t)$ , further  $g(l - \gamma)p + gk = gl(q+t)$ .

Hence  $gk = (l - \gamma)gp + lg(q + t)$ . By lemma 2.1,  $g(q + t) \equiv 0 \pmod{p}$ . Therefore,  $gk \equiv 0 \pmod{p}$ . Clearly,  $gk > 0$ . Hence  $gk > p$ , just  $k > \frac{p}{g}$ .

Case 3: If  $h_{p-st, k+1-sq} = h_{x,0}$  for  $0 \leq x \leq k$ .

Subcase 3.1: If  $0 \leq x \leq k - 1$ . According to  $h_{p-st, k-sq} = h_{x,0}$ , we have  $k - sq - q = 0$  and  $p - st - t = x$ . Further,  $k = (1 + s)q$  and  $0 \leq p - (1 + s)t < k \pmod{p}$ . Then there exists  $\eta \in \mathbb{Z}$  such that  $0 \leq \eta p - (1 + s)t < k$ .

By lemma 2.1,  $g(q + t) \equiv 0 \pmod{p}$ . So there exists  $\theta \in \mathbb{Z}$  such that  $\theta p = g(q + t)$ , then  $gq = \theta p - gt$ . Hence

$$gk = g(1 + s)q = (1 + s)(\theta p - gt) = (1 + s)\theta p - (1 + s)gt$$

and

$$gk > g[\eta p - (1 + s)t] = g\eta p - (1 + s)gt \geq 0.$$

Therefore  $(1 + s)\theta > g\eta$ , further  $(1 + s)\theta \geq 1 + g\eta$ . Then  $gk = (1 + s)\theta p - (1 + s)gt \geq (1 + g\eta)p - (1 + s)gt = p + [g\eta p - (1 + s)gt] \geq p$ . So  $k \geq \frac{p}{g}$ .

Subcase 3.2: If  $x = k$ , then  $k \equiv p - (s + 1)t \pmod{p}$ . Hence there exists  $\eta \in \mathbb{Z}^+$  such that  $k = \eta p - (s + 1)t$ . Then  $g'k = \eta g'p - (s + 1)g't$ . By lemma 2.1,  $g't \equiv 0 \pmod{p}$ . There exists  $\theta \in \mathbb{Z}$  such that  $g'k = [\eta g' - (s + 1)\theta]p$ . Since  $g'k > 0$ , hence  $g'k \geq p$ . So  $k \geq \frac{p}{g'}$ . □

Let  $G \subset H$ , an edge  $e \in E(G)$  is called a *pendant edge* if  $\beta(e)$  is a 1-degree vertex. Clearly, a pendant edge  $e$  is  $B$ -forced by  $V(H - G)$ .

**Lemma 4.6.** Let  $\Delta_k$  be the characteristic triangle of toroidal polyhex  $H$ . Then  $D(\Delta_k) = V(H)$ .

*Proof.* Let  $\Delta_k$  consist of  $s$  trapeziums  $P_{l+1}$  ( $0 \leq l \leq s - 1$ ) and a triangle  $P_{s+1}$ ,  $H_0 := H[\bar{\Delta}_k]$  is the subgraph of  $H$  induced by  $\bar{\Delta}_k$  (see Figure 4).

Case 1: There exists  $0 \leq l \leq s$  such that  $P_1$  and  $P_{l+1}$  have the same corner  $h_{k,0}$ . Let  $S^1 = E(H_0) \cap M_1$ . Then we have the following claim:

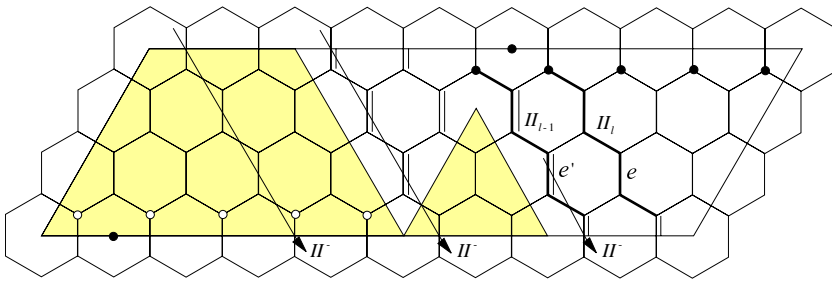


Figure 4. Illustration for case 1 in proof of lemma 4.6.

Claim 1:  $S^1$  is  $B$ -forced by  $\Delta_k$ .

Proof. Clearly,  $b_{k,0}w_{k-1,1}$  is a pendant edge of  $H_0$  and is forced by  $\Delta_k$ . Let  $e_1 = b_{k,0}w_{k-1,1}$  and  $H_1 = H_0 - \{b_{k,0}, w_{k-1,1}\}$ . Define  $S_i$  as the vertical pendant edge set of  $H_i$  and  $H_{i+1} := H_i - V(S_i), i = 0, 1, 2, \dots$

Suppose to the contrary that there exist edges in  $S^1$  not  $B$ -forced by  $\Delta_k$ , equivalently, there exists  $H_m \subset H_0$  such that  $E(H_m)$  contains no pendant vertical edge and  $E(H_m) \cap S^1 \neq \emptyset$ . Choose one edge  $e \in E(H_m) \cap S^1$  such that  $e \in II_l$  and  $l$  is minimal. By the minimality of  $l$ , for any  $e' \in E(II_{l-1})$ , either  $e' \in E(H[\Delta_k])$  or  $e'$  is a pendant edge of some  $H_i$  with  $i < m$ . Let  $R_{l-1}$  and  $R_l$  be the  $II$ -cycle containing  $II_{l-1}$  and  $II_l$ , respectively. By lemma 4.5, every  $II$ -cycle contains at least one edge in  $E' = \{w_{j,0}b_{j+t+1,q-1} | 0 \leq j \leq k-1\}$ . Hence, all vertical edges in  $E(R_{l-1})$  starting from  $e'$  along  $II^-$ -direction and stopping at some edge in  $E' \cap E(R_{l-1})$  are not in  $E(H_m)$ . Since  $e$  is not a pendent edge, therefore all vertical edge in  $E(R_l)$  starting from  $e$  along  $II^-$ -direction and stopping at some edge in  $E' \cap E(R_l)$  belong to  $E(H_m)$ ; If not,  $E(H_m)$  contains vertical pendant edge which contradicts the supposition. But  $E' \cap E(H_0) = \emptyset$ , which contradicts  $H_m \subset H_0$  and  $E' \cap E(R_l) \cap E(H_m) \neq \emptyset$ . The contradiction implies claim 1.

Since  $S^1 = E(H_0) \cap M_1$ , then  $H - (V(S^1) \cup \Delta_k)$  consists of  $k$  isolated vertices:  $b_{t+i,q-1} (1 \leq i \leq k)$ . Then  $N(b_{t+i,q-1}) \subset \Delta_k \cup V(S^1)$ , so  $b_{t+i,q-1} \in D(\Delta_k)$  since  $S^1$  is  $B$ -forced by  $\Delta_k$ . Further,  $D(\Delta_k) = V(H)$ .

Case 2: There exists  $0 \leq l \leq s$  such that  $P_l$  and  $P_{l+1}$  have the same corner  $h_{0,0}$ . Let  $S^2 = E(H_0) \cap M_2$ . Then we have following claim (see Figure 5):

Claim 2:  $S^2$  is  $B$ -forced by  $\Delta_k$ .

Proof. Since  $P_l = h_{p-(l-1)t,0}h_{k-(l-1)(q+t),0}h_{k-l(q+t),0}h_{p-lt,0}$ , hence  $k-l(q+t) \equiv 0 \pmod p$  and further  $k - (l - 1)(q + t) - q \equiv t \pmod p$ , which implies the black vertex  $b_{t+i,q-1} (1 \leq i \leq k)$  is adjacent to  $w_{i-1,0}$  belonging to  $P_l$ . Hence,  $b_{t+1,q-1}w_{t+1,q-1}$  is a pendant edge of  $H_0$  since  $w_{t,q-1} \in P_l \cap N(b_{t+1,q-1})$  and  $w_{0,0} \in P_l \cap N(b_{t+1,q-1})$ . Let  $H_1 = H_0 - \{b_{t+1,q-1}, w_{t+1,q-1}\}$ . Define  $S_i \subset S^2$  is the pendant edge set of  $H_i$  and  $H_{i+1} := H_i - V(S_i), i = 0, 1, \dots$

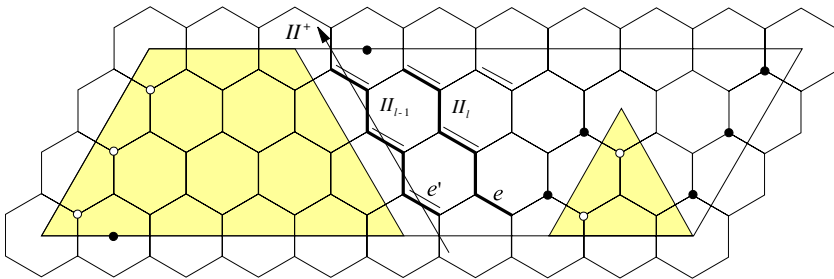


Figure 5. Illustration for case 2 in proof of lemma 4.6.

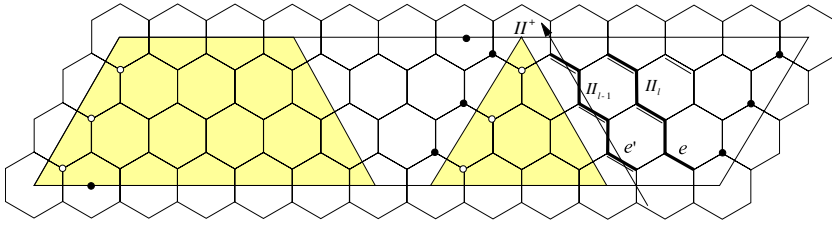


Figure 6. Illustration for subcase 3.1 in proof of lemma 4.6.

Suppose to the contrary that there exist edges in  $S^2$  not  $B$ -forced by  $\Delta_k$ , equivalently, there exists  $H_m \subset H_0$  such that every edge in  $E(H_m) \cap S^2 \neq \emptyset$  is not a pendant edge of  $H_m$ . Choose one edge  $e \in E(H_m) \cap S^2$  such that  $e \in II_l$  and  $l$  is minimal. By the minimality of  $l$ , for any  $e' \in E(II_{l-1}) \cap M_2$ , either  $e' \in E(H[\Delta_k])$  or  $e'$  is a pendant edge of some  $H_i$  with  $i < m$ . By lemma 4.5, every  $II$ -cycle contains at least one edge in  $E' = \{w_{j,0}b_{j,0} | 0 \leq j \leq k-1\}$ . Hence, all edges in  $E(R_{l-1}) \cap M_2$  starting from  $e'$  along  $II^+$ -direction and stopping at some edge in  $E' \cap E(R_{l-1})$  are not in  $E(H_m)$ . Since  $e$  is not a pendent edge, all vertical edge in  $E(R_l)$  starting from  $e$  along  $II^+$ -direction and stopping at some edge in  $E' \cap E(R_l)$  belong to  $E(H_m)$ ; If not,  $E(H_m)$  contains pendant edge in  $S^2$  which contradicts the supposition. But  $E' \cap E(H_0) = \emptyset$ , which contradicts  $H_m \subset H_0$  and  $E' \cap E(R_l) \cap E(H_m) \neq \emptyset$ . The contradiction implies claim 2.

Since  $S^2$  is  $B$ -forced by  $\Delta_k$ ,  $H_0 - V(S^2)$  has no edges, hence for any vertex in  $H_0 - V(S^2)$ , its neighbors belongs to  $\Delta_k \cup V(S^2)$ . Hence  $D(\Delta_k) = V(H)$ .

Case 3: The corner  $h_{p-st,k-sq}$  of  $P_{s+1}$  coincides with  $h_{x,0}$  where  $0 \leq x \leq k$ .

Subcase 3.1: If  $x < k$ . Then  $b_{x+1,q-1}w_{x+1,q-1}$  is a pendant edge of  $H_0$ . Let  $H_1 = H_0 - \{b_{x+1,q-1}, w_{x+1,q-1}\}$  (see Figure 6).

Further, by the same discussion as that of case 2, we have  $E(H_0) \cap M_2$  is  $B$ -forced by  $\Delta_k$ . Since  $H_0 - V(E(H_0) \cap M_2)$  has only  $k$  isolated vertices,  $D(\Delta_k) = V(H)$ .

Subcase 3.2: If  $x = k$ . Then  $b_{x,q-1}w_{x-1,q-1}$  is a pendant edge of  $H_0$ . Let  $H_1 = H_0 - \{b_{x,q-1}, w_{x-1,q-1}\}$ .

By the same discussion of subcase 3.1 but changing  $II$ -cycle to  $I$ -cycle, we have  $D(\Delta_k) = V(H)$ . □

**Lemma 4.7.** Let  $\Delta_k$  be the characteristic triangle of  $H$ . Then  $f(H) \leq k$ .

*Proof.* It suffices to find a perfect matching  $M$  of  $H$  such that  $f(H, M) \leq k$ . Let  $\Delta_k$  consist of  $s$  trapeziums  $P_{l+1}$  ( $0 \leq l \leq s-1$ ) and a triangle  $P_{s+1}$ .

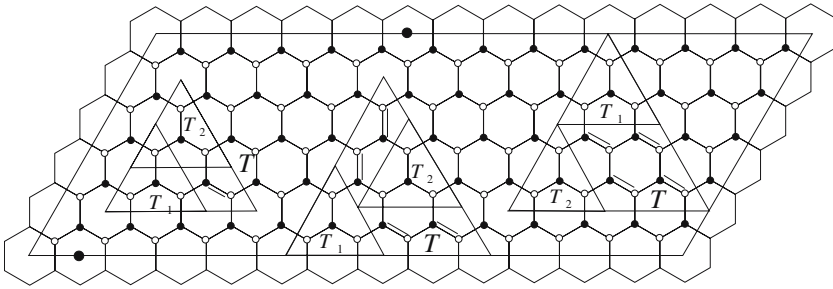


Figure 7.  $T_1$  and  $T_2$ , the double edges are  $B$ -forced by  $T_1 \cup T_2$ .

*Case 1:* If there exists  $0 \leq l \leq s$  such that  $P_l$  and  $P_{l+1}$  have the same corner  $h_{k,0}$ . Let  $S = \{w_{i,0}b_{i+t+1,q-1} \mid 0 \leq i \leq k-1\}$ . Then  $S$  forces  $E(H[\Delta_k]) \cap M_1$ . By lemma 4.6, in this case,  $\Delta_k$  forces  $E(H[\bar{\Delta}_k]) \cap M_1$ . Since  $M_1 = S \cup (E(H[\Delta_k]) \cap M_1) \cup (E(H[\bar{\Delta}_k]) \cap M_1)$ , we have  $S$  forces  $M_1$ . Further,  $f(H(p, q, t), M_1) \leq |S| = k$ .

*Case 2:* If there exists  $0 \leq l \leq s$  such that  $P_l$  and  $P_{l+1}$  have the same corner  $h_{0,0}$ . Let  $S = \{b_{p-rt,i}w_{p-rt,i} \mid 0 \leq r \leq \lfloor \frac{k}{q} \rfloor, 0 \leq i \leq q-1$  and  $r = \lceil \frac{k}{q} \rceil, 0 \leq i \leq k - (r-1)q - 1\}$ . Then  $S$  forces  $E(H[\Delta_k]) \cap M_2$ . Since  $\Delta_k$  forces  $E(H[\bar{\Delta}_k]) \cap M_2$  and  $M_2 = S \cup (E(H[\Delta_k]) \cap M_2) \cup (E(H[\bar{\Delta}_k]) \cap M_2)$ , we have  $S$  forces  $M_2$  and then  $f(H(p, q, t), M_2) \leq |S| = k$ .

*Case 3:* The corner  $h_{p-st,k-sq}$  of  $P_{s+1}$  coincides with  $h_{x,0}$  where  $0 \leq x \leq k$ .

*Subcase 3.1:* For  $0 \leq x < k$ . Let  $S = \{b_{p-rt,i}w_{p-rt,i} \mid 0 \leq r \leq \lfloor \frac{k}{q} \rfloor, 0 \leq i \leq q-1$  and  $r = \lceil \frac{k}{q} \rceil, 0 \leq i \leq k - (r-1)q - 1\}$ . As discussion in case 2, we have  $S$  forces  $M_2$  and then  $f(H, M_2) \leq |S| = k$ .

*Subcase 3.2:* For  $x = k$ . Let  $S = \{b_{k-r(p+t),i}w_{k-r(p+t)-1,i} \mid 0 \leq r \leq \lfloor \frac{k}{q} \rfloor, 0 \leq i \leq q-1$  and  $r = \lceil \frac{k}{q} \rceil, 0 \leq i \leq k - (r-1)q - 1\}$ . Then  $S$  forces  $E(H[\Delta_k]) \cap M_3$ . Since  $\Delta_k$  forces  $E(H[\bar{\Delta}_k]) \cap M_3$  and  $M_3 = S \cup (E(H[\Delta_k]) \cap M_3) \cup (E(H[\bar{\Delta}_k]) \cap M_3)$ , we have  $S$  forces  $M_3$  and further  $f(H, M_3) \leq |S| = k$ .  $\square$

Let triangles  $T_1$  and  $T_2$  satisfy  $T_1 = N[b_{x_1,y_1}]$  and  $T_2 = N[b_{x_2,y_2}]$ . If  $T_1$  and  $T_2$  have a common point, then  $D(T_1 \cup T_2)$  is the minimal triangle  $T$  such that  $T_1 \cup T_2 \subset T$  if  $\Delta_k$  satisfies  $k > \delta(T)$  (see figure 7). For generality, let  $T_1$  and  $T_2$  be two triangles with  $\delta(T_i) < k$  ( $i = 1, 2$ ). We say  $T_1$  and  $T_2$  are *disjoint* if they have no common point. If  $T_1$  and  $T_2$  have a common point, let  $T_*$  be the region of intersection of  $T_1$  and  $T_2$ , then  $D(T_1 \cup T_2)$  is the minimal triangle containing  $T_1 \cup T_2$  if  $\delta(T_1) + \delta(T_2) - \delta(T_*) < k$  and  $D(T_1 \cup T_2) = V(H)$  if  $\delta(T_1) + \delta(T_2) - \delta(T_*) \geq k$ , where  $k$  is the side length of the characteristic triangle of  $H$ . We omit the proof here.

**Lemma 4.8.** Let  $\Delta_k$  be the characteristic triangle of  $H$  and  $b_{pq} > b_{pq-1} > \dots > b_1$  be any canonical ordering of  $B$  whose key vertices are  $b_{j_1} > \dots > b_{j_l}$ . Then  $\sum_{i=1}^l \epsilon(b_{j_i}) \geq k$ .

*Proof.* Since  $H$  is a 3-regular graph and  $b_{j_i}$  ( $1 \leq i \leq l$ ) is key vertex, we have  $1 \leq \epsilon(b_{j_i}) \leq 2$ . Clearly we have  $b_{pq} = b_{j_1}$ ,  $\epsilon(b_{j_1}) = 2$  and  $D(b_{j_1}) = V(H)$ . If  $l = 1$ , then  $D(N[b_{j_1}]) = V(H)$ . According to the isomorphism  $\phi_{tb}$  and  $\phi_{r1}$ , let  $b_{j_1} = b_{1,0}$ . Then  $\Delta_2 = N[b_{j_1}]$ , so  $D(\Delta_2) = V(H)$ , hence  $\Delta_2$  is a characteristic triangle. Therefore,  $k = 2 \leq \epsilon(b_{j_1})$  and the assertion holds.

So, in the following, we suppose  $l > 1$ . Then  $D(b_{j_{l-1}}) \subsetneq V(H)$ .

*Claim:*  $D(b_{j_i})$  ( $1 \leq i \leq l - 1$ ) consists of some disjoint triangles  $T$  such that  $\delta(T) < k$  and  $\sum_{b_{j_i} \in T} \epsilon(b_{j_i}) \geq \delta(T)$  for  $1 \leq t \leq i$ .

*Proof.* We prove it by induction on  $i$ . If  $i = 1$ , let  $b_{j_1} = b_{x,y}$ . Then  $D(b_{j_1}) = N[b_{x,y}]$ . So  $D(b_{j_1})$  consists only of one triangle  $T = N[b_{x,y}]$  with side length 2. On the other hand,  $b_{j_1}$  is the maximum key vertex of the ordering  $B$ , so  $\epsilon(b_{j_1}) = 2 \geq \delta(T)$ . Hence the claim holds for  $i = 1$ .

In the following, we assume claim is true for  $i - 1$ , then  $D(b_{j_{i-1}})$  consists of some disjoint triangles  $T_1, \dots, T_r$  and  $\sum_{b_{j_i} \in T_m} \epsilon(b_{j_i}) \geq \delta(T_m)$  ( $1 \leq t \leq i - 1, 1 \leq m \leq r$ ). Let  $\mathcal{T} = \{T_1, T_2, \dots, T_r\}$ . For the key vertex  $b_{j_i}$ , let  $T^0$  be the triangle such that  $T^0 = N[b_{j_i}]$ . If  $T^0$  has no common points with  $T_m$  ( $1 \leq m \leq r$ ), then  $\epsilon(b_{j_i}) = 2$  and claim is true since  $\delta(T) = 2$ . Without loss of generality, suppose there exists a sequence of triangles  $T_{m_1}, \dots, T_{m_{r_1}} \in \mathcal{T}$  such that  $T_{m_{j+1}}$  has a common point with  $T^j$ , where  $T^j$  is the minimal triangle satisfying  $T^{j-1} \cup T_{m_j} \subseteq T^j$ , and for every  $T' \in \mathcal{T}$ ,  $T'$  has a common point with  $T^{r_1}$  if and only if  $T' \subseteq T^{r_1}$ . Let  $T_*^j = T^{j-1} \cap T_{m_j}$  ( $1 \leq j \leq r_1$ ). Then  $\delta(T^j) = \delta(T_{m_j}) + \delta(T^{j-1}) - \delta(T_*^j)$  and  $\delta(T^{r_1}) < k$ , otherwise contradict with  $i \leq l - 1$ . Let  $\mathcal{T}_m = \{T_{m_1}, T_{m_2}, \dots, T_{m_{r_1}}\}$ . We have

$$\begin{aligned} \delta(T^{r_1}) &= \delta(T^{r_1-1}) + \delta(T_{m_{r_1}}) - \delta(T_*^{r_1}) \leq \delta(T^{r_1-1}) + \delta(T_{m_{r_1}}) \leq \sum_{j=1}^{r_1} \delta(T_{m_j}) + \delta(T^0) - \delta(T_*^1) \\ &\leq \sum_{j=1}^{r_1} \sum_{b_{j_i} \in T_{m_j}} \epsilon(b_{j_i}) + \sum_{T' \in \mathcal{T} \setminus \mathcal{T}_m \text{ and } T' \subset T^{r_1}} \delta(T') \leq \sum_{b_{j_i} \in T^{r_1}} \epsilon(b_{j_i}). \end{aligned}$$

Therefore, the claim holds.

In the following, we will prove  $\sum_{i=1}^l \epsilon(b_{j_i}) \geq k$ . Suppose that  $D(b_{j_{l-1}})$  consists of  $r$  disjoint triangles  $T_1, \dots, T_r$ . Let  $T^0 = N[b_{j_l}]$ . Since  $1 \leq \epsilon(b_{j_l}) \leq 2$  and  $D(b_{j_l}) = V(H)$ , there exists  $T_{m_1}$  ( $1 \leq m_1 \leq r$ ) such that  $T_{m_1}$  has a common point with  $T^0$ . Then either  $\delta(T_{m_1}) + \delta(T^0) - \delta(T_*^1) \geq k$  where  $T_*^1 = T^0 \cap T_{m_1}$  or there is a minimal triangle  $T^1$  such that  $T^0 \cup T_{m_1} \subset T^1$  and  $\delta(T^1) = \delta(T_{m_1}) + \delta(T^0) - \delta(T_*^1) < k$ .



If the former holds, we have

$$k \leq \delta(T_{m_1}) + \delta(T^0) - \delta(T_*^1) \leq \sum_{b_{j_i} \in T_{m_1}} \epsilon(b_{j_i}) + \epsilon(b_{j_i}) \leq \sum_{i=1}^l \epsilon(b_{j_i}),$$

the assertion holds. If the latter holds, without loss of generality, suppose there exists a sequence of triangles  $T_{m_1}, T_{m_2}, \dots, T_{m_{r_1}}$  ( $1 \leq m_i \leq r$  for  $i = 1, 2, \dots, r_1$ ) and triangles  $T^0, T^1, T^2, \dots, T^{r_1}$ , such that  $T^j$  has a common point with  $T_{m_{j+1}}$  and is minimal subject to  $T^{j-1} \cup T_{m_j} \subseteq T^j$ , and every  $T_i$  ( $1 \leq i \leq r$ ) has a common point with  $T^{r_1}$  if and only if  $T_i \subseteq T^{r_1}$ . Let  $T_*^j = T^{j-1} \cap T_{m_j}$ . Then  $\delta(T^{r_1}) = \delta(T^{r_1-1}) + \delta(T_{m_{r_1}}) - \delta(T_*^{r_1}) \geq k$  by  $D(b_{j_i}) = V(H)$ . According to the claim, we have

$$\begin{aligned} k &\leq \delta(T^{r_1-1}) + \delta(T_{m_{r_1}}) - \delta(T_*^{r_1}) \leq \delta(T^{r_1-1}) + \delta(T_{m_{r_1}}) \\ &\leq \sum_{j=1}^{r_1} \delta(T_{m_j}) + \delta(T^0) - \delta(T_*^1) \leq \sum_{j=1}^{r_1} \sum_{b_{j_i} \in T_{m_j}} \epsilon(b_{j_i}) + \epsilon(b_{j_i}) \leq \sum_{i=1}^l \epsilon(b_{j_i}). \end{aligned}$$

The assertion holds. □

**Theorem 4.9.** Let  $\Delta_k$  be the characteristic triangle of  $H(p, q, t)$ . Then  $f(H(p, q, t)) = k$ .

*Proof.* By lemmas 3.9 and 4.8, we know the smallest possible maximum excess over all canonical orderings of  $B$  is no less than  $k$ . Hence  $f(H(p, q, t)) \geq k$  by lemma 3.6 and theorem 3.8. By lemma 4.7,  $f(H(p, q, t)) \leq k$ . So  $f(H(p, q, t)) = k$ . □

### 5. An algorithm

We conclude this paper with a fast algorithm to compute  $f(H(p, q, t))$  with  $p > q \geq 1$  and  $1 \leq t \leq p - q - 1$ , based on theorem 4.2, which gives the forcing number of a toroidal polyhex  $H(p, q, t)$  with  $1 \leq p \leq q$  or  $p > q \geq 1$  and  $t \in \{p - q, p - q + 1, \dots, p - 1, 0\}$ .

According to the triangle extension introduced in section 4 and theorems 4.4 and 4.9, we have the following algorithm of complexity  $O(n)$ , where  $n$  is the number of vertices of  $H(p, q, t)$ .

**Algorithm 5.1. Input:** A toroidal polyhex  $H(p, q, t)$  with  $p > q \geq 1$  and  $1 \leq t \leq p - q - 1$ .

**Output:** The forcing number of  $H(p, q, t)$ .

**Step 0.** Set  $a := p - 1$ ,  $b := 1$ , and  $k := q + 1$  ( $a$  is the minimal  $x$ -coordinate over all bottom-left vertices of trapeziums except  $P_1$ ,  $b$  is the maximal  $x$ -coordinate over all the bottom-right vertices of the trapeziums except  $P_1$ , and  $k$  is the side length of the normal triangle).

**Step 1.** Set  $s := \lfloor \frac{k}{q} \rfloor$  and  $r := k - sq$ ; If  $r = 0$ , set  $s := s - 1$ ,  $r := q$ .

**Step 2.** If  $r = q$  and  $0 \leq p - (s + 1)t \pmod{p} \leq k$ , obtain the characteristic triangle and output  $k$ , stop.

**Step 3.** If  $r = 1$ , set  $a := \min\{a, p - st \pmod{p}\}$ ,  $b := \max\{b + 1, (p - st) \pmod{p} + 1\}$ ; else, set  $b := b + 1$ .

**Step 4.** If  $a = k$  or  $b = q$ , obtain the characteristic triangle and output  $k$ , then stop.

**Step 5.** Set  $k := k + 1$ . Then go to step 1. □

A program of algorithm 5.1 in Microsoft Visual FoxPro 6.0 has been accomplished on micro computer.

## Acknowledgments

This work was supported by NSFC grant 10471058, TRAPOYT, and the Priority Academic Discipline Foundation of Linyi Normal University.

## References

- [1] P. Adams, M. Mahdian and E.S. Mahmoodian, *Discrete Math.* 281 (2004) 1–12.
- [2] P. Afshani, H. Hatami and E.S. Mahmoodian, *Aust. J. Comb.* 30 (2004) 147–160.
- [3] T. Došlić, *J. Math. Chem.* (2006). Online First, DOI: 10.1007/s10910-006-9056-2.
- [4] F. Harary, D.J. Klein and T.P. Živković, *J. Math. Chem.* 6 (1991) 295–306.
- [5] D.J. Klein and M. Randić, *J. Comput. Chem.* 8 (1987) 516–521.
- [6] D.J. Klein and H. Zhu, *Discrete Appl. Math.* 67 (1996) 157–173.
- [7] S. Kleinerman, *Discrete Math.* 306 (2006) 66–73.
- [8] E.C. Kirby, D.J. Klein, R.B. Mallion, P. Pollak and H. Sachs, *Croat. Chem. Acta* 77(1–2) (2004) 263–278.
- [9] E.C. Kirby, R.B. Mallion and P. Pollak, *J. Chem. Soc. Faraday Trans.* 89(12) (1993) 1945–1953.
- [10] E.C. Kirby and P. Pollak, *J. Chem. Inf. Comput. Sci.* 38 (1998) 66–70.
- [11] K. Kutnar, A. Malnič and D. Marušič, *J. Chem. Inf. Comput. Sci.* 45 (2005) 1527–1535.
- [12] F. Lam and L. Pachter, *Theor. Comput. Sci.* 303 (2003) 409–416.
- [13] J. Liu, H. Dai, J.H. Hafner, D.T. Colbert, R.E. Smalley, S.J. Tans and C. Dekker, *Nature* 385 (1997) 780–781.
- [14] L. Pechter and P. Kim, *Discrete Math.* 190 (1998) 287–294.
- [15] M. Randić and D.J. Klein, in: *Mathematical and Computational Concepts in Chemistry*, ed. N. Trinajstić (Wiley, New York, 1985) pp. 274–282.
- [16] M.E. Riddle, *Discrete Math.* 245 (2002) 283–292.
- [17] W.C. Shiu, P.C.B. Lam and H. Zhang, *J. Math. Chem.* 38(4) (2005) 451–466.
- [18] D. Vukičević, H.W. Kroto and M. Randić, *Croat. Chem. Acta* 78 (2005) 223–234.
- [19] D. Vukičević and J. Sedlar, *Math. Commun.* 9 (2004) 169–179.
- [20] D. Vukičević and N. Trinajstić, *J. Math. Chem.* (2006) Online-first, DOI: 10.1007/s10910-006-9133-6.

- [21] F. Zhang and X. Li, *Discrete Math.* 140 (1995) 253–263.
- [22] F. Zhang and X. Li, *Acta Math. Appl. Sinica (English Series)* 12(2) (1996) 209–215.
- [23] F. Zhang and H. Zhang, *J. Mol. Struct. (Theochem)* 331 (1995) 255–260.
- [24] H. Zhang and F. Zhang, *Discrete Appl. Math.* 105 (2000) 291–311.