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Wiener index of toroidal polyhexes*

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Abstract

The Wiener index of a graph is the sum of distances between all pairs of vertices. A toroidal polyhex (or toroidal graphitoid) $H(p,q,t)$ can be described by a string (p,q,t) of three integers $(p \geqslant 1, q \geqslant 1, 0 \leqslant t \leqslant p-1)$. In a recent work (*MATCH* **45** (2002) 109-122) M.V. Diudea obtained Wiener index formulae for several classes of toroidal nets, including toroidal polyhexes with $t \equiv -\frac{q}{2} (\text{mod } p)$. In this paper, we obtain formulae for calculating the Wiener index of toroidal polyhexes $H(p,q,t)$ with either $t = 0$ or $p \leqslant 2q$ or $p \leqslant q+t$.

1 Introduction

The Wiener index of a graph is a well-known topological index based on the distances, introduced originally for alkanes by H. Wiener [20] and extensively studied since the middle of the 1970s. For researches on the Wiener index we refer to [1, 3, 8, 17] and two special issues of MATCH [6] and Discrete Appl. Math. [7]. Two recent surveys on the Wiener index of trees [4] and hexagonal systems [5] were given.

The *Wiener index* of a graph G, denoted by $W(G)$, is defined as the sum of distances between all pairs of vertices in G [9],

$$W(G) := \sum_{\{u,v\} \subseteq V(G)} d_G(u,v)$$

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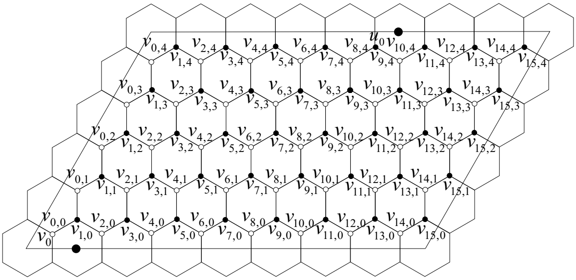

Fig. 1. A toroidal polyhex $H(p,q,t)$ for $p = 8, q = 5$ and $t = 4$, a pair of specified vertices v_0 and u_0 and the labelling of vertices.

where $d_G(u,v)$ is the distance (i.e. the number of edges in a shortest path) between a pair of vertices u and v of G.

A *toroidal polyhex* (or *toroidal graphitoid, torene*) $H(p,q,t)$ [15, 18], described by three parameters p, q and t, is a 3-regular (cubic or trivalent) bipartite graph embedded on the torus such that each face is a hexagon and represented by a $p \times q$-parallelogram M in the plane (equipped with the regular hexagonal lattice L) with the usual boundary identification (see Fig. 1): each side of M connects the centers of two hexagons, and is perpendicular to an edge-direction of L, both top and bottom sides pass through p vertical edges of L; while two lateral sides pass through q edges. First identify its two lateral sides, then rotate the top cycle t hexagons $(0 \leqslant t \leqslant p-1)$, finally identify the top and bottom at their corresponding points. If we carry only out the lateral boundary identification, then we obtain a *zig-zag open-ended nanotube* (or *tubule*), denoted by $T(p,q)$. Toroidal polyhexes have been recently experimentally detected [13]. Various researches on toroidal polyhexes appeared in both chemical and mathematical literatures, such as theoretical background [16, 19], the enumeration of Kekulé structures [10, 11, 12] and k-resonance [18], etc.

Theorem 1.1 ([15, 19]). *Every toroidal polyhex $H(p,q,t)$ is a vertex-transitive graph.*

In this paper we consider the Wiener index of toroidal polyhexes $H(p,q,t)$. In fact, M.V. Diudea [2] gave a formula for the Wiener index of $H(p,q,t)$ with $t \equiv -\frac{q}{2} (\text{mod } p)$. We denote by Θ the sum of distances from a fixed vertex v to all other vertices of $H(p,q,t)$. Then by the vertex-transitivity of a toroidal polyhex $H(p,q,t)$ with $2pq$ vertices (Theorem 1.1), we have

$$W(H(p,q,t)) = pq\Theta. \tag{1}$$

So our main object is to compute Θ. By establishing a relation between distances in tubule $T(p,q)$ and in toroidal polyhex $H(p,q,t)$ (Lemma 2.4 or 2.5), we give the distances from the fixed vertex v to all other vertices in $H(p,q,t)$ (Subsections 3.1 and 3.2), further we obtain formulae for $W(H(p,q,t))$ for either $t=0$ or $p \leqslant 2q$ or $p \leqslant q+t$ (Theorem 3.6), which includes the case when $t \equiv -\frac{q}{2} (\text{mod } p)$. Finally we give some examples that our approach is not suitable for other cases.

2 From tubule to torus

For convenience, we denote by *layer* $0, 1, 2, \cdots, q-1$ horizontal zig-zag lines in M from bottom to top in defining $H(p,q,t)$, and by $v_{0,k}, v_{1,k}, \cdots, v_{2p-1,k}$ (in the sense that the first subscript modules $2p$) the vertices of layer k from left to right ($0 \leqslant k \leqslant q-1$). In $H(p,q,t)$, $v_{0,k}$ and $v_{2p-1,k}$ are adjacent for $0 \leqslant k \leqslant q-1$ and $v_{i,0}$ and $v_{i+2t+1,q-1}$ are adjacent for all even i. In a 2-coloring of $V(H(p,q,t))$, $v_{i,j}$ is colored white or black according as i is even or odd. Two adjacent vertices $v_{0,0}$ and $v_{2t+1,q-1}$ are specified as v_0 and u_0, respectively (see Fig. 1). However tubule $T(p,q)$ can also be obtained from $H(p,q,t)$ by deleting all edges passing through the bottom side of M. For $r \leqslant q$, $T(p,r)$ is a subgraph of $T(p,q)$ that is the part between layers 0 and $r-1$.

Let G_1 be a connected subgraph of a graph G. Then $d_{G_1}(u,v) \geqslant d_G(u,v)$ for any pair of vertices u and v of G_1. G_1 is a *convex subgraph* of G if any shortest path of G between two vertices of G_1 is already in G_1. Hence if G_1 is convex, $d_{G_1}(u,v) = d_G(u,v)$.

Lemma 2.1. *For any integer r with $1 \leqslant r \leqslant q-1$, $T(p,r)$ is convex in $T(p,q)$.*

Proof. Suppose to the contrary that $T(p,r)$ is not convex in $T(p,q)$. Then $T(p,q)$ has a shortest path P between a pair of vertices u and v of $T(p,r)$ which is not completely in $T(p,r)$. We choose such a pair of vertices u and v such that $d_{T(p,q)}(u,v)$ is as minimal as possible. Then only the end vertices of P lie in $T(p,r)$, precisely in layer $r-1$. Thus P and each of the two paths in layer $r-1$ with end vertices u and v form a cycle. One contractible cycle bounds a benzenoid system B on the tubule, which can be unfolded on the plane. However, there is a unique shortest path between u and v in B which lies completely in layer $r-1$ [14]. This contradicts that P is a shortest path. □

In the following we define some notations. From now on, it will be understood that H and T represent $H(p,q,t)$ and $T(p,q)$ respectively. We denote by G the graph H or T. For a fixed vertex v of G, $0 \leqslant l \leqslant 2p-1$, $0 \leqslant k \leqslant q-1$, the sequence of distances from v to the vertices in layer k started at $v_{l,k}$ is defined:

$$S_G(l,k;v) := \big(d_G(v_{l,k},v), d_G(v_{l+1,k},v), \cdots, d_G(v_{l+2p-1,k},v)\big),$$

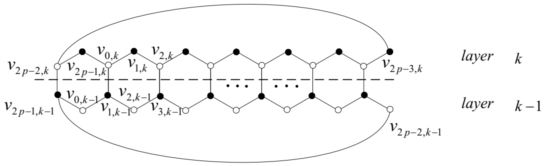

Fig. 2. The induced subgraph of T by layers $k-1$ and k.

and $S_G(k;v)$ is the cyclic permutation of $S_G(l,k;v)$. For a sequence $A=(a_i)_{i\geqslant 0}$, let

$$A+\vec{1}:=(a_i+1)_{i\geqslant 0}.$$

For convenience, for nonnegative integers m, n and s we define 5 sequences of integers as follows.

$$m,\nearrow,n:=\big(m,m+1,m+2,\cdots,n\big);\qquad (m\leqslant n)$$

$$m,\searrow,n:=\big(m,m-1,m-2,\cdots,n\big);\qquad (m\geqslant n)$$

$$m,\leftrightsquigarrow 2s,n:=\overbrace{m,n,m,n,\cdots,m,n}^{2s\text{ terms}}\;;\qquad (m\neq n)$$

$$S_1:=(2k,\nearrow,p+k,\searrow,2k,\leftrightsquigarrow 2k,2k+1);$$

$$S_2:=\big(2(q-k)-1,\leftrightsquigarrow 2(q-k),2(q-k),\nearrow,p+q-k,\searrow,2(q-k)\big).$$

Lemma 2.2.

$$S_T(0,k;v_0)=\begin{cases} S_1, & 0\leqslant k\leqslant p-1;\\ (2k,\leftrightsquigarrow 2p,2k+1), & p\leqslant k\leqslant q-1.\end{cases}\tag{2}$$

and

$$S_T(2t+1,k;u_0)+\vec{1}=\begin{cases} \big(2(q-k)-1,\leftrightsquigarrow 2p,2(q-k)\big), & 0\leqslant k\leqslant q-p-1;\\ S_2, & q-p\leqslant k\leqslant q-1.\end{cases}\tag{3}$$

Proof. We first prove Eq. (2) by applying induction on k. For the induction start, let $k=0$. Since the cycle $T(p,1)$ is a convex subgraph of T by Lemma 2.1,

$$S_T(0,0;v_0)=S_{T(p,1)}(0,0;v_0)=(0,\nearrow,p,\searrow,1).$$

So the assertion holds for $k=0$. Now let $0<k\leqslant q-1$ and suppose that the assertion holds for $k-1$. The induced subgraph of T by layers $k-1$ and k is shown in Fig. 2. For even i, since $v_{i,k}$ and $v_{i+1,k-1}$ are precisely ends of a vertical edge, by the bipartition of T and Lemma 2.1 we have

$$d_T(v_{i,k},v_0)=d_T(v_{i+1,k-1},v_0)+1\tag{4}$$

$$=\min\{d_T(v_{i,k-1},v_0),d_T(v_{i+2,k-1},v_0)\}+2.\tag{5}$$

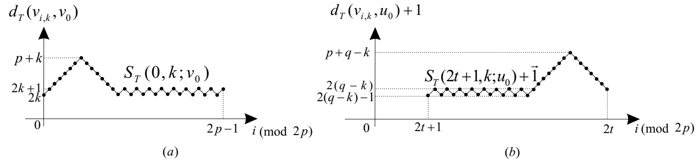

Fig. 3. (a). $S_T(0, k; v_0)$ for $k \leqslant p-1$ and (b). $S_T(2t+1, k; u_0) + \vec{1}$ for $p-q \leqslant k \leqslant q-1$.

For odd i, by the convexity of $T(p, k+1)$ and Eq. (4) we have

$$\begin{aligned} d_T(v_{i,k}, v_0) &= \min\{d_T(v_{i-1,k}, v_0), d_T(v_{i+1,k}, v_0)\} + 1 \\ &= \min\{d_T(v_{i,k-1}, v_0), d_T(v_{i+2,k-1}, v_0)\} + 2. \end{aligned} \tag{6}$$

By Eqs. (5) and (6), we have for any i,

$$d_T(v_{i,k}, v_0) = \begin{cases} d_T(v_{i,k-1}, v_0), & \text{if } d_T(v_{i,k-1}, v_0) > d_T(v_{i+2,k-1}, v_0); \\ d_T(v_{i,k-1}, v_0) + 2, & \text{otherwise.} \end{cases} \tag{7}$$

By the induction hypothesis, we have that for $0 \leqslant k-1 < p-1$,

$$S_T(0, k-1; v_0) = \big(2(k-1), \nearrow, p+k-1, \searrow, 2(k-1), \leftrightsquigarrow 2(k-1), 2k-1\big),$$

and for $p-1 \leqslant k-1 \leqslant q-1$,

$$S_T(0, k-1; v_0) = \big(2(k-1), \leftrightsquigarrow 2p, 2k-1\big).$$

Eq. (7) implies that the assertion holds for k.

Since there is an automorphism g of T such that $g(v_{2t+1-i,q-1-k}) = v_{i,k}$ for all i, k, in particular $g(v_0) = g(v_{0,0}) = v_{2t+1,q-1} = u_0$, $d_T(v_{i,k}, u_0) = d_T(v_{2t+1-i,q-1-k}, v_0)$ for any i, k. So Eq. (3) follows from Eq. (2). $\square$

Fig. 3 illustrates $S_T(0, k; v_0)$ for $k \leqslant p-1$ and $S_T(2t+1, k; u_0) + \vec{1}$ for $q-p \leqslant k \leqslant q-1$.

From now on we always suppose that parameters p, q and t satisfy

$$\text{either } t = 0 \text{ or } p \leqslant 2q \text{ or } p \leqslant q+t. \tag{$*$}$$

Lemma 2.3. *$d_T(v_{i-2t-1,0}, v_0) \leqslant d_T(v_{i,q-1}, v_0) + 1$ for odd i.*

Proof. Let i be odd. By Eq. (2) in Lemma 2.2, $2q-1 = 2(q-1)+1 \leqslant d_T(v_{i,q-1}, v_0)$. So, if $p \leqslant 2q$, $d_T(v_{i-2t-1,0}, v_0) \leqslant p \leqslant 2q \leqslant d_T(v_{i,q-1}, v_0) + 1$. Otherwise, we assume that $p \geqslant 2q+1$. By Eq. (2) we have

$$d_T(v_{i,q-1}, v_0) + 1 = \begin{cases} 2q+i-1, & 0 \leqslant i \leqslant p-q+1; \\ 2p-i+1, & p-q+2 \leqslant i \leqslant 2p-2q+2; \\ 2q, & 2p-2q+3 \leqslant i \leqslant 2p-1. \end{cases} \tag{8}$$

While

$$d_T(v_{i-2t-1,0}, v_0) = \begin{cases} \min\{2t-i+1, 2p+i-2t-1\}, & 0 \leqslant i \leqslant 2t+1; \\ \min\{i-2t-1, 2p+2t-i+1\}, & 2t+1 \leqslant i \leqslant 2p-1. \end{cases}$$

If $t = 0$,

$$d_T(v_{i-2t-1,0}, v_0) = \min\{i-1, 2p-i+1\}, 1 \leqslant i \leqslant 2p-1. \quad (9)$$

For $0 \leqslant i \leqslant 2p-2q+2$, by Eqs. (8) and (9), we have $d_T(v_{i-2t-1,0}, v_0) \leqslant d_T(v_{i,q-1}, v_0)+1$. For $2p-2q+3 \leqslant i \leqslant 2p-1$, $2p-i+1 < 2q$. By Eqs. (8) and (9), we have $d_T(v_{i-2t-1,0}, v_0) < d_T(v_{i,q-1}, v_0)+1$.

For the remaining case $p \leqslant q+t$, we distinguish the following three cases according to Eq. (8).

Case 1. $0 \leqslant i \leqslant p-q+1$. Since $p \leqslant q+t$, $i \leqslant t+1$. So $d_T(v_{i-2t-1,0}, v_0) \leqslant 2p+i-2t-1 \leqslant 2q+i-1 = d_T(v_{i,q-1}, v_0)+1$.

Case 2. $p-q+2 \leqslant i \leqslant 2p-2q+2$. If $i \leqslant 2t+1$, $d_T(v_{i-2t-1,0}, v_0) \leqslant 2t-i+1 \leqslant 2p-i+1 = d_T(v_{i,q-1}, v_0)+1$. If $i \geqslant 2t+1$, since $2i \leqslant 4p-4q+4 \leqslant 2t+2p-2q+4 \leqslant 2p+2t+2$, $d_T(v_{i-2t-1,0}, v_0) \leqslant i-2t-1 \leqslant 2p-i+1 = d_T(v_{i,q-1}, v_0)+1$.

Case 3. $2p-2q+3 \leqslant i \leqslant 2p-1$. Either $2t-i+1 \leqslant 2p-i+1 \leqslant 2q$ or $i-2t-1 \leqslant 2p-2t-1 \leqslant 2q$. So $d_T(v_{i-2t-1,0}, v_0) \leqslant d_T(v_{i,q-1}, v_0)+1$. □

Under Condition $(*)$ we give a crucial relation between distances in tubule $T(p,q)$ and in toroidal polyhex $H(p,q,t)$ as follows.

Lemma 2.4. $d_H(v_0, u) = \min\{d_T(v_0, u), d_T(u_0, u)+1\}$ *for every vertex* u *of* H.

Proof. Let u be any vertex in H. Then $d_H(v_0, u) \leqslant \min\{d_T(v_0, u), d_T(u_0, u)+1\}$. So it is sufficient to show that $d_H(v_0, u) \geqslant \min\{d_T(v_0, u), d_T(u_0, u)+1\}$.

Among all shortest paths from v_0 to u in H, we choose one, say P, such that the number N of edges at which P passes through the bottom side L_1 of the parallelogram M is as minimal as possible.

If $N = 0$, P is also a path of T. Then $d_H(v_0, u) \geqslant d_T(v_0, u)$.

Let $N \geqslant 1$. Let v_1v_2 be any edge in P passing through the bottom side L_1 from v_1 to v_2. Then

Claim 1. v_1 and v_2 belong to layers 0 and $q-1$ respectively.

Suppose not and let v_1v_2 be the first edge of P such that v_1 and v_2 lie in layers $q-1$ and 0 respectively. If v_0Pv_1 (i.e. the subpath of P from v_0 to v_1) lies entirely in T (see Fig. 4(a)), then

$$d_H(v_2, v_0) = d_H(v_1, v_0)+1 = d_T(v_1, v_0)+1. \quad (10)$$

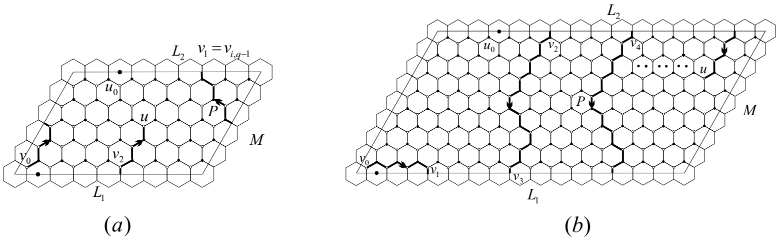

Fig. 4. Illustrations for Claims 1 and 2 in Lemma 2.4.

Let $v_1 = v_{i,q-1}$. Then i is odd and $v_2 = v_{i-2t-1,0}$. By Lemma 2.3 and Eq. (10),

$$d_T(v_2, v_0) = d_T(v_{i-2t-1,0}, v_0) \leqslant d_T(v_{i,q-1}, v_0) + 1 = d_T(v_1, v_0) + 1 = d_H(v_2, v_0),$$

which contradicts the choice of P. Otherwise, v_0Pv_1 has an edge v_3v_4 passing through L_1 such that v_3 and v_4 lie in layers 0 and $q-1$ respectively and v_4Pv_1 lies completely in T, precisely in layer $q-1$ by Lemma 2.1. We can replace $v_3v_4Pv_1v_2$ with a shorter path between v_3 and v_2 lying entirely in layer 0. This contradicts that P is a shortest path.

Claim 2. $N \leqslant 1$.

Suppose $N \geqslant 2$, we denote by v_1v_2 and v_3v_4 the first two edges of P passing through L_1 such that v_1 and v_3 belong to layer 0 (see Fig. 4(b)). Then

$$d_H(v_1, v_3) = d_H(v_2, v_3) + 1 = d_T(v_2, v_3) + 1. \tag{11}$$

We can shift horizontally backward all vertices some units such that v_3 is moved to the position of v_0. Then By Lemma 2.3 and Eq. (11),

$$d_T(v_1, v_3) \leqslant d_T(v_2, v_3) + 1 = d_H(v_1, v_3),$$

which contradicts the choice of P.

By Claims 1 and 2 v_0Pv_1 and v_2Pu lie entirely in T. By Lemma 2.1 v_0Pv_1 lies entirely in layer 0. Hence $d_H(v_0, v_1) = d_T(v_0, v_1) = d_T(u_0, v_2)$. Further, $d_H(v_0, u) = d_H(v_0, v_1) + 1 + d_H(v_2, u) = d_T(u_0, v_2) + d_T(v_2, u) + 1 \geqslant d_T(u_0, u) + 1$. □

For two sequences with length m: $A = (a_i)_{1\leqslant i\leqslant m}$ and $B = (b_i)_{1\leqslant i\leqslant m}$, let

$$A \wedge B := \big(\min\{a_i, b_i\}\big)_{1\leqslant i\leqslant m}.$$

From Lemma 2.4 we arrive at a main distance relation between torus and tubule.

Lemma 2.5. *$S_H(l, k; v_0) = S_T(l, k; v_0) \wedge \big(S_T(l, k; u_0) + \vec{1}\big)$ for any l, k.*

3 Computation for the Wiener index

In this section we shall obtain formulae for the Wiener index of $H(p,q,t)$. By Eq. (1), it needs to evaluate the sum Θ of distances from the vertex v_0 to all other vertices. For the sake of computation, we evaluate $S_H(k;v_0)$ for every layer k $(0 \leqslant k \leqslant q-1)$ in two ways.

For convenience, we further define 8 sequences with length $2p$ as follows.

$S_3 := \big(2k, \nearrow, 2(q-k)-1, \leftrightsquigarrow 2(p-2q+3k+1), 2(q-k), \searrow, 2k, \leftrightsquigarrow 2k, 2k+1\big)$,
$S_4 := \big(2k, \nearrow, 2(q-k)-1, \leftrightsquigarrow 2(p+k-i_0+1), 2(q-k), \nearrow, i_0, \searrow, 2k, \leftrightsquigarrow 2k, 2k+1\big)$,
$S_5 := \big(2k, \nearrow, q+t, \searrow, 2(q-k)-1, \leftrightsquigarrow 2(p+k-q-t), 2(q-k), \searrow, 2k, \leftrightsquigarrow 2k, 2k+1\big)$,
$S_6 := \big(2k, \nearrow, q+t, \searrow, 2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, p-t, \searrow, 2k, \leftrightsquigarrow 2k, 2k+1\big)$,
$S_7 := \big(2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, p-t, \searrow, 2k, \leftrightsquigarrow 2(k+1), 2k+1, \nearrow, q+t, \searrow, 2(q-k)\big)$,
$S_8 := \big(2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, 2k, \leftrightsquigarrow 2(p+q-3k), 2k+1, \searrow, 2(q-k)\big)$,
$S_9 := \big(2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, 2k, \leftrightsquigarrow 2(p-k-t+1), 2k+1, \nearrow, q+t, \searrow, 2(q-k)\big)$,
$S_{10} := \big(2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, i_0, \searrow, 2k, \leftrightsquigarrow 2(p+q-i_0-k), 2k+1, \searrow, 2(q-k)\big)$,
where $i_0 = p-t$ or $2p-t$ in S_4 and S_{10}.

3.1 Evaluating $S_H(k;v_0)$ according to k

We partition the interval of the parameter k into three ranges: $0 \leqslant k \leqslant \min\{p-1, q-p-1\}$, $\min\{p, q-p\} \leqslant k \leqslant \max\{p, q-p\}-1$ and $\max\{p, q-p\} \leqslant k \leqslant q-1$. The second one is equivalent to either $p \leqslant k \leqslant q-p-1$ or $q-p \leqslant k \leqslant p-1$.

Proposition 3.1. *(i) For* $0 \leqslant k \leqslant \min\{p-1, q-p-1\}$, $S_H(0,k;v_0) = S_1$.
(ii) For $\max\{p, q-p\} \leqslant k \leqslant q-1$, $S_H(2t+1,k;v_0) = S_2$.

Proof. For $0 \leqslant k \leqslant \min\{p-1, q-p-1\}$, from Lemma 2.2 we have $p+k = \max_i\{d_T(v_{i,k}, v_0)\}$ and $2(q-k)-1 = \min_i\{d_T(v_{i,k}, u_0)+1\}$. Since $k \leqslant \min\{p-1, q-p-1\} \leqslant \frac{2q-p-1}{3}$, $p+k \leqslant 2(q-k)-1$. Thus $d_T(v_{i,k}, v_0) \leqslant d_T(v_{i,k}, u_0)+1$ for each i. By Lemma 2.4, $d_H(v_{i,k}, v_0) = d_T(v_{i,k}, v_0)$. By Lemmas 2.2 and 2.5, $S_H(0,k;v_0) = S_T(0,k;v_0) = S_1$. For $\max\{p, q-p\} \leqslant k \leqslant q-1$, $2k = \min_i\{d_T(v_{i,k}, v_0)\}$ and $p+q-k = \max_i\{d_T(v_{i,k}, u_0)+1\}$. Since $k \geqslant \max\{p, q-p\} \geqslant \frac{p+q}{3}$, $2k \geqslant p+q-k$. By Lemmas 2.2, 2.4 and 2.5, $S_H(2t+1,k;v_0) = S_T(2t+1,k;u_0) + \vec{1} = S_2$. □

Similar to the proof of Proposition 3.1, we have

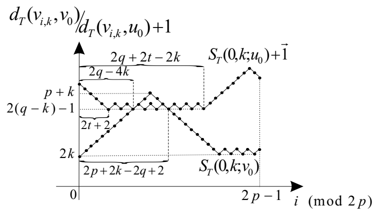

Fig. 5. Illustration for the proof of Proposition 3.4.

Proposition 3.2. *For* $p \leqslant k \leqslant q-p-1$,

$$S_H(0,k;v_0) = \begin{cases} (2k, \leftrightsquigarrow 2p, 2k+1), & p \leqslant k \leqslant \frac{q-1}{2}; \\ \big(2(q-k), \leftrightsquigarrow 2p, 2(q-k)-1\big), & \frac{q}{2} \leqslant k \leqslant q-p-1. \end{cases}$$

From now on suppose $q-p \leqslant k \leqslant p-1$. Since $\frac{2q-p-1}{3} = \frac{2}{3}(q-p) + \frac{1}{3}(p-1)$, $\frac{q-1}{2} = \frac{1}{2}(q-p) + \frac{1}{2}(p-1)$ and $\frac{q+p-2}{3} = \frac{2}{3}(q-p) + \frac{1}{3}(p-1)$, $q-p \leqslant \frac{2q-p-1}{3} \leqslant \frac{q-1}{2} \leqslant \frac{q+p-2}{3} \leqslant p-1$. So we further partition it into such four ranges.

Similar to the proof of Proposition 3.1, we obtain

Proposition 3.3. *(i) For* $q-p \leqslant k \leqslant \frac{2q-p-1}{3}$, $S_H(0,k;v_0) = S_1$.
(ii) For $\frac{p+q}{3} \leqslant k \leqslant p-1$, $S_H(2t+1,k;v_0) = S_2$.

We now discuss two remaining ranges: $\frac{2q-p}{3} \leqslant k \leqslant \frac{q-1}{2}$ and $\frac{q}{2} \leqslant k \leqslant \frac{q+p-1}{3}$.

Proposition 3.4. *For* $\frac{2q-p}{3} \leqslant k \leqslant \frac{q-1}{2}$,

$$S_H(0,k;v_0) = \begin{cases} S_3, & k \leqslant \min\{\frac{q-t-1}{2}, \frac{2q+t-p-1}{2}\}, \\ S_4, i_0 = p-t, & \frac{2q+t-p}{2} \leqslant k \leqslant \frac{q-t-1}{2}, \\ S_5, & \max\{\frac{q-t}{2}, q+t-p\} \leqslant k \leqslant \frac{2q+t-p-1}{2}, \\ S_6, & \max\{\frac{q-t}{2}, \frac{2q+t-p}{2}\} \leqslant k, \\ S_1, & k \leqslant \min\{p-t, q+t-p-1\}, \\ S_4, i_0 = 2p-t, & \max\{p-t+1, \frac{2q+t-2p}{2}\} \leqslant k \leqslant q+t-p-1, \\ S_3, & k \leqslant \frac{2q+t-2p-1}{2}. \end{cases}$$

Proof. For $\frac{2q-p}{3} \leqslant k \leqslant \frac{q-1}{2}$, $S_T(0,k;v_0) = S_1 = (2k, \nearrow, p+k, \searrow, 2k, \leftrightsquigarrow 2k, 2k+1)$ and $S_T(2t+1,k;u_0) + \vec{1} = S_2 = \big(2(q-k)-1, \leftrightsquigarrow 2(q-k), 2(q-k), \nearrow, p+q-k, \searrow, 2(q-k)\big)$. Obviously, $2k = \min_i\{d_T(v_{i,k},v_0)\} < 2(q-k)-1 = \min_i\{d_T(v_{i,k},u_0)+1\} < p+k = \max_i\{d_T(v_{i,k},v_0)\}$ (see Fig. 5). We now compute $S_H(0,k;v_0)$.

Since the $(2q-4k)$-th and $(2p+2k-2q+2)$-th terms of subsequence $(2k, \nearrow, p+k, \searrow, 2k)$ of $S_T(0,k;v_0)$ are all equal to $2(q-k)-1$,

$$\max_{\substack{0 \leqslant i \leqslant 2q-4k-1 \text{ or} \\ 2p+2k-2q+1 \leqslant i \leqslant 2p-1}} \{d_T(v_{i,k},v_0)\} = 2(q-k)-1, \tag{12}$$

and

$$\min_{2q-4k\leqslant i\leqslant 2p+2k-2q}\{d_T(v_{i,k},v_0)\}=2(q-k). \tag{13}$$

Combining $\min_i\{d_T(v_{i,k},u_0)+1\}=2(q-k)-1$ and Eq. (12) with Lemma 2.4, we have

$$d_H(v_{i,k},v_0)=d_T(v_{i,k},v_0), 0\leqslant i\leqslant 2q-4k-1 \text{ or } 2p+2k-2q+1\leqslant i\leqslant 2p-1. \tag{14}$$

If $k\leqslant \min\{\frac{q-t-1}{2},\frac{2q+t-p-1}{2}\}$, then

$$2t+2\leqslant 2q-4k, \tag{15}$$

and

$$2p+2k-2q+2\leqslant 2q+2t-2k. \tag{16}$$

From $\frac{2q-p}{3}\leqslant k$ and Eq. (15), we have $2q+2t-2k<2p$. Since $2(q-k)-1$ and $2(q-k)$ appear alternately from the $(2t+2)$-th to the $(2q+2t-2k)$-th term in $S_T(0,k;u_0)+\vec{1}$, by Eqs. (15) and (16) we have

$$\max_{2q-4k\leqslant i\leqslant 2p+2k-2q}\{d_T(v_{i,k},u_0)+1\}\leqslant 2(q-k). \tag{17}$$

Combining Eqs. (13) and (17) with Lemma 2.4, we have

$$d_H(v_{i,k},v_0)=d_T(v_{i,k},u_0)+1, 2q-4k\leqslant i\leqslant 2p+2k-2q. \tag{18}$$

By Eqs. (14) and (18), we have $S_H(0,k;v_0)=S_3$.

For the other cases, we can give proofs in similar ways. □

For $\frac{q}{2}\leqslant k\leqslant \frac{p+q-1}{3}$, similar to the above proof we can obtain the following result.

Proposition 3.5. *For* $\frac{q}{2}\leqslant k\leqslant \frac{p+q-1}{3}$,

$$S_H(2t+1,k;v_0)=\begin{cases} S_7, & k\leqslant \min\{\frac{q+t-1}{2},\frac{p-t-1}{2}\},\\ S_{10}, i_0=p-t, & \frac{q+t}{2}\leqslant k\leqslant \frac{p-t-1}{2},\\ S_9, & \frac{p-t}{2}\leqslant k\leqslant \min\{\frac{q+t-1}{2},p-t\}\\ S_8, & \max\{\frac{q+t}{2},\frac{p-t}{2}\}\leqslant k\leqslant p-t,\\ S_2, & \max\{q+t-p,p-t+1\}\leqslant k,\\ S_{10}, i_0=2p-t, & p-t+1\leqslant k\leqslant \min\{q+t-p-1,p-\frac{t+1}{2}\},\\ S_8, & p-\frac{t}{2}\leqslant k. \end{cases}$$

3.2 Evaluating $S_H(k;v_0)$ according to p

To compute the Wiener index of H according to $S_H(k,v_0)$, we tidy renewedly up the above propositions 3.1-3.5 in the following cases. We only give proofs for Cases 1 and 2.

Case 1. $p \leqslant \frac{q}{2}$,

$$S_H(k;v_0)=\begin{cases} S_1, & 0\leqslant k\leqslant p-1;\\ (2k,\leftrightsquigarrow 2p,2k+1), & p\leqslant k\leqslant \frac{q-1}{2};\\ \big(2(q-k),\leftrightsquigarrow 2p,2(q-k)-1\big), & \frac{q}{2}\leqslant k\leqslant q-p-1;\\ S_2, & q-p\leqslant k\leqslant q-1.\end{cases}$$

The interval $0\leqslant k\leqslant q-1$ is partitioned into three intervals $0\leqslant k\leqslant \min\{p-1,q-p-1\}=p-1$, $p\leqslant k\leqslant q-p-1$ and $q-p=\max\{p,q-p\}\leqslant k\leqslant q-1$. For $0\leqslant k\leqslant \min\{p-1,q-p-1\}$, by Proposition 3.1(i), $S_H(0,k;v_0)=S_1$. For $\max\{p,q-p\}\leqslant k\leqslant q-1$, by Proposition 3.1(ii), $S_H(2t+1,k;v_0)=S_2$. Similarly, we can obtain $S_H(0,k;v_0)$ for $p\leqslant k\leqslant q-p-1$ by Proposition 3.2.

Case 2. $\frac{q}{2}<p\leqslant \frac{q}{2}+\frac{t}{2}$,

$$S_H(k;v_0)=\begin{cases} S_1, & 0\leqslant k\leqslant \frac{2q-p-1}{3};\\ S_3, & \frac{2q-p}{3}\leqslant k\leqslant \frac{q-1}{2};\\ S_8, & \frac{q}{2}\leqslant k\leqslant \frac{p+q-1}{3};\\ S_2, & \frac{p+q}{3}\leqslant k\leqslant q-1.\end{cases}$$

Since $\frac{p-t}{2}<p-t\leqslant \frac{q-t}{2}\leqslant \frac{2q-p-1}{3}\leqslant \frac{q-1}{2}\leqslant \frac{2q+t-2p-1}{2}<q+t-p<\frac{2q+t-p}{2}$, Proposition 3.4 is equivalent to the statement: $S_H(0,k;v_0)=S_3$ for $\frac{2q-p}{3}\leqslant k\leqslant \frac{q-1}{2}$. Since $\frac{p-t-1}{2}<p-t<p-\frac{t}{2}\leqslant \frac{q}{2}<\frac{p+q}{3}<q+t-p$, similarly, Proposition 3.5 is equivalent to the statement: $S_H(2t+1,k;v_0)=S_8$ for $\frac{q}{2}\leqslant k\leqslant \frac{p+q-1}{3}$. Combining the above discussions with Propositions 3.1 and 3.3, the assertions hold.

Case 3. $\frac{q}{2}+\frac{t}{2}<p\leqslant \frac{q}{2}+\frac{3t}{4}$,

$$S_H(k;v_0)=\begin{cases} S_1, & & 0\leqslant k\leqslant \frac{2q-p-1}{3};\\ S_3, & & \frac{2q-p}{3}\leqslant k\leqslant \frac{2q+t-2p-1}{2};\\ S_4, & i_0=2p-t, & \frac{2q+t-2p}{2}\leqslant k\leqslant \frac{q-1}{2};\\ S_{10}, & i_0=2p-t, & \frac{q}{2}\leqslant k\leqslant p-\frac{t+1}{2};\\ S_8, & & p-\frac{t}{2}\leqslant k\leqslant \frac{p+q-1}{3};\\ S_2, & & \frac{p+q}{3}\leqslant k\leqslant q-1.\end{cases}$$

Case 4. $\frac{q}{2}+\frac{3t}{4}<p<\frac{q}{2}+t$,

$$S_H(k;v_0)=\begin{cases} S_1, & & 0\leqslant k\leqslant p-t;\\ S_4, & i_0=2p-t, & p-t+1\leqslant k\leqslant \frac{q-1}{2};\\ S_{10}, & i_0=2p-t, & \frac{q}{2}\leqslant k\leqslant q+t-p-1;\\ S_2, & & q+t-p\leqslant k\leqslant q-1.\end{cases}$$

Case 5. $p\geqslant \frac{q}{2}+t$. We distinguish three subcases:

Subcase 5.1. $q\leqslant t$,

$$S_H(k;v_0)=\begin{cases} S_1, & 0\leqslant k\leqslant q+t-p-1;\\ S_5, & q+t-p\leqslant k\leqslant \frac{q-1}{2};\\ S_9, & \frac{q}{2}\leqslant k\leqslant p-t;\\ S_2, & p-t+1\leqslant k\leqslant q-1.\end{cases}$$

Subcase 5.2. $q > t$ and $p \leqslant 2q$.

Subsubcase 5.2.1. $\frac{q}{2} + t \leqslant p \leqslant \frac{q}{2} + \frac{3t}{2}$,

$$S_H(k; v_0) = \begin{cases} S_1, & 0 \leqslant k \leqslant q + t - p - 1; \\ S_5, & q + t - p \leqslant k \leqslant \frac{q-1}{2}; \\ S_9, & \frac{q}{2} \leqslant k \leqslant p - t; \\ S_2, & p - t + 1 \leqslant k \leqslant q - 1. \end{cases}$$

Subsubcase 5.2.2. $\frac{q}{2} + \frac{3t}{2} < p < q + t$,

$$S_H(k; v_0) = \begin{cases} S_1, & 0 \leqslant k \leqslant \frac{2q-p-1}{3}; \\ S_3, & \frac{2q-p}{3} \leqslant k \leqslant \frac{q-t-1}{2}; \\ S_5, & \frac{q-t}{2} \leqslant k \leqslant \frac{q-1}{2}; \\ S_9, & \frac{q}{2} \leqslant k \leqslant \frac{q+t-1}{2}; \\ S_8, & \frac{q+t}{2} \leqslant k \leqslant \frac{p+q-1}{3}; \\ S_2, & \frac{p+q}{3} \leqslant k \leqslant q - 1. \end{cases}$$

Subsubcase 5.2.3. $q + t \leqslant p < q + 2t$,

$$S_H(k; v_0) = \begin{cases} S_1, & 0 \leqslant k \leqslant \frac{2q-p-1}{3}; \\ S_3, & \frac{2q-p}{3} \leqslant k \leqslant \frac{q-t-1}{2}; \\ S_5, & \frac{q-t}{2} \leqslant k \leqslant \frac{2q+t-p-1}{2}; \\ S_6, & \frac{2q+t-p}{2} \leqslant k \leqslant \frac{p-t-1}{2}; \\ S_9, & \frac{p-t}{2} \leqslant k \leqslant \frac{q+t-1}{2}; \\ S_8, & \frac{q+t}{2} \leqslant k \leqslant \frac{p+q-1}{3}; \\ S_2, & \frac{p+q}{3} \leqslant k \leqslant q - 1. \end{cases}$$

Subsubcase 5.2.4. $p \geqslant q + 2t$,

$$S_H(k; v_0) = \begin{cases} S_1, & & 0 \leqslant k \leqslant \frac{2q-p-1}{3}; \\ S_3, & & \frac{2q-p}{3} \leqslant k \leqslant \frac{2q+t-p-1}{2}; \\ S_4, & i_0 = p - t, & \frac{2q+t-p}{2} \leqslant k \leqslant \frac{q-t-1}{2}; \\ S_6, & & \frac{q-t}{2} \leqslant k \leqslant \frac{q+t-1}{2}; \\ S_{10}, & i_0 = p - t, & \frac{q+t}{2} \leqslant k \leqslant \frac{p-t-1}{2}; \\ S_8, & & \frac{p-t}{2} \leqslant k \leqslant \frac{p+q-1}{3}; \\ S_2, & & \frac{p+q}{3} \leqslant k \leqslant q - 1. \end{cases}$$

Subcase 5.3. $q > t$ and $p > 2q$,

$$S_H(k; v_0) = \begin{cases} S_4, & i_0 = p - t, & 0 \leqslant k \leqslant \frac{q-t-1}{2}; \\ S_6, & & \frac{q-t}{2} \leqslant k \leqslant \frac{q+t-1}{2}; \\ S_{10}, & i_0 = p - t, & \frac{q+t}{2} \leqslant k \leqslant q - 1. \end{cases}$$

3.3 Formulae for the Wiener index of $H(p, q, t)$

In this subsection we obtain algebraic expressions for the Wiener index of $H(p, q, t)$. Firstly, we compute the sum of all terms of S_i for $1 \leqslant i \leqslant 10$. Then, by the discussion of Subsection 3.2 we give the sum Θ of distances from v_0 to all other vertices. Finally,

TABLE I. Wiener index of $H(p,q,t)$ for $t=0$ or $p \leqslant 2q$.

p	q	t	W	p	q	t	W	p	q	t	W	p	q	t	W
4	20	0	131200	7	21	0	486717	4	8	1	9472	7	4	1	6440
4	15	0	56400	7	16	0	225792	4	5	1	2760	7	5	2	11305
4	10	0	17600	7	11	0	82313	4	6	2	4416	7	8	3	36736
4	7	0	6608	7	8	0	36400	4	3	2	792	7	10	4	64260
4	3	0	768	7	5	0	11305	4	7	3	6608	7	13	5	128037
4	1	0	64	7	1	0	343	4	2	3	320	7	14	6	156408

TABLE 2. Wiener index of $H(p,q,t)$ for $p \leqslant q+t$.

p	q	t	W	p	q	t	W	p	q	t	W
10	4	6	17600	19	9	11	655443	28	13	18	4485208
10	4	9	18800	19	8	13	522272	28	10	20	2513280
10	3	8	10260	19	6	14	275424	28	7	22	1163064
10	3	7	9480	19	4	17	121600	28	5	23	560000
10	2	9	4400	19	4	18	119168	28	4	25	371168
10	1	9	1000	19	2	18	28880	28	2	27	90944

according to Eq. (1) we obtain the main results of this article (Theorem 3.6). Some computations are accomplished by applying the Software package MATHEMATICA 5.0.

For convenience, we let

$$z = \begin{cases} 0, & q+p \equiv 0 (\mathrm{mod}\ 3); \\ 2, & q+p \equiv 1 (\mathrm{mod}\ 3); \\ -2, & q+p \equiv 2 (\mathrm{mod}\ 3). \end{cases}$$

Theorem 3.6. *For either $t=0$ or $p \leqslant 2q$ or $p \leqslant q+t$,*

$$W(H(p,q,t)) = \begin{cases} \frac{1}{3}p^2q(3q^2+2p^2-2), & p \leqslant \frac{q}{2}; \\ \frac{1}{9}pq(\Theta_1+z), & \frac{q}{2} < p \leqslant \frac{q}{2}+\frac{t}{2}; \\ \frac{1}{9}pq(\Theta_2+z), & \frac{q}{2}+\frac{t}{2} < p \leqslant \frac{q}{2}+\frac{3}{4}t; \\ \frac{1}{3}pq\Theta_3, & \frac{q}{2}+\frac{3}{4}t < p \leqslant \frac{q}{2}+t; \\ \frac{1}{3}pq\Theta_4, & \frac{q}{2}+t < p \leqslant \min\{\frac{q}{2}+\frac{3}{2}t, q+t\}; \\ \frac{1}{9}pq(\Theta_1-3t+3t^3+z), & \min\{\frac{q}{2}+\frac{3}{2}t, q+t\} < p \leqslant q+t; \\ \frac{1}{9}pq(\Theta_5+z), & q+t < p \leqslant 2q; \\ \frac{1}{3}q^2p(3p^2+2q^2-2), & t=0 \text{ and } 2q < p. \end{cases}$$

where

$\Theta_1 = -2p^3 - 3q + 12p^2q + 3pq^2 + q^3$,

$\Theta_2 = -6p + 22p^3 - 24p^2q + 21pq^2 - 2q^3 + 3t - 36p^2t + 36pqt - 9p^2t + 18pt^2 - 9qt^2 - 3t^3$,

$\Theta_3 = 2p - 14p^3 - 2q + 24p^2q - 9pq^2 + 2q^3 - 2t + 36p^2t - 36pqt + 9q^2t - 30pt^2 + 15qt^2 + 8t^3$,

$\Theta_4 = -2p + 2p^3 + 3pq^2 + 2t - 12p^2t + 12pqt - 3q^2t + 18pt^2 - 9qt^2 - 8t^3$,

$\Theta_5 = -3p + p^3 + 3p^2q + 12pq^2 - 2q^3 - 9p^2t + 18pqt - 9q^2t + 9pt^2 - 9qt^2$.

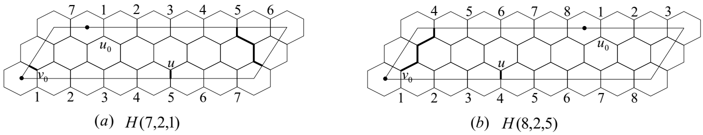

Fig. 6. Counterexamples to Lemma 2.4.

Corollary 3.7.

$$(i)\ W(H(p,q,0)) = \begin{cases} \frac{1}{3}p^2q(3q^2+2p^2-2), & p \leqslant \frac{q}{2}; \\ \frac{1}{9}pq(z-2p^3-3q+12p^2q+3pq^2+q^3), & \frac{q}{2} < p \leqslant q; \\ \frac{1}{9}pq(z-2q^3-3p+12q^2p+3qp^2+p^3), & q < p \leqslant 2q; \\ \frac{1}{3}q^2p(3p^2+2q^2-2), & 2q < p. \end{cases}$$

$$(ii)\ W(H(p,p,0)) = \begin{cases} \frac{1}{9}p^2(14p^3-3p), & p \equiv 0 (\text{mod } 3); \\ \frac{1}{9}p^2(14p^3-3p-2), & p \equiv 1 (\text{mod } 3); \\ \frac{1}{9}p^2(14p^3-3p+2), & p \equiv 2 (\text{mod } 3). \end{cases}$$

(iii) $W(H(p,1,0)) = W(C_{2p}) = p^3$.

Tables I and II list some numerical results for the Wiener index of toroidal polyhex $H(p,q,t)$.

4 Discussions

We have given formulae for calculating Wiener index of toroidal polyhexes $H(p,q,t)$ under Condition $(*)$: either $t=0$ or $p \leqslant 2q$ or $p \leqslant q+t$. But we cannot obtain Wiener index formulae of $H(p,q,t)$ for the other cases, i.e. $p \geqslant 2q+1$ and $0 < t < p-q$. In fact, our approach in this article is not suitable for such cases. For example, for $H(7,2,1)$ with two vertices v_0 and u (cf. Fig. 6(a)), $d_{H(7,2,1)}(u,v_0) = 4$ and the bold line represents a shortest path between v_0 and u. However $\min\{d_{T(7,2)}(u,v_0), d_{T(7,2)}(u,u_0)+1\} = 6$. Hence Lemma 2.4 does not holds for $H(7,2,1)$. $H(8,2,5)$ is another counterexample to Lemma 2.4 (cf. Fig. 6(b)).

From Theorem 3.6, we note that different toroidal polyhexes may have the same Wiener index. For example, the Wiener indices of two non-equivalent toroidal polyhexes [10, 11] $H(3,6,0)$ and $H(3,6,1)$ are both equal to 2232.

M.V. Diudea [2] obtained Hosoya polynomials for two classes of toroidal polyhexes: $HC6\ c,n$ and $VC6\ c,n$ with $n \geqslant c$ (in notations of [2]). In fact, $HC6\ c,n$ and $VC6\ c,n$ are precisely $H(\frac{c}{2}, n, -\frac{n}{2} (\text{mod } \frac{c}{2}))$ and $H(\frac{n}{2}, c, -\frac{c}{2} (\text{mod } \frac{n}{2}))$ respectively.

For $H(\frac{c}{2}, n, -\frac{n}{2} (\text{mod } \frac{c}{2}))$, let $p = \frac{c}{2}, q = n, t \equiv -\frac{n}{2} (\text{mod } \frac{c}{2}) \equiv -\frac{q}{2} (\text{mod } p)$. The condition $n \geqslant c$ is equivalent to $p \leqslant \frac{q}{2}$, and thus satisfies the condition $p \leqslant 2q$ of Theorem 3.6. So

$$W(HC6\ c, n) = \frac{1}{3} p^2 q (3q^2 + 2p^2 - 2) = \frac{1}{24} n c^2 (6n^2 + c^2 - 4), \quad n \geqslant c. \tag{19}$$

For $H(\frac{n}{2}, c, -\frac{c}{2} (\text{mod } \frac{n}{2}))$, let $p = \frac{n}{2}, q = c, t \equiv -\frac{c}{2} (\text{mod } \frac{n}{2}) \equiv -\frac{q}{2} (\text{mod } p)$. The condition $n \geqslant c$ is equivalent to $p \geqslant \frac{q}{2}$. Hence $t = p - \frac{q}{2}$ and the condition $p \leqslant q + t$ of Theorem 3.6 is satisfied. So

$$W(VC6\ c, n) = \frac{1}{3} pq\Theta_3 = \frac{1}{24} n c^2 (3n^2 + c^2 + 3nc - 4), \quad n \geqslant c. \tag{20}$$

We can see that Eqs. (19) and (20) are consistent with Eqs. (11) and (12) of [2] respectively. We also know that $HC6\ c, n$ and $VC6\ c, n$ with $n \geqslant c$ are precisely $H(p, q, t)$ with $t \equiv -\frac{q}{2} (\text{mod } p)$.

Usually, toroidal polyhexes have other notations, such as Kirby's notation $TPH(a, b, d)$ and Diudea's notation VH$t[c, n]$, which correspond to $H(a, d, b - d)$ and $H(\frac{c}{2}, n, \frac{t-n}{2})$ respectively.

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