

k -resonant toroidal polyhexes

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Abstract A toroidal polyhex $H(p, q, t)$ is a cubic bipartite graph embedded on the torus such that each face is a hexagon, which can be described by a string (p, q, t) of three integers ($p \geq 1, q \geq 1, 0 \leq t \leq p - 1$). A set \mathcal{H} of mutually disjoint hexagons of $H(p, q, t)$ is called a resonant pattern if $H(p, q, t)$ has a perfect matching M such that all hexagons in \mathcal{H} are M -alternating. A toroidal polyhex $H(p, q, t)$ is k -resonant if any i ($1 \leq i \leq k$) mutually disjoint hexagons form a resonant pattern. In [16], Shiu, Lam and Zhang characterized 1, 2 and 3-resonant toroidal polyhexes $H(p, q, t)$ for $\min(p, q) \geq 2$. In this paper, we characterize k -resonant toroidal polyhexes $H(p, 1, t)$. Furthermore, we show that a toroidal polyhex $H(p, q, t)$ is k -resonant ($k \geq 3$) if and only if it is 3-resonant.

Keywords Toroidal polyhex · Perfect matching · Resonant pattern · k -resonant

AMS 2000 Subject Classification 05C10 · 05C70 · 05C90

1 Introduction

A *toroidal polyhex* is a cubic bipartite graph embedded on torus such that each face is a hexagon, described by a string (p, q, t) of three integers ($p \geq 1, q \geq 1, 0 \leq t \leq p - 1$) and denoted by $H(p, q, t)$ [11, 16]. Toroidal polyhex had been considered in mathematics as hexagonal tessellation (or dually triangulation) on torus [1, 12, 18]. In chem-

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istry, toroidal polyhex has been thought as a new possible carbon cage different from spherical fullerene [4], also named toroidal fullerene or elementary benzenoid [9]. We refer readers to surveys of toroidal polyhex [7,8].

Let G be a graph admitting a 2-cell embedding on torus. A face is even if it is bound by a cycle with even size. In this paper, a face also means the cycle bounding it. A set M of independent edges of G is called a *perfect matching* (a *Kekulé structure* in chemistry) if every vertex of G is incident with exactly one edge of M . A cycle C of G is M -*alternating* (or conjugated circuit) if the edges of C appear alternately in and off M . A set \mathcal{H} of mutually disjoint even faces of G is called a *resonant pattern* if G has a perfect matching M such that all faces in \mathcal{H} are simultaneously M -alternating. For a positive integer k , a graph is k -*resonant* if any i ($i \leq k$) mutually disjoint even faces form a resonant pattern. A resonant pattern \mathcal{H} is also called a *sextet pattern* if every even face in \mathcal{H} is a hexagon. In this paper, all hexagons in a sextet pattern will be designated by depicting circles within them; see Fig. 4.

In the Clar's aromatic sextet theory [3], Clar found that various electronic properties of polycyclic aromatic hydrocarbons can be predicted by sextet patterns from a purely empirical standpoint, by which an aromatic hydrocarbon molecule with larger number of mutually resonant hexagons is more stable. From Randić's conjugated circuits model [13–15], the conjugated circuits with different sizes have different resonance energies and the conjugated hexagons contribute the largest resonant energy among all $(4n + 2)$ -length circuits which contribute positively to resonant energy of molecular. Zhang and Chen [19] characterized completely 1-resonant benzenoid systems: a 1-resonant benzenoid system coincides with a normal benzenoid system. The similar result was extended to coronoid systems [2,21] and plane bipartite graphs [23]. Later, Zheng [24,25] characterized general k -resonant benzenoid systems and showed that any 3-resonant benzenoid system are also k -resonant ($k \geq 3$). For coronoid benzenoid systems [10] and open-end nanotubes [20], the result is still valid. Recently, the concept of k -resonance was extended to toroidal polyhexes and Klein-bottle polyhexes [16,17]. We refer readers to recent surveys [5,6].

Each toroidal polyhex $H(p, q, t)$ is elementary [16]. Different from plane elementary bipartite graph which is also 1-resonant, $H(2, 2, 0)$ is the unique non-1-resonant toroidal polyhex [16]. In [16], Shiu, Lam and Zhang have characterized 1, 2 and 3-resonant toroidal polyhexes $H(p, q, t)$ for $\min(p, q) \geq 2$. In this paper, we characterize k -resonant toroidal polyhexes $H(p, 1, t)$ which are not discussed in [16] (except the degenerated cases $H(1, q, 0)$, $H(p, 1, 0)$ and $H(p, 1, p-1)$ since each hexagonal face is not bounded by a cycle). Moreover, we prove that a toroidal polyhex $H(p, q, t)$ ($p \geq 1, q \geq 1$ and $0 \leq t \leq p-1$) is k -resonant ($k \geq 3$) if and only if it is 3-resonant, and thus settle an open problem of Guo [5]. For convenience, a toroidal polyhex $H(p, q, t)$ in question always means a non-degenerated case throughout this paper.

2 Preliminaries

A *toroidal polyhex* is generated from a $p \times q$ -parallelogram P of the hexagonal lattice with the usual torus boundary identification with torsion t . A $p \times q$ -parallelogram

Fig. 1 Toroidal polyhex $H(7, 3, 3)$ arising from a 7×3 -parallelogram of the hexagonal lattice

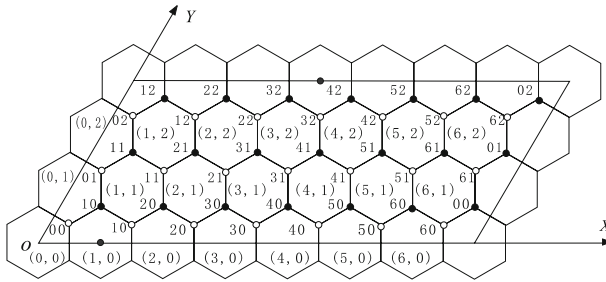
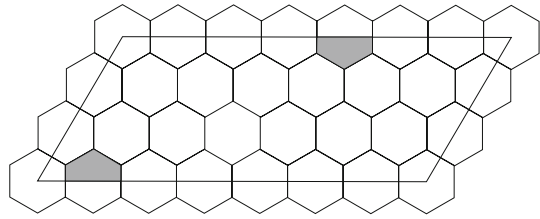


Fig. 2 The affine coordinate system XOY for $H(7, 3, 2)$

P considered here has two horizontal sides and two lateral sides: Each side connects two hexagon centers; Two horizontal sides pass perpendicularly through p edges and two lateral sides pass perpendicularly through q edges (see Fig. 1). In order to form a toroidal polyhex $H(p, q, t)$, first identify two lateral sides of P to form a tube, and then identify the top side of the tube with its bottom side after rotating it through t hexagons.

Let $H(p, q, t)$ be a toroidal polyhex and $V(H), E(H)$ be vertex set and edge set respectively. Clearly, $V(H)$ admits a proper 2-coloring: the vertices which are incident with one downward vertical edge and two upwardly oblique edges are colored black and other vertices white (see Fig. 2). Establish an affine coordinate system XOY for $H(p, q, t)$ as introduced in [16]: Take one horizontal side and one lateral side of the $p \times q$ -parallelogram P as x -axis and y -axis such that two axes form an angle of 60° and P lies in non-negative region; The origin O is the intersection of two axes; Define one unit length to be the distance between a pair of parallel edges in a hexagon. For any positive integer n , let $\mathbb{Z}_n := \{0, 1, \dots, n - 1\}$ with module additions. Now, we give a labeling to vertices and hexagons of $H(p, q, t)$. Label each hexagon by its center coordinate (x, y) ($x \in \mathbb{Z}_p, y \in \mathbb{Z}_q$) and denote it by $h_{x,y}$ or (x, y) . For the upper edge of (x, y) perpendicular to y -axis, label its black end by $b_{x,y}$ and its white end by $w_{x,y}$ (see Fig. 2). So $w_{0,y}b_{0,y} \in E(H)$ and $w_{x,0}b_{x+t+1,q-1} \in E(H)$. We also call the 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 th layer, denoted by L_y .

Let G_1 and G_2 be two simple graphs. An *isomorphism* between them is a bijection $\phi : V(G_1) \rightarrow V(G_2)$ such that, for any $u, v \in V(G_1), uv \in E(G_1)$ if and only if $\phi(u)\phi(v) \in E(G_2)$. An *automorphism* of a simple graph G is an isomorphism G to itself. For a toroidal polyhex $H(p, q, t)$, there are three hexagon-preserving automorphisms: the r -l shift ϕ_{rl} moving every vertex horizontally backwards a unit, the t -b shift ϕ_{tb} moving every vertex downwards a unit along the y -axis, and the 180°

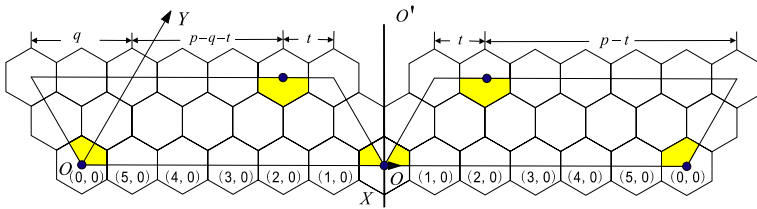
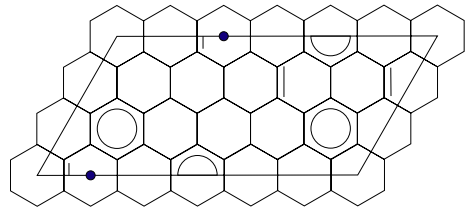


Fig. 3 Illustration of the reflective symmetry against OO'

Fig. 4 An ideal configuration of $H(6, 3, 1)$: the hexagons depicted with circles and the vertical double edges



rotation R_2 surrounding the center of the parallelogram P . The generated subgroup $\langle \phi_{rl}, \phi_{tb}, R_2 \rangle$ is transitive on both vertex set and hexagon set of $H(p, q, t)$ ([16]).

Lemma 2.1 [16] $H(p, q, t)$ is hexagon-transitive. □

Two toroidal polyhexes are *equivalent* if there exists a hexagon-preserving isomorphism between them. Let OO' be a vertical line through the origin O of affine coordinate of $H(p, q, t)$ and let ψ be the reflective symmetry of $H(p, q, t)$ against OO' (see Fig. 3). Then ψ is a hexagon-preserving isomorphism and $\psi(H(p, q, t)) = H(p, q, t')$ where $t' \equiv p - q - t \pmod p$.

Lemma 2.2 $H(p, q, t)$ is equivalent to $H(p, q, t')$ where $t' \equiv p - q - t \pmod p$. □

Let S be a subgraph of a toroidal polyhex $H(p, q, t)$ such that every component is either hexagon or K_2 (a complete graph with two vertices). S is an *ideal configuration* [16] if it is alternately incident with white and black vertices along any direction of every y th layer (see Fig. 4); S is a *Clar cover* [22] if it is a spanning subgraph of $H(p, q, t)$.

Lemma 2.3 [16] An ideal configuration S of a toroidal polyhex $H(p, q, t)$ can be extended to a Clar cover, and the hexagons in S are thus mutually resonant. □

Let u, v be two vertices of y th layer with x -coordinates i and j , respectively. We use $P(u, v) \subset L_y$ to denote the path from u to v such that the x -coordinate set of all vertices of $P(u, v)$ is $\{i, i + 1, \dots, j - 1, j\}$. For example, $P(b_{i,y}, w_{j,y}) = b_{i,y}w_{i,y}b_{i+1,y} \cdots w_{j-1,y}b_{j,y}w_{j,y}$. A path is *odd* if it has odd number of edges, and it is *even*, otherwise.

Lemma 2.4 Let S be a subgraph of $H(p, q, t)$ such that every component is either hexagon or K_2 . For any $y \in \mathbb{Z}_q$, if $L_y - S = \emptyset$ or each component of $L_y - S$ is an odd path, then S is an ideal configuration.

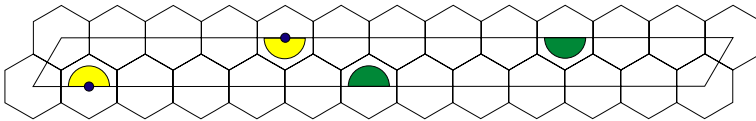


Fig. 5 $H(12, 1, 3)$ and $x = 6 \geq t + 3$

Proof If $L_y - \mathcal{S} = \emptyset$, \mathcal{S} is alterningly incident with white and black vertices along any direction of y th layer. If $L_y - \mathcal{S} \neq \emptyset$, let $P(u, v)$ be an odd path which is a component of $L_y - \mathcal{S}$. Since $H(p, q, t)$ is bipartite graph, the white vertices and the black vertices appear alterningly in $P(u, v)$. So u and v have different colors. Immediately we have \mathcal{S} is alterningly incident with white and black vertices along any direction of y th layer. So \mathcal{S} is an ideal configuration of $H(p, q, t)$. \square

3 k -resonant $H(p, 1, t)$

In this section, the y -coordinate of all labels of vertices and hexagons of $H(p, 1, t)$ are omitted since they have the same value 0. For example $L_0 = w_0b_1w_1b_2w_2 \dots w_{p-1}b_0w_0$.

Since any hexagon of toroidal polyhexes $H(p, 1, t)$ itself exactly forms an ideal configuration, $H(p, 1, t)$ is 1-resonant by Lemma 2.3.

Theorem 3.1 $H(p, 1, t)$ is 1-resonant. \square

Theorem 3.2 $H(p, 1, t)$ is 2-resonant if and only if either $p < 8$, or $p \geq 8$ is odd, or $p \geq 8$ is even and $t \neq \frac{p}{2} - 1$ or $\frac{p}{2}$.

Proof It is enough to prove that $H(p, 1, t)$ is non-2-resonant if and only if $p \geq 8$ is even and $t = \frac{p}{2} - 1$ or $\frac{p}{2}$.

We first suppose that $p \geq 8$ is even and $t = \frac{p}{2} - 1$ or $\frac{p}{2}$ and show that $H(p, 1, t)$ is non-2-resonant. Choose a pair of hexagons $(1, 0)$ and $(3, 0)$, which can be expressed as $w_0b_1w_1b_{t+2}w_{t+1}b_{t+1}$ and $w_2b_3w_3b_{4+t}w_{3+t}b_{3+t}$ respectively, and are thus disjoint since $3 < t + 1$ and $4 + t \leq p$. Further the vertex w_{2+t} outside the hexagons has three neighbors b_{3+t}, b_{t+2} and b_1 (or b_3), since $(2 + t) + t + 1 \equiv 1$ or $3 \pmod{p}$ according as $t = \frac{p}{2} - 1$ or $\frac{p}{2}$. That is, $H(p, 1, t) - h_1 - h_3$ has an isolated vertex w_{2+t} . This shows that such two hexagons are not mutually resonant.

For the other cases it is sufficient to choose a pair of disjoint hexagons and show their mutual resonance. We consider $H(p, 1, t)$ with $1 \leq t \leq p - 2$, and only choose a pair of disjoint hexagons $(1, 0)$ and $(x, 0)$ with $3 \leq x \leq \frac{p}{2} + 1$. Then $p \geq 6$ since $2p \geq 12$. If $p = 6$, it is easy to see that $x = 4$ and $t = 1$ or 4 . Hence, from now on we suppose that $1 \leq t < \frac{p}{2} - 1$ or $\frac{p}{2} < t \leq p - 2$. Since the hexagon $(1, 0)$ and hexagon $(x, 0)$ (i.e. $w_{x-1}b_xw_xb_{x+t+1}w_{x+t}b_{x+t}$) are disjoint, $t + 1 \notin \{x, x - 1\}$ and $x + t \notin \{0, 1\}$. Hence there are the following five cases to be considered.

Case 1 $1 \leq t \leq x - 3$. It follows that on the the unique layer both 3-paths of lower half parts of hexagons $(1, 0)$ and $(x, 0)$ are separated by both 3-paths of their upper

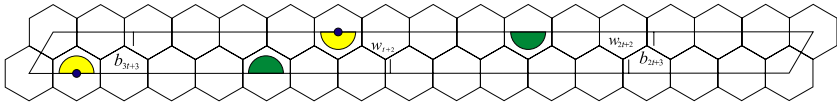


Fig. 6 $H(16, 1, 5)$ and $x = 5 \leq t < \frac{p}{2} - 1$

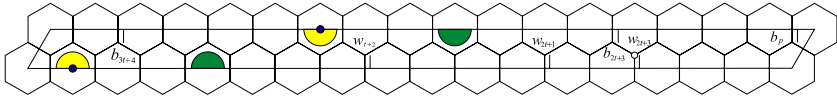


Fig. 7 $H(17, 1, 5)$ and $x = 4 \leq t < \frac{p}{2} - 1, (r + 1)t + 3 = p + 1$

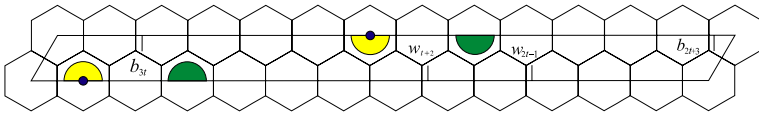


Fig. 8 $H(13, 1, 5)$ and $x = 3 \leq t < \frac{p}{2} - 1, p + x \leq (r + 1)t + 3 \leq p + t$

parts since $2 \leq t + 1 \leq x - 2$ and $x < x + t \leq 2x - 3 \leq p - 1$ (see Fig. 5). Hence such two hexagons form an ideal configuration.

Case 2 $x \leq t < \frac{p}{2} - 1$. The above result no longer holds since $x + 1 \leq t + 1 < t + 2 < x + t < p$. So we must choose a series of vertical edges so that the chosen hexagons together with such vertical edges form an ideal configuration. We first choose the following edges: $w_{it+2}b_{(i+1)t+3}$ ($i = 1, \dots, r$) such that $rt + 3 \leq p$ and $(r + 1)t + 3 \geq p + 1$ (see Fig. 6). Then $(r + 1)t + 3 \leq p + t$. Since $x + t + 3 \leq 2t + 3 \leq p, r \geq 2$. If $p + 2 \leq (r + 1)t + 3 \leq p + x - 1$ (see Fig. 6), the required is verified.

If $(r + 1)t + 3 = p + 1$, the edge $w_{rt+2}b_{(r+1)t+3}$ is replaced by $w_{rt+1}b_p$, and further choose the edge $w_{rt+j}b_{(r+1)t+j+1}$ with $3 \leq j \leq x$ (see Fig. 7). Then $rt + 3 \leq rt + j \leq (r + 1)t$ and $p + 2 \leq (r + 1)t + j + 1 \leq p + x - 1$. The requirement is also verified.

The last case $p + x \leq (r + 1)t + 3 \leq p + t$ is now considered. Let $j_0 := (r + 1)t + 3 - (p + x)$. Then $0 \leq j_0 \leq t - x$. The edge $w_{rt+2}b_{(r+1)t+3}$ is replaced by $w_{rt+1-j_0}b_{(r+1)t+2-j_0}$ (see Fig. 8). Since $rt + 1 \geq rt + 1 - j_0 \geq (r - 1)t + x + 1$ and $(r + 1)t + 2 - j_0 = p + x - 1 \equiv x - 1 \pmod{p}$, the required is verified.

Case 3 $p - x + 2 \leq t \leq p - 2$. The result in Case 1 still holds since $x + 1 \leq t + 1 \leq p - 1$ and $p + 2 \leq x + t \leq p + x - 2$.

Case 4 $\frac{p}{2} < t \leq p - x - 1$. Since $x < t + 1 < t + 2 < x + t \leq p - 1$, then the chosen hexagons $(1, 0)$ and $(x, 0)$ is not an ideal configuration. So it is necessary to choose additional edges. We choose the following certain edges:

$$w_{t+2+i_0}b_{2t+3+i_0}, w_{x+1+j_0}b_{x+t+2+j_0}, \tag{1}$$

with

$$0 \leq i_0 \leq x - 3 \text{ and } 1 \leq j_0 \leq t - x - 1. \tag{2}$$

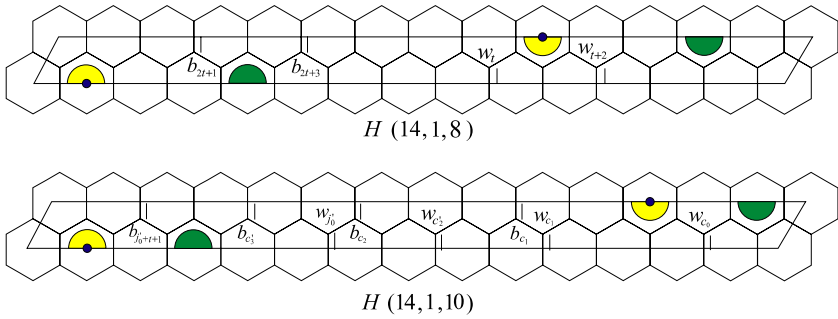


Fig. 9 Illustration for Case 4 in the proof of Theorem 3.2

Hence w_{t+2+i_0} lies between w_{t+2} and w_{t+x-1} , and w_{x+1+j_0} lies between w_{x+2} and w_t .

We suppose firstly that $p+x \geq 2t+2$. Let $i_0 := p+x-2t-2$ and $j_0 := t-x-1$. Clearly, the inequalities (2) holds. On the other hand, $2t+3+i_0 = p+x+1 \leq p+t$ and $x+t+2+j_0 = 2t+1 < p+x$ (see $H(14, 1, 8)$ in Fig. 9). Hence the chosen hexagons together with both edges in (1) form an ideal configuration.

From now on, suppose that $p+x \leq 2t+1$ (see $H(14, 1, 10)$ in Fig. 9). For convenience we construct the following arithmetic sequence of integers:

$$c_k := (t+2) + k(t+1-p), k = 0, 1, \dots$$

with the inequality $t+1-p \leq -x \leq -3$. Let $i_0 := 0$, $j_0 := p-t-3$ and $j'_0 := x+1+j_0 = p+x-t-2$. Since $1 \leq p-t-x \leq j_0 < t-x-1$, $x+2 \leq j'_0 < t$ and the inequalities (2) also holds. Then both edges in (1) can be expressed as $w_{c_0}b_{c_1}$ and $w_{j'_0}b_{j'_0+t+1}$. Further $j'_0+t+1 = p+x-1$, and $x+2 \leq c_1 < t$. Hence b_{c_1} lies between b_{x+2} and b_{t-1} . Put

$$k_0 := \min\{k : c_k \leq j'_0\}.$$

Since $c_0 > j'_0$, $k_0 \geq 1$. If $k_0 = 1$, the vertex b_{c_1} lies on the left side of $w_{j'_0}$ and the required is verified. Otherwise, $k_0 \geq 2$, i.e. $2p+x-3t \leq 4$, which together with $t \leq p-x-1$ and $x \geq 3$ imply that

$$x+2 \leq j'_0 \leq t-x+1 \leq t-2.$$

If $c_{k_0-1} \geq j'_0+2$, since $c_{k_0} = c_{k_0-1} + (t+1-p) \geq j'_0+2 + (t+1-p) = x+1$ we have

$$x+1 \leq c_{k_0} \leq j'_0 < c_{k_0-1} < \dots < c_1 < t.$$

We now choose further edges $w_{c_1}b_{c_2}, w_{c_2}b_{c_3}, \dots, w_{c_{k_0-1}}b_{c_{k_0}}$. Hence the chosen part has such incident vertices $w_x, b_{c_{k_0}}, w_{j'_0}, b_{c_{k_0-1}}, w_{c_{k_0-1}}, \dots, b_{c_1}, w_{c_1}, b_{t+1}$ from w_x to b_{t+1} , and is thus an ideal configuration.

If $c_{k_0-1} = j'_0 + 1, c_{k_0} = x$. Let $c'_{k_0-1} := c_{k_0-1} + 1 = j'_0 + 2$ and $c'_{k_0} := c_{k_0} + 1$ (see $H(14, 1, 10)$ in Fig. 9). Then

$$x + 1 = c'_{k_0} < j'_0 < c_{k_0-1} < c'_{k_0-1} < c_{k_0-2} < \dots < c_1 < t.$$

We now choose further edges $w_{c_1}b_{c_2}, w_{c_2}b_{c_3}, \dots, w_{c_{k_0-2}}b_{c_{k_0-1}}, w_{c'_{k_0-1}}b_{c'_{k_0}}$. Hence the chosen part has such incident vertices $w_x, b_{c'_{k_0}}, w_{j'_0}, b_{c_{k_0-1}}, w_{c'_{k_0-1}}, b_{c_{k_0-2}}, w_{c_{k_0-2}}, \dots, b_{c_1}, w_{c_1}, b_{t+1}$ from w_x to b_{t+1} , and is thus an ideal configuration.

Case 5 p is odd and $t = \frac{p-1}{2}$. The chosen hexagons $(1, 0)$ and $(x, 0)$ together with the additional edge $w_{t+3}b_{2t+3}$ form an ideal configuration since $1 < 2t + 3 - p = 2 < x < 1 + t < t + 2 < t + x < p$.

Hence the chosen pair of disjoint hexagons are mutually resonant in any cases by Lemma 2.3. So the entire proof is completed. \square

In the following, we consider k -resonant ($k \geq 3$) toroidal polyhexes $H(p, 1, t)$.

Lemma 3.3 *If $H(p, 1, t)$ is 3-resonant, then $t \in \{1, 2, p - 2, p - 3, \frac{p-3}{2}, \frac{p-1}{2}, \frac{p+1}{2}\}$ or $\frac{2p-3}{2} \leq t \leq \frac{2p}{3}$ or $\frac{p-3}{3} \leq t \leq \frac{p}{3}$.*

Proof Let $H(p, 1, t)$ be a 3-resonant toroidal polyhex where $t \notin \{1, 2, p - 2, p - 3\}$. Then hexagons $(1, 0)$ and $(3, 0)$ are disjoint. For the vertex $w_{t+2}, b_{t+2}, b_{t+3}$ and b_{2t+3} are its three neighbors. Clearly, $b_{t+2} \in h_1, b_{t+3} \in h_3$ and $b_{2t+3} \in h_{2t+3}$. Let $\mathcal{H} := \{h_1, h_3, h_{2t+3}\}$. Since $H(p, 1, t)$ is 3-resonant and w_{t+2} is an isolated vertex of $H(p, 1, t) - \mathcal{H}$, the hexagons in \mathcal{H} must not be mutually disjoint. Thus either $h_1 \cap h_{2t+3} \neq \emptyset$ or $h_3 \cap h_{2t+3} \neq \emptyset$.

For $p \leq 2t + 3$, since $h_1 \cap h_{2t+3} \neq \emptyset$ or $h_3 \cap h_{2t+3} \neq \emptyset$, we have $p \leq 2t + 3 \leq p + 4$ or $2p \leq 3t + 3 \leq 2p + 3$. Further, $\frac{p-3}{2} \leq t \leq \frac{p+1}{2}$ or $\frac{2p-3}{2} \leq t \leq \frac{2p}{3}$. By Lemma 3.2, $t \neq \frac{p}{2} - 1, \frac{p}{2}$. So $t \in \{\frac{p-3}{2}, \frac{p-1}{2}, \frac{p+1}{2}\}$ or $\frac{2p-3}{2} \leq t \leq \frac{2p}{3}$.

For $p > 2t + 3$, since $h_1 \cap h_{2t+3} \neq \emptyset$ or $h_3 \cap h_{2t+3} \neq \emptyset$, we have $p \leq 3t + 3 \leq p + 3$. So $\frac{p-3}{3} \leq t \leq \frac{p}{3}$. \square

Lemma 3.4 *$H(p, 1, t)$ is k -resonant ($k \geq 3$) for $t \in \{1, 2, p - 2, p - 3\}$.*

Proof Let $\mathcal{H} := \{S_0, S_1, \dots, S_{k-1}\}$ be a set of any k mutually disjoint hexagons such that $S_i = (x_i, 0)$. We may assume $1 = x_0 < x_1 < \dots < x_{k-1} < p$ by Lemma 2.1.

If $t = 1$ or 2 , any hexagon $(x, 0)$ with $x_i - (t + 1) \leq x \leq x_i + t + 1$ satisfies $h_x \cap h_{x_i} \neq \emptyset$. So $h_x \notin \mathcal{H}$. Clearly, h_{x_i} is incident with L_0 at $w_{x_i-1}, b_{x_i}, w_{x_i}, b_{x_i+t}, w_{x_i+t}$ and b_{x_i+t+1} , and $x_i - 1 < x_i < x_i + t < x_i + t + 1 \leq x_{i+1} - 1$ for $i \in \mathbb{Z}_k$. Therefore \mathcal{H} forms an ideal configuration of $H(p, 1, t)$. By Lemma 2.3, \mathcal{H} is a resonant pattern. So $H(p, 1, t)$ with $t = 1$ or 2 is k -resonant.

By Lemma 2.2, we immediately have $H(p, 1, t)$ is k -resonant for $t \in \{1, 2, p - 2, p - 3\}$. \square

Lemma 3.5 *$H(p, 1, t)$ is k -resonant ($k \geq 3$) for $t \in \{\frac{p-3}{2}, \frac{p-1}{2}, \frac{p+1}{2}\}$.*

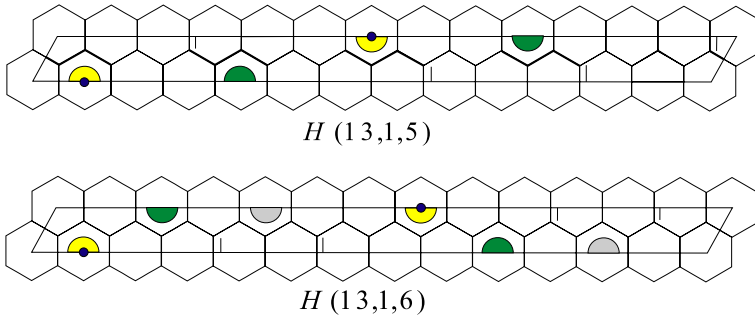


Fig. 10 Illustration for the proof of Lemma 3.5

Proof By Lemma 2.2, $H(p, 1, \frac{p-3}{2})$ is equivalent to $H(p, 1, \frac{p+1}{2})$ since $p-1-\frac{p-3}{2} = \frac{p+1}{2}$. It is enough to prove $H(p, 1, t)$ is k -resonant for $t = \frac{p-3}{2}$ and $\frac{p+1}{2}$. By Lemma 3.4, assume $t \notin \{1, 2, p-2, p-3\}$. Let $\mathcal{H} := \{S_0, S_1, \dots, S_{k-1}\}$ be a set of any k mutually disjoint hexagons such that $S_i = (x_i, 0)$.

Case 1 $t = \frac{p-3}{2}$. For $x = x_i + t + 1$ or $x_i + t + 2$, $h_x \notin \mathcal{H}$ since $h_x \cap S_i \neq \emptyset$. Choose the vertical edge $w_{x_i+t+1}b_{x_i+2t+2} = w_{x_i+t+1}b_{x_i-1}$. Let G_i be the subgraph consisting of S_i and $w_{x_i+t+1}b_{x_i-1}$. Then G_i induces two paths on L_0 , i.e., $P(b_{x_i-1}, w_{x_i})$ and $P(b_{x_i+t}, w_{x_i+t+1})$ (see the paths illustrated by thick lines in $H(13, 1, 5)$ in Fig. 10). Let $\mathcal{S} := \mathcal{H} \cup \{w_{x_i+t+1}b_{x_i-1} | i \in \mathbb{Z}_k\}$. Then \mathcal{S} is alternating incident with black vertices and white vertices along any direction of L_0 . Hence \mathcal{S} is an ideal configuration of $H(p, q, t)$.

Case 2 $t = \frac{p-1}{2}$. If $L_0 - \mathcal{H} = \emptyset$ or every component of $L_0 - \mathcal{H}$ is an odd path, then \mathcal{H} is a resonant pattern by Lemma 2.4. So we suppose $L_0 - \mathcal{H}$ contains an even path.

Claim $P(b_{x_i+1}, b_{x_{i+1}-1})$ is a component of $L_0 - \mathcal{H}$ if and only if $P(w_{x_i+t+1}, w_{x_{i+1}+t-1})$ is.

Proof of Claim Suppose that $P(b_{x_i+1}, b_{x_{i+1}-1})$ is a component of $L_0 - \mathcal{H}$. That is $S_j \cap P(b_{x_i+1}, b_{x_{i+1}-1}) = \emptyset$ for any $j \in \mathbb{Z}_k$. If $P(w_{x_i+t+1}, w_{x_{i+1}+t-1})$ is not a component of $L_0 - \mathcal{H}$, then $S_j \cap P(w_{x_i+t+1}, w_{x_{i+1}+t-1}) \neq \emptyset$ for some $j \in \mathbb{Z}_k$. Hence $S_j = (x_j, 0)$ satisfies $x_i + t + 1 \leq x_j \leq x_{i+1} + t - 2$ or $x_i + t + 1 \leq x_j + t \leq x_{i+1} + t - 1$. Further $x_i \leq x_j + t \leq x_{i+1} - 3$ or $x_i + 1 \leq x_j \leq x_{i+1} - 1$. So $S_j \cap P(b_{x_i+1}, b_{x_{i+1}-1}) \neq \emptyset$, which contradicts that $P(b_{x_i+1}, b_{x_{i+1}-1})$ is a component of $L - \mathcal{H}$.

A similar discussion proves the sufficiency of Claim. □

For each pair of $P(b_{x_i+1}, b_{x_{i+1}-1})$ and $P(w_{x_i+t+1}, w_{x_{i+1}+t-1})$, choose the vertical edge $w_{x_i+t+1}b_{x_i+1}$ (see $H(13, 1, 6)$ in Fig. 10). Delete b_{x_i+1} and w_{x_i+t+1} from $P(b_{x_i+1}, b_{x_{i+1}-1})$ and $P(w_{x_i+t+1}, w_{x_{i+1}+t-1})$, respectively. Then obtain two odd paths $P(w_{x_i+1}, b_{x_{i+1}-1})$ and $P(b_{x_i+t+2}, w_{x_{i+1}+t-1})$. Let \mathcal{S} be the set of all hexagons in \mathcal{H} together with all chosen edges. Then either $L_0 - \mathcal{S} = \emptyset$ or every component of $L_0 - \mathcal{S}$ is an odd path. Therefore, \mathcal{S} is a required ideal configuration by Lemma 2.4.

By Lemma 2.3, \mathcal{H} is a resonant pattern. So $H(p, 1, t)$ is k -resonant for $t \in \left\{ \frac{p-3}{2}, \frac{p-1}{2}, \frac{p+1}{2} \right\}$. □

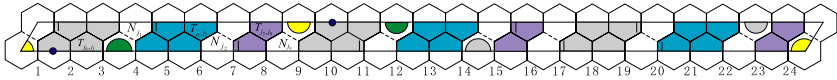


Fig. 11 $H(24, 1, 8)$ and S_2 with $x_2 \leq t$

In the following, we turn to $H(p, 1, t)$ with $\frac{2p-3}{2} \leq t \leq \frac{2p}{3}$ or $\frac{p-3}{3} \leq t \leq \frac{p}{3}$. By Lemma 2.2, $H(p, 1, \frac{p-i}{3})$ is equivalent to $H(p, 1, \frac{2p-(3-i)}{3})$ since $p - 1 - \frac{p-i}{3} = \frac{2p-(3-i)}{3}$. So it suffices to consider $H(p, 1, t)$ with $\frac{p-3}{3} \leq t \leq \frac{p}{3}$. Let N_x be the subgraph consisting of three hexagons $(x, 0)$, $(x + \delta, 0)$ and $(x + 2\delta, 0)$ where δ satisfies

$$\delta := \begin{cases} t & \text{if } t = \frac{p}{3} \text{ or } \frac{p-1}{3}; \\ t + 1 & \text{if } t = \frac{p-3}{3} \text{ or } \frac{p-2}{3}. \end{cases}$$

Any two hexagons in N_x are adjacent. Let $\sigma(N_x) := \min\{x, x + \delta, x + 2\delta\} \pmod{p}$, then $\sigma(N_x) \leq t$. Let $E_{\sigma(N_x)} := \{h_x \cap h_{x+\delta}, h_{x+\delta} \cap h_{x+2\delta}, h_{x+2\delta} \cap h_x\}$ (for example, see Fig. 11, $E_0 = \{b_0w_0, b_8w_8, b_{16}w_{16}\}$ illustrated by dash lines in $H(24, 1, 8)$). Clearly, $E_i \cup E_j$ ($i \neq j$) is an edge cut of $H(p, 1, t)$ which separates $H(p, 1, t)$ into two components. Let $T_{i,j}$ and $T_{j,i}$ be the components containing $P(w_i, w_{j-1})$ and $P(w_j, w_{i-1})$, respectively (see T_{j_0, j_1} in Fig. 11).

Lemma 3.6 $H(p, 1, t)$ is k -resonant ($k \geq 3$) for $\frac{p-3}{3} \leq t \leq \frac{p}{3}$ or $\frac{2p-3}{3} \leq t \leq \frac{2p}{3}$.

Proof It suffices to prove $H(p, 1, t)$ is k -resonant for $\frac{p-3}{3} \leq t \leq \frac{p}{3}$.

Let $\mathcal{H} = \{S_0, S_1, \dots, S_{k-1}\}$ be a set of any k mutually disjoint hexagons of $H(p, q, t)$, and let $S_i = (x_i, 0) \in N_{x_i}$ and $j_i = \sigma(N_{x_i}) \leq t$. By Lemma 2.1, we may assume $S_0 = (0, 0)$ and $0 = j_0 < j_1 \dots < j_{k-1} \leq t$. According to Lemma 2.3, it is sufficient to construct an ideal configuration \mathcal{S} such that $\mathcal{H} \subseteq \mathcal{S}$. For $i, i + 1 \in \mathbb{Z}_k$, $T_{j_i, j_{i+1}}$ is one component of $H(p, 1, t)$ separated by the edge cut $E_{j_i} \cup E_{j_{i+1}}$.

Case 1 $t = \frac{p}{3}$ or $t = \frac{p-3}{3}$. We only show the lemma holds for $t = \frac{p}{3}$ here. A similar discussion shows the lemma is true for $t = \frac{p-3}{3}$. For $t = \frac{p}{3}$, we have $\delta = t$, i.e. $N_x = h_x \cup h_{x+t} \cup h_{x+2t}$.

If $x_2 \leq t$, then $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$ consists of paths $P(b_1, b_{x_2-1})$, $P(w_{t+1}, w_{x_2+t-1})$ and $P(w_{2t}, b_{x_2+2t})$. Choose two additional vertical edges $w_{2t}b_1$ and $w_{x_2+t-1}b_{x_2+2t}$. Let $E'_{0,1} := \{w_{2t}b_1, w_{x_2+t-1}b_{x_2+2t}\}$ (see T_{j_0, j_1} in Fig. 11).

If $t < x_2 \leq 2t$ (i.e., $x_2 + t \leq 3t = p$), paths $P(b_1, b_{x_2+2t})$, $P(w_{t+1}, b_{x_2-1})$ and $P(w_{2t}, w_{x_2+t-1})$ are three components of $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$. Choose the additional vertical edge $w_{2t}b_1$ and let $E'_{0,1} := \{w_{2t}b_1\}$ (see T_{j_1, j_2} in Fig. 11).

If $2t < x_2 < p$ (i.e., $p < x_2 + t < p + t$), then paths $P(b_1, w_{x_2+t-1})$, $P(w_{t+1}, b_{x_2-t})$ and $P(w_{2t}, b_{x_2-1})$ are three components of $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$ and all of them are odd paths. Let $E'_{0,1} := \emptyset$.

Every component of $(T_{j_0, j_1} \cap L_0) - \mathcal{H} \cup E'_{0,1}$ is an odd path. For any $S_i, S_{i+1} \in \mathcal{H}$, let ϕ be the automorphism moving every vertex horizontally backwards $x_i - 1$ units. Then $\phi(N_{j_i}) = N_{j_0}$. So we can choose vertical edge set $E'_{i, i+1}$ for S_i and S_{i+1} as we

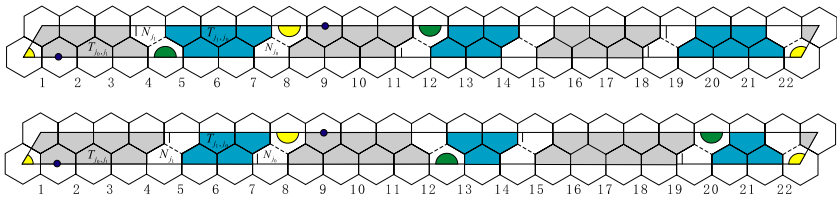


Fig. 12 $H(22, 1, 7)$ and illustration for the proof of Case 2

choose $E'_{0,1}$ for S_0 and S_1 . Let $\mathcal{S} := \mathcal{H} \cup (\cup_{i=0}^{k-1} E'_{i,i+1})$. Then every component of $(T_{j_i, j_{i+1}} \cap L_0) - \mathcal{S}$ for any $i \in \mathbb{Z}_k$ is an odd path. By Lemma 2.4, $\mathcal{H} \cup (\cup_{i=0}^{k-1} E'_{i,i+1})$ is a desired ideal configuration.

Case 2 $t = \frac{p-1}{3}$ or $t = \frac{p-2}{3}$. We only show the lemma is true for $t = \frac{p-1}{3}$. A similar discussion implies the lemma holds for $t = \frac{p-2}{3}$. For $t = \frac{p-1}{3}$, we have $\delta = t$ (i.e., $N_i = h_i \cup h_{i+t} \cup h_{i+2t}$).

If $x_2 \leq t$, then $P(b_1, b_{x_2-1})$, $P(w_{t+1}, w_{x_2+t-1})$ and $P(w_{2t}, b_{x_2+2t})$ are the three components of $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$. Let $E'_{0,1} := \{w_{x_2+t-1}b_{x_2+2t}, w_{x_2+2t-1}b_{x_2-1}\}$ (see T_{j_0, j_1} in Fig. 12 (up)).

If $t < x_2 \leq 2t$ (i.e., $0 < x_2 + 2t \leq t \pmod{p}$), then $P(b_1, b_{x_2+2t})$, $P(w_{t+1}, b_{x_2-1})$ and $P(w_{2t}, w_{x_2+t-1})$ are the three components of $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$. Let $E'_{0,1} := \{w_{x_2+t-1}b_{x_2+2t}\}$ (see T_{j_0, j_1} in Fig. 12 (below)).

If $2t < x_2 < p$ (i.e., $0 < x_2 + t < t \pmod{p}$), then $P(b_1, w_{x_2+t-1})$, $P(w_{t+1}, b_{x_2+2t})$ and $P(w_{2t}, b_{x_2-1})$ are the three components of $(T_{j_0, j_1} \cap L_0) - \mathcal{H}$. Let $E'_{0,1} := \emptyset$.

It is easy to see that every component of $(T_{j_0, j_1} \cap L_0) - \mathcal{H} \cup E'_{0,1}$ is an odd path. For any $S_i, S_{i+1} \in \mathcal{H}$ ($i \in \mathbb{Z}_k$), then $\phi(N_{j_i}) = N_{j_0}$ where ϕ is the automorphism moving every vertex horizontally backward $x_i - 1$ units. We choose vertical edge set $E'_{i,i+1}$ for S_i and S_{i+1} as we choose $E'_{0,1}$ for S_0 and S_1 . Then let $\mathcal{S} := \mathcal{H} \cup (\cup_{i=0}^{k-1} E'_{i,i+1})$. So every component of $(T_{j_i, j_{i+1}} \cap L_0) - \mathcal{S}$ for $i \in \mathbb{Z}_k$ is an odd path. Therefore, \mathcal{S} is a required ideal configuration according to Lemma 2.4. \square

Combining Lemmas 3.3, 3.4, 3.5 and 3.6, we have following theorem.

Theorem 3.7 $H(p, 1, t)$ is k -resonant ($k \geq 3$) if and only if one of the following cases appears:

1. $\frac{p-3}{3} \leq t \leq \frac{p}{3}$,
2. $\frac{2p-3}{2} \leq t \leq \frac{2p}{3}$,
3. $t \in \{1, 2, p-2, p-3, \frac{p-3}{2}, \frac{p-1}{2}, \frac{p+1}{2}\}$.

\square

4 k -resonant $H(p, q, t)$ with $\min(p, q) \geq 2$

In this section, we consider k -resonant ($k \geq 3$) $H(p, q, t)$ with $\min(p, q) \geq 2$.

Theorem 4.1 [16] $H(p, q, t)$ with $\min(p, q) \geq 2$ is 3-resonant if and only if one of the following cases appears:

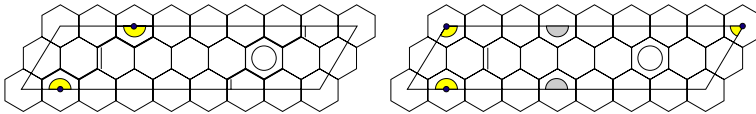


Fig. 14 Toroidal polyhexes $H(8, 2, 1)$ (left) and $H(8, 2, 7)$ (right)

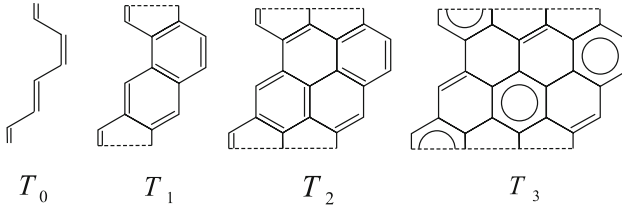
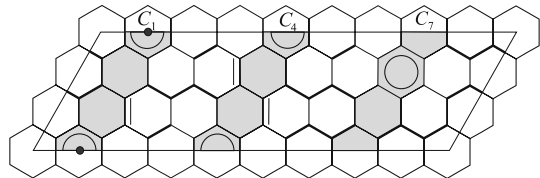


Fig. 15 The dangling double edges in T_0 and dashed lines in T_1, T_2, T_3 are identified

Fig. 16 k -resonant $H(9, 3, 0)$



Case 2 $t = p - 1$. For any two consecutive hexagons $S_i, S_{i+1} \in \mathcal{H}$ with $y_i = y_{i+1}$, choose (see $H(8, 2, 7)$ in Fig. 14)

$$e'_i = \begin{cases} w_{x_i, y_i+1} b_{x_i+1, y_i} & \text{if } y_i = 0; \\ w_{x_i+1, y_i-1} b_{x_i+1, y_i} & \text{if } y_i = 1. \end{cases}$$

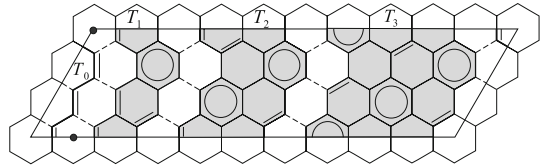
Let $\mathcal{S} := \mathcal{H} \cup \{e'_i | y_i = y_{i+1} \text{ and } i \in \mathbb{Z}_k\}$. Then it is easy to check that \mathcal{S} is a required ideal configuration. □

In the following, we will consider $H(p, 3, t)$ with $p \geq 4$ and $t \in \{0, p - 3, p - 2, p - 1\}$. By Lemma 2.2, we know that $H(p, 3, 0)$ and $H(p, 3, p - 1)$ are equivalent to $H(p, 3, p - 3)$ and $H(p, 3, p - 2)$, respectively. Therefore it is enough to consider $H(p, 3, 0)$ and $H(p, 3, p - 1)$.

For toroidal polyhexes $H(p, 3, 0)$ and $H(p, 3, p - 1)$, hexagons $(x, 0), (x, 1)$ and $(x, 2)$ form a cyclic hexagonal chain, denoted by C_x (see C_1 in Fig. 16 and T_1 in Fig. 17). Clearly, hexagons in C_x are pairwise adjacent. Use $T_{x,y}$ ($x \neq y$) to denote the subgraph consisting of hexagon columns C_{x+1}, \dots, C_{y-1} for $y \neq x + 1$, and $T_{x,x+1} = C_x \cap C_{x+1}$ for $y = x + 1$. For example, $T_{x,x+i}$ ($i = 1, 2, 3$ and 4) of $H(p, 3, p - 1)$ are illustrated in Fig. 15, where $T_0 = T_{x,x+1}, T_1 = T_{x,x+2}, T_2 = T_{x,x+3}$ and $T_3 = T_{x,x+4}$. It can be verified that each set of disjoint hexagons of T_i ($i = 1, 2, 3$) is a resonant pattern of T_i and T_3 contains a unique resonant pattern with three disjoint hexagons as shown in Fig. 15.

Lemma 4.4 For $p \geq 4$ and $t \in \{0, p - 3, p - 2, p - 1\}$, $H(p, 3, t)$ is k -resonant ($k \geq 3$).

Fig. 17 k -resonant $H(10, 3, 9)$



Proof It suffices to prove that $H(p, 3, t)$ is k -resonant for $p \geq 4$ and $t = 0, p - 1$. Let $\mathcal{H} = \{S_0, S_1, \dots, S_{k-1}\}$ be a set of any k disjoint hexagons and let $S_i = (x_i, y_i) \in C_{x_i}$ where $C_{x_i} = h_{x_i,0} \cup h_{x_i,1} \cup h_{x_i,2}$. By Lemma 2.1, let $S_0 = (1, 0)$, i.e. $x_0 = 1$. Since every C_x contains at most one hexagon in \mathcal{H} , we may assume that $1 = x_0 < x_1 < x_2 < \dots < x_{k-1}$. Now we turn to construct an ideal configuration \mathcal{S} containing \mathcal{H} .

Case 1 $t = 0$.

If $y_1 = 0$, then $x_1 \geq 3$. Then $(T_{1,x_1} \cap L_0) - (S_0 \cup S_1) = P(b_{2,0}, b_{x_1-1,0})$, $(T_{1,x_1} \cap L_1) - (S_0 \cup S_1) = P(w_{1,1}, b_{x_1,1})$ and $(T_{1,x_1} \cap L_2) - (S_0 \cup S_1) = P(w_{2,2}, w_{x_1+t-1,2}) = P(w_{2,2}, w_{x_1-1,2})$ (see $T_{1,4}$ of $H(9, 3, 0)$ in Fig. 16). Choose additional vertical edges $w_{1,1}b_{2,0}, w_{x_1-1,2}b_{x_1,1}$ and let $E_{0,1} := \{w_{1,1}b_{2,0}, w_{x_1-1,2}b_{x_1,1}\}$.

If $y_1 = 1$, then $x_1 \geq 2$. Then $(T_{1,x_1} \cap L_0) - (S_0 \cup S_1) = P(b_{2,0}, w_{x_1-1,0})$, $(T_{1,x_1} \cap L_1) - (S_0 \cup S_1) = P(w_{1,1}, b_{x_1-1,1})$ and $(T_{1,x_1} \cap L_2) - (S_0 \cup S_1) = P(w_{2,2}, b_{x_1,2})$. All these three paths are odd. Let $E_{0,1} := \emptyset$.

If $y_1 = 2$, then $x_1 \geq 3$. Then $(T_{1,x_1} \cap L_0) - (S_0 \cup S_1) = P(b_{2,0}, b_{x_1,0})$, $(T_{1,x_1} \cap L_1) - (S_0 \cup S_1) = P(w_{1,1}, w_{x_1-1,1})$ and $(T_{1,x_1} \cap L_2) - (S_0 \cup S_1) = P(w_{2,2}, b_{x_1-1,2})$ (see $T_{4,7}$ of $H(9, 3, 0)$ in Fig. 16). Choose the additional edge $w_{1,1}b_{2,0}$ and let $E_{0,1} := \{w_{1,1}b_{2,0}\}$.

Therefore, $(T_{1,x_1} \cap L_y) - (S_1 \cup S_2 \cup E_{0,1})$ is an odd path for each $y \in \mathbb{Z}_3$. For any $S_i, S_{i+1} \in \mathcal{H}$ ($i, i + 1 \in \mathbb{Z}_k$), let $\phi \in \langle \phi_{rl}, \phi_{tb} \rangle$ be the automorphism moving every vertex horizontally backwards $x_i - 1$ units and downwards y_i units. Then $\phi(S_i) = S_0$ and $\phi(C_{x_i}) = C_{x_0}$. So we can choose a vertical edge set $E_{i,i+1}$ as we choose $E_{0,1}$. Then $(T_{x_i,x_{i+1}} \cap L_y) - (S_i \cup S_{i+1} \cup E_{i,i+1})$ is an odd path for each $y \in \mathbb{Z}_3$. Hence $\mathcal{S} = \mathcal{H} \cup (\bigcup_{i=0}^{k-1} E_{i,i+1})$ is a desired ideal configuration of $H(p, 3, 0)$ by Lemma 2.4.

Case 2 $t = p - 1$.

Notice that the hexagon $(x, 0)$ is adjacent to every hexagons in C_{x-1} and the hexagon $(x, 2)$ is adjacent to every hexagons in C_{x+1} , and T_3 has a unique set consisting of three disjoint hexagons as illustrated in Fig. 15. If \mathcal{H} contains three hexagons in three consecutive cyclic hexagonal chains, say C_{x-1}, C_x and C_{x+1} , then $C_{x-2} \cap \mathcal{H} = \emptyset$ and $C_{x+2} \cap \mathcal{H} = \emptyset$. So the number of consecutive cyclic hexagonal chains such that each of them contains one hexagon in \mathcal{H} is no more than three.

For any given \mathcal{H} , $H(p, 3, p - 1)$ can be decomposed to a series of T_0, T_1, T_2 and T_3 subject to \mathcal{H} (see Fig. 17): C_x, C_{x+1} and C_{x+2} together correspond to a T_3 if $C_{x+i} \cap \mathcal{H} \neq \emptyset$ ($i = 0, 1, 2$); C_x and C_{x+1} together correspond to a T_2 if $C_{x+i} \cap \mathcal{H} \neq \emptyset$ ($i = 0, 1$) and $C_{x+2} \cap \mathcal{H} = \emptyset$ ($i = -1, 2$); C_x corresponds to T_1 if $C_x \cap \mathcal{H} \neq \emptyset$ and $C_{x+i} \cap \mathcal{H} = \emptyset$ ($i = -1, 2$); others are treated as T_0 s. Since T_0 has a perfect matching as illustrated in Fig. 15 and any mutually disjoint hexagons in T_i form a resonant pattern of T_i ($i = 1, 2, 3$), immediately we have \mathcal{H} is a resonant pattern of $H(p, 3, p - 1)$. Hence $H(p, 3, p - 1)$ is k -resonant. \square

For toroidal polyhexes $H(2, 2, 1)$ and $H(2, 3, t)$ ($0 \leq t \leq 1$), any two hexagons in them are adjacent. So they are the degenerated cases of k -resonant ($k \geq 3$) toroidal polyhexes. By Lemmas 4.2, 4.3, 4.4 and Theorem 4.1, we have following result:

Theorem 4.5 A 3-resonant $H(p, q, t)$ with $\min(p, q) \geq 2$ is k -resonant ($k \geq 3$). \square

5 Remark

Benzenoid systems [25], coronoid benzenoid systems [2, 10], open-end nanotubes [20] and Klein-bottle polyhexes [17] are k -resonant ($k \geq 3$) if and only if they are 3-resonant. Here, by Theorems 3.7 and 4.5, we immediately have a parallel result for toroidal polyhexes.

Theorem 5.1 $H(p, q, t)$ is k -resonant ($k \geq 3$) if and only if it is 3-resonant. \square

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