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k-resonance in toroidal polyhexes[⋆]

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This paper considers the k -resonance of a toroidal polyhex (or toroidal graphitoid) with a string (p, q, t) of three integers ($p \geqslant 2$, $q \geqslant 2$, $0 \leqslant t \leqslant p-1$). A toroidal polyhex G is said to be k-resonant if, for $1 \leqslant i \leqslant k$, any i disjoint hexagons are mutually resonant, that is, G has a Kekulé structure (perfect matching) M such that these hexagons are M-alternating (in and off M). Characterizations for 1, 2 and 3-resonant toroidal polyhexes are given respectively in this paper.

KEY WORDS: Fullerene, toroidal polyhex, Kekulé structure, k-resonance

AMS 2000 MSC: 05C10, 05C70, 05C90

1. Introduction

The discovery of the fullerene molecules and nanotubes has stimulated much interests in other possibilities for carbons. Classical fullerene is an all-carbon molecule in which the atoms are arranged on a pseudospherical framework made up entirely of pentagons and hexagons. Its molecular graph is a finite trivalent graph embedded on the surface of a sphere with only hexagonal and (exactly 12) pentagonal faces. Deza et al. [4] considered fullerene's extension to other closed surfaces and showed that only four surfaces are possible: sphere, torus, Klein bottle and projective plane. Unlike spherical fullerenes, toroidal and Klein bottle's fullerenes have been regarded as tessellations of entire hexagons on their surfaces since they must contain no pentagons [4, 11]. For the theoretical consideration and detailed classifications of hexagonal tilings (dually, triangulations) on the torus and the Klein bottle, see [17, 22]. Toroidal fullerenes are likely

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to have direct experimental relevance since "crop circles fullerenes" discovered by Liu et al. [14] in 1997 are presumably torus-shaped.

A *toroidal polyhex* (or *toroidal graphitoid, torene*) is a toroidal fullerene that can be described by a string (p, q, t) of three integers $(p \geqslant 1, q \geqslant 1, 0 \leqslant t \leqslant p-1)$; its definition is referred to the next section. Some features of toroidal polyhexes with chemical relevance were discussed [9, 10]. For example, a systematic coding and classification scheme were given for the enumeration of isomers of toroidal polyhexes, the calculation of the spectrum and the count for spanning trees. There have been a few work in the enumeration of perfect matchings of toroidal polyhexes by applying various techniques, such as transfer-matrix [12, 21], permanent of the adjacency matrix [1], and Pfaffian orientation [8].

This paper considers the k-resonance of toroidal polyhexes. The concept of k-resonance originates from Clar's aromatic sextet theory [3] and Randić's conjugated circuit model [18,19,20]. In the former Clar found that various electronic properties of polycyclic aromatic hydrocarbons can be predicted by defining mutually resonant sextets [7] (i.e., disjoint hexagons that are all alternating with respect to a Kekulé structure). In Randić's model a conjugated hexagon has the largest contribution of the resonance energy among all $4n + 2$ conjugated circuits (a cycle is said to be conjugated or resonant if it is alternating with respect to a Kekulé structure). A benzenoid system is said to be *k-resonant* if, for $1 \leqslant i \leqslant k$, any i disjoint hexagons are mutually resonant. For a recent survey on k-resonant benzenoids and k-cycle resonant graphs, see [5]. Zhang and Chen [24] characterized completely 1-resonant benzenoid systems, solved such a problem proposed by Gutman [6] and showed its equivalence to normal benzenoid systems (i.e., each edge is contained in a Kekulé structure). The similar results were extended to coronoid systems (benzenoids with holes) [2] and plane bipartite graphs [26]. Later, Zheng [27, 28] characterized general k-resonant benzenoid systems. In particular he showed that any 3-resonant benzenoid systems are also k-resonant for any integer $k \geqslant 3$ and gave their systematic construction. The same result and similar construction are still valid for coronoid systems [2,13] and open-ended carbon nanotubes [23].

In this paper mutually resonant hexagons and k-resonance are naturally extended to toroidal polyhexes $H(p, q, t)(p \geqslant 2, q \geqslant 2)$ (in some degenerated cases, for instance, $H(1, q, 0)$, $H(p, 1, 0)$ and $H(p, 1, p-1)$, a hexagonal face is not bounded by a cycle). We point out several hexagon-preserving automorphisms of toroidal polyhexes and thus show the vertex- and hexagon-transitivity of this kind of graphs. Then we give a sufficient condition for some disjoint hexagons being mutually resonant whereby we show that all toroidal polyhexes are 1-resonant only except for (2, 2, 0), though they are all elementary bipartite graphs. This exception demonstrates a great difference with the plane situation. Further a simple characterization for 2-resonant toroidal polyhexes are given. Finally we completely characterize 3-resonant toroidal polyhexes.

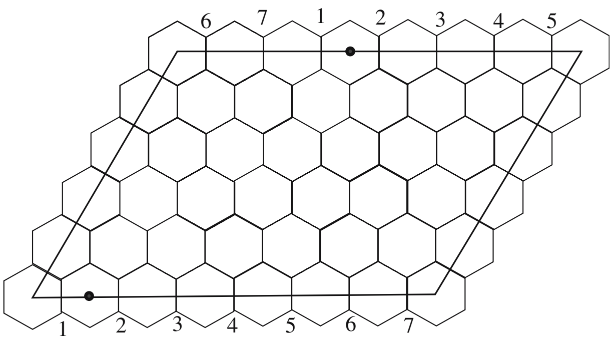

Figure 1. A toroidal polyhex $H(p,q,t)$ for $p=7,\ q=5,\ t=2$.

2. Toroidal polyhex with symmetry

A *toroidal polyhex* is a 3-regular (cubic or trivalent) graph embedded on the torus such that each face is a hexagon, described by three parameters p, q and t, denoted by $H(p,q,t)$ [16, 22], and drawn in the plane (equipped with the regular hexagonal lattice L) using the representation of the torus by a $p \times q$-parallelogram P with the usual boundary identification (see figure 1): each side of P 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, finally identify the top and bottom at their corresponding points. From this we get a toroidal polyhex $H(p,q,t)$ with the torsion $t (0 \leqslant t \leqslant p-1)$. In fact there is at least two ways to get such a toroidal polyhex. For example, see [8,16].

We easily know that $H(p,q,t)$ has pq hexagons. $2pq$ vertices and $3pq$ edges. The graph lying in the interior of the parallelogram P has a proper 2-coloring (white-black): the vertices incident with a downward vertical edge and with two upwardly oblique edges are colored black, and the other vertices white (see figure 2). Such a 2-coloring is a proper 2-coloring of $H(p,q,t)$, i.e., the end-vertices of each edge receive distinct colors. Hence we have

Proposition 2.1. $H(p,q,t)$ is a bipartite graph.

For convenience, the hexagons and vertices of $H(p,q,t)$ are labeled as an ordered pair of non-negative integers in the sense that we take the first component to be congruent modulo p and the second modulo q. We first establish an affine coordinate system XOY (see figure 2) : take the bottom side as x-axis, a lateral side as y-axis, their intersection as the origin O such that both sides form an angle of 60°, and P lies on non-negative region. For any positive integer n, we shall use $\mathbb{Z}_n$ to denote the set $\{0, 1, \ldots, n-1\}$ with arithmetic modulo n. The distance between a pair of parallel edges in a hexagon is a unit length.

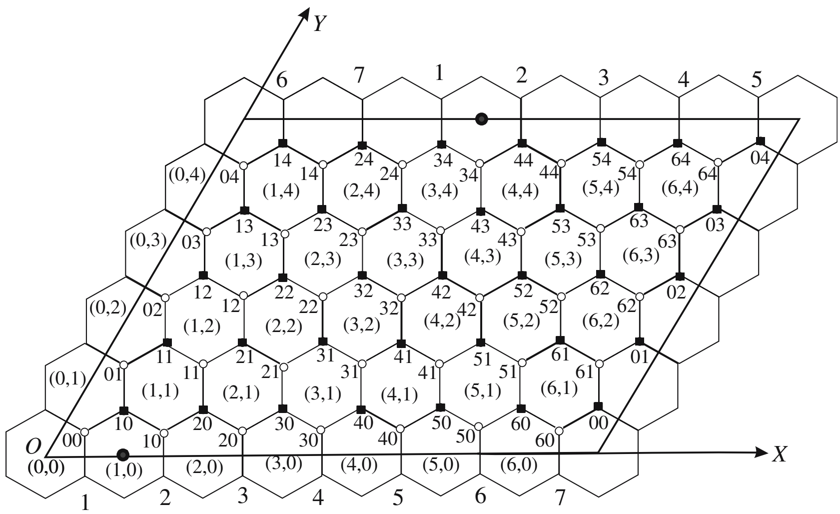

Figure 2. Labeling for the hexagons and vertices of toroidal polyhex $H(p, q, t)$ for $p = 7$, $q = 5$, $t = 2$.

Each hexagon is labeled by the coordinates (x, y) of its center, where $x \in \mathbb{Z}_p$ and $y \in \mathbb{Z}_q$. Hence such a hexagon is denoted by its label (x, y)(or $h_{xy}, h_{x,y}$). For each hexagon h_{xy}, choosing the upper one of a pair of parallel edges perpendicular to y-axis, the black end-vertex is named by b_{xy} (or $b_{x,y}$) and the white end-vertex by w_{xy} (or $w_{x,y}$) (for example, see figure 2). In this notations, each $w_{0,y}$, is adjacent to $b_{0,y}$ and each $w_{x,0}$ to $b_{x+t+1,q-1}$; the yth *layer* is the even cycle $w_{0,y}b_{1,y}w_{1,y}b_{2,y}\cdots w_{p-1,y}b_{0,y}w_{0,y}$, $0 \leqslant y \leqslant q-1$.

An *automorphism* ϕ of a simple graph is a bijection from the vertex-set to itself so that both ϕ and the inverse ϕ^{-1} preserve the adjacency between vertices. We now define three types of automorpllisms of toroidal polyhex $H(p, q, t)$ as follows: the l - r shift ϕ_{lr} moves horizontally backward every vertex a unit, i.e.,

$$\phi_{lr}(w_{x,y}) = w_{x-1,y} \text{ and } \phi_{lr}(b_{x,y}) = b_{x-1,y}, \text{ for every pair } (x, y). \tag{1}$$

The t-b shift ϕ_{tb} moves downwards every vertex a unit from the y-axis, but the x-coordinates may change. More precisely,

$$\phi_{tb}(w_{x,y}) = w_{x,y-1} \text{ and } \phi_{tb}(b_{x,y}) = b_{x,y-1}, \text{ for } 1 \leqslant y \leqslant q-1, \tag{2}$$

and

$$\phi_{tb}(w_{x,0}) = w_{x+t,q-1} \text{ and } \phi_{tb}(b_{x,0}) = b_{x+t,q-1}. \tag{3}$$

It can be seen that both shifts ϕ_{lr} and ϕ_{tb} are hexagon-preserving automorphism of $H(p, q, t)$. Further ϕ_{lr} and ϕ_{tb} generate a subgroup of the automorphism group of $H(p, q, t)$, denoted by $\langle \phi_{lr}, \phi_{tb} \rangle$, which acts transitively on the set of hexagons of $H(p, q, t)$; that is, for each pair of hexagons h and h' there is a hexagon-preserving automorphism $g \in \langle \phi_{lr}, \phi_{tb} \rangle$ so that $g(h) = h'$. Hence we have the following result.

Lemma 2.2. $H(p, q, t)$ is hexagon-transitive.

Finally, let R_2 be the rotation of 180° about the center of the parallelogram P. Then R_2 is also a hexagon-preserving automorphism of $H(p, q, t)$ that interchanges the black and white vertices. The generated subgroup $\langle \phi_{lr}, \phi_{tb} R_2 \rangle$ is transitive on the vertex-set of $H(p, q, t)$.

Lemma 2.3 (22,16). $H(p, q, t)$ is vertex-transitive.

3. 1-and 2-Resonance

A *perfect matching* or 1-*factor* M (Kekulé structure in chemistry) of a graph G is a set of pairwise disjoint edges of G such that every vertex of G is incident with an edge in M. A bipartite graph is called *elementary* [15] if it is connected and each edge is contained in a perfect matching. We easily know that any toroidal polyhex is an elementary bipartite graph since it is 3-regular. In fact the edge-set of a toroidal polyhex can be decomposed into three perfect matchings so that each consists of all edges with the same edge-direction [8].

The concept for k-resonance is now extended to toroidal polyhexes. The set of some disjoint hexagons of $H(p, q, t)$ is called a *resonant pattern*, or these hexagons are *mutually resonant*, if $H(p, q, t)$ has a perfect matching M such that these hexagons are all M-alternating (in and off M) cycles. In some degenerated cases of toroidal polyhexes, for instance, $H(1, q, 0)$, $H(p, 1, 0)$ and $H(p, 1, p-1)$, a hexagonal face is not bounded by a cycle. So we only consider toroidal polyhexes $H(p, q, t)$ with $p \geqslant 2$ and $q \geqslant 2$. In such cases disjoint hexagons of $H(p, q, t)$ are mutually resonant if and only if the subgraph obtained from $H(p, q, t)$ by deleting the vertices of the hexagons either has a perfect matching or is empty (since each hexagonal face is bounded by a cycle with length 6).

Definition 3.1. For some positive integer k, a toroidal polyhex $H(p, q, t)$ is called *k-resonant* if for any $i (\leqslant k)$ disjoint hexagons of $H(p, q, t)$ are mutually resonant.

Remark 3.1. By the definition above, a toroidal polyhex $H(p, q, t)$ is k-resonant if it is $(k-1)$ –resonant and does not contain any k disjoint hexagons.

To obtain our characterizations (the main results in this paper) for k-resonance of toroidal polyhexes, the following provides us a crucial approach. Let $\mathcal{S}$ be a subgraph of a toroidal polyhex $H(p,q,t)$ for which each component is either a hexagon or an edge with the end-vertices. Then $\mathcal{S}$ is called a *Clar cover* [25] if $\mathcal{S}$ includes all vertices of $H(p,q,t)$; an *ideal configuration* if $\mathcal{S}$ is alternately incident with white and black vertices along any direction of each layer.

Lemma 3.1. Any ideal configuration $\mathcal{S}$ of a toroidal polyhex $H(p,q,t)$ can be extended to a Clar cover, and the hexagons in $\mathcal{S}$ are thus mutually resonant.

Proof. Let L_y be the yth layer of $H(p,q,t), 0 \leqslant y \leqslant q-1$. Let $L_y - \mathcal{S}$ be the subgraph obtained from L_y by deleting all vertices of $\mathcal{S}$ together with their incident edges. If $\mathcal{S}$ contains a vertex of L_y, each component of $L_y - \mathcal{S}$ is a path with odd length for which the end-vertices have different colors because $\mathcal{S}$ is alternately incident with white and black vertices along the cycle L_y. Hence each $L_y - \mathcal{S}$ has a perfect matching. This implies that $H(p,q,t) - \mathcal{S}$ has a perfect matching. Hence S can be extended to a Clar cover, and its hexagons are thus mutually resonant. □

In this section we first give 1-resonant toroidal polyhexes, and then characterize 2-resonant toroidal polyhexes.

Theorem 3.2. A toroidal polyhex $H(p,q,t)(p,q \geqslant 2)$ is 1-resonant if and only if $(p,q,t) \neq (2,2,0)$.

Proof. Since $H(p,q,t)$ is hexagon-transitive (Lemma 2.2), it suffices to check whether any given hexagon is resonant or not.

Case 0: $p = 2 = q$. Choose the hexagon h_{11} (see figure 3). $H(2,2,0) - h_{11}$ consists of exactly two isolated vertices w_{00} and b_{01}. This implies that $H(2,2,0)$ is not 1-resonant. $H(2,2,1) - h_{11}$ consists of exactly two adjacent vertices w_{00} and b_{01}. Hence $H(2,2,1)$ is 1-resonant.

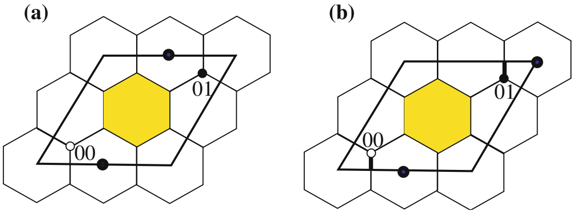

Figure 3. (a) $H(2,2,0)$, (b) $H(2,2,1)$.

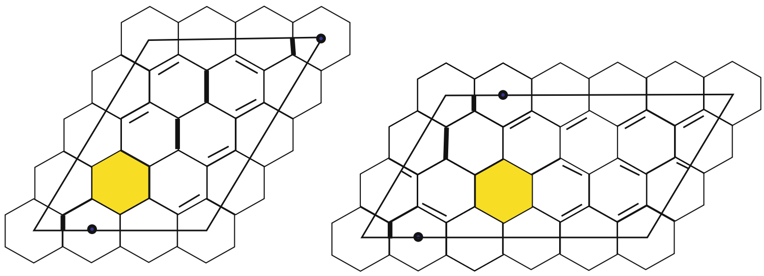

Figure 4. Illustration for the proof of Theorem 3.2.

Case 1: $p \geqslant 2$ and $q \geqslant 3$. Choose the hexagon h_{11} (i.e., the cycle $b_{11}w_{11}b_{20}w_{10}b_{10}w_{01}b_{11}$, which is hatched in figure 4(left)), and the vertical edges $w_{00}b_{t+1,q-1}, w_{12}b_{21}, w_{13}b_{22}, \ldots, w_{1,q-1}b_{2,q-2}$ (indicated by thick lines in figure 4 (left)). The chosen hexagon and vertical edges form an ideal configuration since it is incident with vertices: w_{00}, b_{10}, w_{10} and b_{20} in the 0th layer; w_{01}, b_{11}, w_{11} and b_{21} in the first layer; $w_{1y}, b_{2,y}$, in the yth layers, $2 \leqslant y \leqslant q-2$; and $W_{1,q-1}, b_{t+1,q-1}$ in the $(q-1)$th layer. Hence by Lemma 3.1 h_{11} is a resonant hexagon.

Case 2: $p \geqslant 3$ and $q \geqslant 2$. For $t \neq 0$, the same arguments as Case 1 can be made. For $t = 0$, we choose the hexagon $h_{2,1}$ (i.e., the cycle $b_{21}w_{21}b_{30}w_{20}b_{20}w_{11}b_{21}$), and vertical edges $w_{00}b_{l,q-1}$, $w_{02}b_{11}, \ldots$, $w_{0,q-l}b_{1,q-2}$ (indicated by thick lines, see figure 4(right)). By the same reason as Case 1 the chosen hexagon and vertical edges form an ideal configuration and the hexagon h_{21} is resonant. □

Lemma 3.3. $H(p,q,t)$ is 2-resonant for $p \geqslant 3$ and $q \geqslant 3$.

Proof. It suffices to prove that any pair of disjoint hexagons (x_1, y_1), and (x_2, y_2) are mutually resonant, where $x_i \in \mathbb{Z}_p$ and $y_i \in \mathbb{Z}_q$. By hexagon-preserving automorphisms of $H(p,q,t)$ we need only to consider the following situation:

(i) $1 = y_1 \leqslant y_2 \leqslant \frac{q}{2} + 1 (\leqslant q-1)$, and

(ii) $1 = \min(x_1, x_2) \leqslant \max(x_1, x_2) \leqslant \frac{p}{2} + 1 (\leqslant p-1)$.

We first show this point. Without loss of generality we may assume that $0 \leqslant y_l \leqslant y_2 \leqslant q-1$. If $0 = y_1 \leqslant y_2 \leqslant q/2$, then we make the reversion of the t-b shift operation ϕ_{tb} (see equation (2)) to $H(p,q,t)$, i.e., $\phi_{tb}^{-1}(x_1, 0) = (x_1, 1)$ and $\phi_{tb}^{-1}(x_2, y_2) = (x_2, y_2 + 1)$. The resulting hexagons satisfy statement (i). If $y_2 - y_1 > \frac{q}{2}$, then we make the t-b shift operation $y_2 - 1$ times (see equations (2) and (3)), i.e., $(x_2', y_2') = \phi_{tb}^{y_2-1}(x_2, y_2) = (x_2, y_2 - (y_2 - 1)) = (x_2, 1)$, and $(x_1', y_1') = \phi_{tb}^{y_2-1}(x_1, y_1) \equiv (x_1', y_1 - (y_2 - 1)) \pmod q$. So $y_1' = y_1 - (y_2 - 1) + q \in \mathbb{Z}_q$. Further

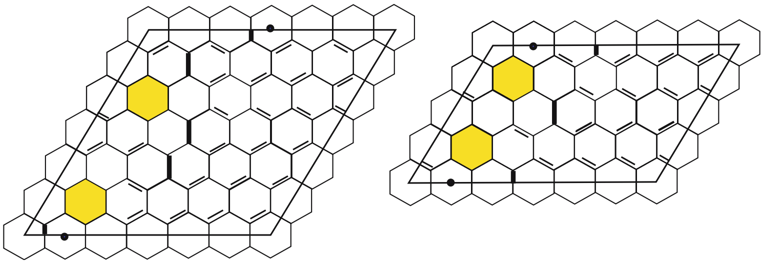

Figure 5. Illustration for Case 1 in the proof of Lemma 3.3.

$1 = y_2' \leqslant y_1' = q - (y_2 - y_1) + 1 < q/2 + 1$. Otherwise, $y_1 \geqslant 1$ and $y_2 - y_1 \leqslant q/2$. Similarly we can reduce this case to (i) by making the t-b shift operation $y_1 - 1$ times. Then, by applying l-r shift operation ϕ_{lr} that makes the y-coordinates to remain unchanged, similarly we can reduce all cases to the situation (ii).

To prove that (x_1, y_1) and (x_2, y_2) are mutually resonant, we will apply mainly the technique in Lemma 3.1: construct an ideal configuration containing such two hexagons by choosing a series of additional edges. We now distinguish the following four cases.

Case 1: $x_1 = y_1 = x_2 = 1$ and $3 \leqslant y_2 \leqslant \frac{q}{2} + 1$. If $y_2 \leqslant q - 2$, then we choose vertical edges $w_{00}b_{t+1,q-1}$; $w_{2,i}b_{3,i-1}$, $i = 2, \ldots, y_2 - 1$; $w_{1,j}b_{2,j-1}$, $j = y_2 + 1, \ldots, q-1$, (indicated by thick lines, see figure 5 (left)). If $y_2 = q-1$, then $q = 4$ only. For $t \neq 0$, we choose two edges $w_{00}b_{t+1,3}$ and $w_{22}b_{31}$. For $t = 0$, $w_{00}b_{13}$ is replaced by $w_{20}b_{33}$ and the edge $w_{22}b_{31}$ remain unchanged (see figure 5 (right)). It is easy to see that the chosen hexagons and vertical edges form an ideal configuration.

Case 2: $1 = x_1 < x_2 \leqslant \frac{p}{2} + 1$ and $1 = y_1 < y_2 \leqslant \frac{q}{2} + 1$. If $y_2 \leqslant q - 2$, then we choose vertical edges $w_{00}b_{t+1,q-1}$; $w_{x_2-1,i}b_{x_2,i-1}$, $i = 2, \ldots, y_2 - 1$; $w_{x_2,j}b_{x_2+1,j-1}$, $j = y_2 + 1, \ldots, q - 1$, which are indicated by thick lines in figure 6 (left). If $y_2 = q - 1$, then $q = 3$ or 4. For $t \neq x_2 - 1$, we choose edges $w_{00}b_{t+1,q-1}$ and $w_{x_2-1,2}b_{x_2,1}$ if $q = 4$, and we only choose the former if $q = 3$ since the edge $w_{00}b_{t+1,q-1}$ is disjoint with the hexagon (x_2, y_2). For $t = x_2 - 1$, $w_{00}b_{t+1,q-1}$ is replaced by $w_{20}b_{x_2+2,q-1}$ since $x_2+2 \not\equiv x_2 \pmod{p}$, and the other choices remain unchanged (see figure 6 (right)). For each subcase, the subgraph formed by the chosen hexagons and vertical edges is an ideal configuration.

Case 3: $1 = x_2 < x_1 \leqslant \frac{p}{2} + 1$ and $1 = y_1 < y_2 \leqslant \frac{q}{2} + 1$. If $y_2 \leqslant q - 2$, then we choose vertical edges $w_{00}b_{t+1,q-1}$; $w_{x_1,i}b_{x_1+1,i-1}$, $i = 2, \ldots, y_2 - 1$; $w_{1,j}b_{2,j-1}$, $j = y_2 + 1, \ldots, q - 1$, (indicated by thick lines, see figure 7 (left)). If $y_2 = q - 1$, then $q = 3$ or 4. For $t \neq 0$, we still choose such edges $w_{00}b_{t+1,q-1}$ and $w_{x_1,i}b_{x_1+1,i-1}$, $i = 2, 3, \ldots, y_2 - 1$, since the edge

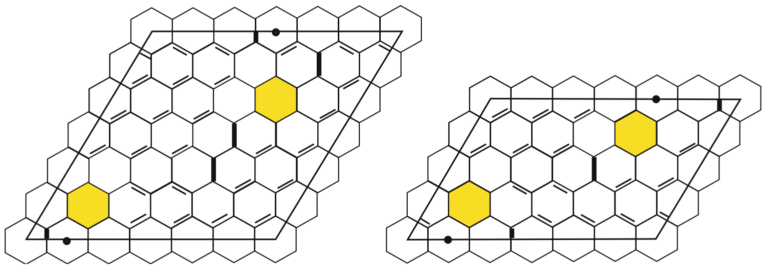

Figure 6. Illustration for Case 2 in the proof of Lemma 3.3.

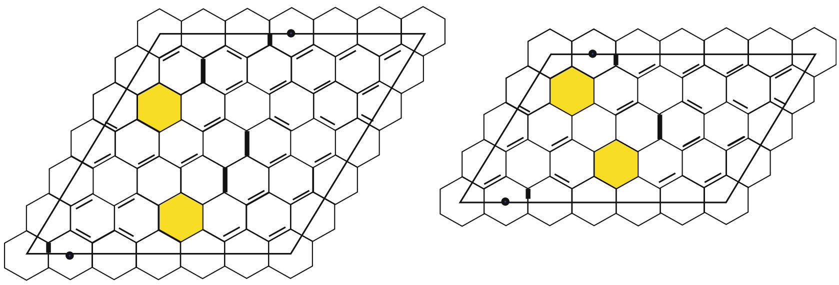

Figure 7. Illustration for Case 3 in the proof of Lemma 3.3.

$w_{00}b_{t+1,q-1}$ is disjoint with the hexagon $(1, y_2)$. For $t = 0$, $w_{00}b_{1,q-1}$ is replaced by $w_{10}b_{2,q-1}$ and the other choices remain unchanged (see figure 7 (right)). For each subcase, the chosen hexagons together with such vertical edges form an ideal configuration.

Case 4: $x_1 = y_1 = y_2 = 1$ and $3 \leqslant x_2 \leqslant \frac{p}{2} + 1$. This situation is more complicated than the previous three cases. Obviously, $p \geqslant 4$ and $1 \leqslant q - 2$. We first choose the vertical edges $w_{1,i}b_{2,i-1}, w_{x_2,i}b_{x_2+1,i-1}, i = 2, \ldots, q-1$ (indicated by thick lines, see figure 8).

For $t = p-1, 0, 1, \ldots, x_2-3$, we further choose two edges $w_{20}b_{t+3,q-1}$ and $w_{x_2+1,0}b_{x_2+2+t,q-1}$. Since $2 \leqslant t+3 \leqslant x_2$ and $x_2+1 \leqslant x_2+2+t \leqslant 2x_2-1 \leqslant p+1$ (note that $t+3, x_2+2+t \in \mathbb{Z}_p$), the chosen part has the incident vertices $w_{1,q-1}, b_{t+3,q-1}, w_{x_2,q-1}$ and $b_{x_2+2+t,q-1}$ in the $(q-1)$th layer that alternate between white and black in one direction of this layer. The same fact holds obviously for the other layers.

For $t = x_2-2, x_2-1, \ldots, p-2$, we further choose two edges $w_{20}b_{t+3,q-1}$ and $w_{x,0}b_{x+1+t,q-1}$, where x will be determined below. If $t = p-2$, then put $x := x_2+1$. Since $x_2 < 3+t = p+1$ and $x+1+t \equiv x_2 \pmod{p}$, the chosen part has the four incident vertices $w_{1,q-1}, b_{x_2,q-1}, w_{x_2,q-1}, b_{3+t,q-1}$, ordered in the $(q-1)$th layer's direction. If $x_2 - 2 \leqslant t \leqslant p-3$, then put $x := x_2 - 2 - t \in \mathbb{Z}_p$. Since $x_2 + 1 \leqslant x \leqslant p$ and $x + 1 + t = x_2 - 1$, the chosen part has the four incident vertices in 0th layer

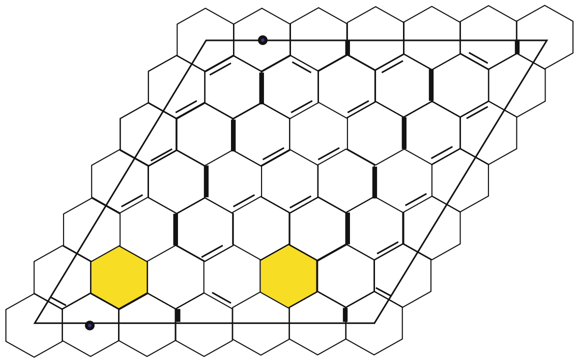

Figure 8. Illustration for Case 4 in the proof of Lemma 3.3.

as ordered $b_{10}, w_{10}, b_{20}, w_{20}, b_{x_2,0}, w_{x_2,0}, b_{x_2+1,0}, w_{x,0}$; in the $(q-1)$th layer as $w_{1,q-1}, b_{x+1+t,q-1}, w_{x_2,q-1}, b_{3+t,q-1}$, which alternate between white and black.

For each subcase mentioned above the chosen hexagons (x_1, y_1) and (x_2, y_2) together with a series of corresponding vertical edges compose of an ideal configuration.

Therefore, by Lemma 3.1 any pair of disjoint hexagons are mutually resonant. Namely, $H(p,q,t)$ is 2-resonant for $p \geqslant 3$ and $q \geqslant 3$. □

Lemma 3.4. For $p \geqslant 4$, $H(p,2,t)$ is 2-resonant if and only if t is neither 0 nor $p-2$.

Proof. Suppose $t = 0$ or $p-2$. We are going to show that $H(p,2,t)$ is not 2-resonant. Choose two disjoint hexagons h_{11} and h_{31}. Then vertices b_{20}, b_{30} and $b_{3+t,1}$ are neighbors of w_{20}. They lie in the hexagon h_{11} or h_{31}. Hence w_{20} is an isolated vertex of $H(p,2,t) - h_{11} - h_{31}$. This shows that such two hexagons are not mutually resonant.

For the other cases, i.e., $t \notin \{0, p-2\}$, we will show that $H(p,2,t)$ is 2-resonant. By a similar argument as in the proof of Lemma 3.3 we consider a pair of disjoint hexagons (x_1, y_1) and (x_2, y_2), where $x_i \in \mathbb{Z}_p$ and $y_i \in \mathbb{Z}_2$. If $y_1 \neq y_2$, then both hexagons compose of an ideal configuration. Hence they are mutually resonant by Lemma 3.1. So we only consider the case $x_1 = y_1 = y_2 = 1$ and $3 \leqslant x_2 \leqslant p/2 + 1 (\leqslant p-1)$ by hexagon-preserving automorphisms of $H(p,q,t)$.

If $t = p-1, 1, 2, \ldots, x_2 - 4$, then we choose $w_{20}b_{t+3,1}$ and $w_{x_2+l,0}b_{x_2+2+t,1}$. Since $2 \leqslant t+3 \leqslant x_2 - 1$ and $x_2 + 1 \leqslant x_2 + 2 + t \leqslant 2x_2 - 2 \leqslant p$, the end-vertices of both chosen edges in the 0th and 1st layers are separated by hexagons $(1,1)$ and $(x_2, 1)$ (see figure 9). If $t = x_2 - 2, x_2 - 1, \ldots, p-3$, then we choose $w_{20}b_{t+3,1}$ and $w_{x,0}b_{x+1+t,1}$, where $x = x_2 - 2 - t + p$. Since $x_2 + 1 \leqslant 3 + t \leqslant p, x_2 + 1 \leqslant x \leqslant p$ and $x + 1 + t = p + x_2 - 1$, the above result also holds. For the last case

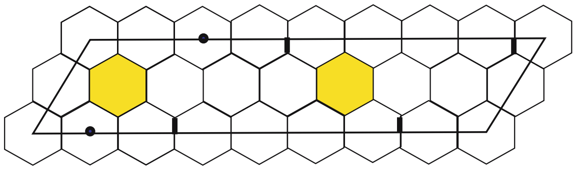

Figure 9. Illustration for the proof of Lemma 3.4 for $p = 8, x_2 = 5$ and $t = 1$.

$t = x_2 - 3$, we have that $x_2 \geqslant 4$ since $t \neq 0$. Since $t + 1 = x_2 - 2 \geqslant 2$ and $x_2 + 1 \leqslant x_2 + t = 2x_2 - 3 \leqslant p - 1$, we choose $w_{00}b_{t+1,1}$ and $w_{x_2-1,0}b_{x_2+t,1}$. For each subcase, the chosen hexagon $(1, 1)$ and $(x_2, 1)$ with the chosen edges form an ideal configuration. Therefore, by Lemma 3.1 the hexagons $(1, 1)$ and $(x_2, 1)$ are mutually resonant. □

Lemma 3.5. For $q \geqslant 1$, $H(2, q, t)$ is not 2-resonant.

Proof. Consider the disjoint hexagons h_{11} and h_{13}. The neighbors of the vertex w_{02}, which are b_{11}, b_{12} and b_{02}, belong to the chosen hexagons. Hence $H(2, q, t) - h_{11} - h_{13}$ has no perfect matching. Namely hexagons h_{11} and h_{13} are not mutually resonant. □

From Lemma 3.2 we know that $H(2, 2, 0)$ is not 1-resonant, $H(2, 2, 1)$, $H(3, 2, t)(t = 0, 1, 2)$ and $H(2, 3, t)(t = 0, 1)$ are 1-resonant. We can see that $H(2, 2, 1)$, $H(3, 2, 0)$, $H(3, 2, 1)$, $H(2, 3, 0)$ and $H(2, 3, 1)$ do not contain two disjoint hexagons. So automatically they are 2-resonant. Further $H(3, 2, 2)$ is 2-resonant since it has exactly 12 vertices, which are all included in any pair of two disjoint hexagons. Combining these facts and Lemmas 3.3–3.5, we summarize the following characterization for the 2-resonance of toroidal polyhexes.

Theorem 3.6. For $p \geqslant 2$ and $q \geqslant 2$, a toroidal polyhex $H(p, q, t)$ is 2-resonant if and only if one of the following cases appears:

1. $\min(p, q) \geqslant 3$,
2. $p \geqslant 4, q = 2$ and $t \notin \{0, p - 2\}$,
3. $(p, q) = (3, 2)$ or $(2, 3)$,
4. $(p, q, t) = (2, 2, 1)$.

4. 3-Resonance

In this section we further consider the 3-resonance of toroidal polyhexes. The following lemma shows that most toroidal polyhexes are not 3-resonant.

Lemma 4.1. For $p, q \geqslant 4$, $H(p, q, t)$ is not 3-resonant.

Proof. Choose three disjoint hexagons h_{11}, h_{13} and h_{31}. Then vertices w_{11}, w_{12} and w_{21} are neighbors of b_{21}. They lie in hexagons h_{11}, h_{13} and h_{31}, respectively. Hence $H(p, q, t) - h_{11} - h_{13} - h_{31}$ has an isolated vertex b_{21}. This implies that such three hexagons are not mutually resonant. $\square$

Lemma 4.2. For $q \geqslant 2$, $H(3, q, t)$ is 3-resonant.

Proof. By Lemma 3.3 or Theorem 3.6 $H(3, 2, t)$ and $H(3, 3, t)$ are 2-resonant. We can easily see that they are 3-resonant since either they contain no three disjoint hexagons or their three disjoint hexagons contain all vertices. So we may assume $q \geqslant 4$.

It suffices to show that any three disjoint hexagons $(x_i, y_i), x_i \in \mathbb{Z}_3$ and $y_i \in \mathbb{Z}_q, i = 1, 2, 3$, are mutually resonant. By l-r and t-b shift operations there are three cases to be considered.

Case 1: $x_1 = 0, x_2 = 1, x_3 = 2$ and $y_1 = 1$. If $2 \leqslant y_2 < y_3 \leqslant q-1$, then we choose vertical edges $w_{0j}b_{1,j-1}, j = 2, \ldots, y_2 - 1$; $w_{1j}b_{2,j-1}, j = y_2 + 1, \ldots, y_3 - 1$; $w_{2j}b_{0,j-1}, j = y_3 + 1, \ldots, q - 1$; we further choose one vertical edge $w_{10}b_{t+2,q-1}$ when $t = 1$ and 2, and $w_{20}b_{0,q-1}$ when $t = 0$ (see figure 10(a)). If $2 < y_3 < y_2 \leqslant q - 1$, then we choose vertical edges $w_{0j}b_{1,j-1}, j = 2, \ldots, y_3 - 1, y_3 + 1, \ldots, y_2 - 1$; $w_{2j}b_{0,j-1}, j = y_2 + 1, \ldots, q - 1$; we further choose one vertical edge $w_{10}b_{t+2,q-1}$ when $t = 0$ and 1, and $w_{20}b_{2,q-1}$ when $t = 2$ (see figure 10(b)). It can be seen that the three hexagons together with the chosen edges for any subcase form an ideal configuration. So by Lemma 3.1 such three hexagons are mutually resonant.

Case 2: $x_1 = x_2 = x_3 = 1$ and $1 = y_1 < y_2 < y_3 \leqslant q - 1$. We choose vertical edges $w_{2j}b_{0,j-1}, j = 2, \ldots, y_2 - 1, y_2 + 1, \ldots, y_3 - 1, y_3 + 1, \ldots, q - 1$. We further choose one vertical edge $w_{00}b_{t+1,q-1}$ when $t = 1$ and 2, and $w_{20}b_{0,q-1}$ when $t = 0$. By the same reason as the above such three hexagons are mutually resonant.

Case 3: $\{x_1, x_2, x_3\} = \{1, 2\}$ and $1 = y_1 < y_2 < y_3 \leqslant q - 1$. If $x_1 = 1, x_2 = 2$ and $x_3 = 1$, then we choose vertical edges $w_{1j}b_{2,j-1}, j = 2, \ldots, y_2 - 1$; $w_{2j}b_{0,j-1}, j = y_2 + 1, \ldots, y_3 - 1, y_3 + 1 \ldots, q - 1 (y_2 + 1 < y_3)$. We further choose one vertical edge $w_{00}b_{t+1,q-1}$ when $t = 1$ and 2, and $w_{20}b_{0,q-1}$ when $t = 0$. The chosen hexagons and edges form an ideal configuration. Similarly, we can show the remaining subcases to have an ideal configuration containing the chosen hexagons. Hence such three hexagons are mutually resonant. $\square$

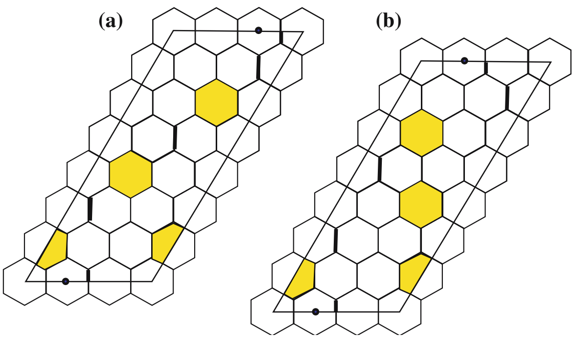

Figure 10. An ideal configuration of $(3, 7, t)$ for (a) $y_2 = 3$, $y_3 = 5$ and $t = 1$, (b) $y_2 = 5$, $y_3 = 3$ and $t = 0$.

Lemma 4.3. For $p \geqslant 4$, $H(p, 3, t)$ is 3-resonant if and only if $t = 0, p-3, p-2$ or $p-1$.

Proof. For $p \geqslant 5$ and $t \in \mathbb{Z}_p \setminus \{0, p-3, p-2, p-1\}$, we choose three disjoint hexagons $(1, 1)$, $(p-1, 1)$ and $(t+1, 2)$. Then the vertex w_{00}'s neighbors b_{10}, b_{00} and $b_{t+1,2}$ are vertices in hexagons $(1, 1), (p-1, 1)$ and $(t+1, 2)$, respectively. Hence the chosen hexagons are not mutually resonant. That says that $H(p, 3, t)$ is not 3-resonant if $t \notin \{0, p-3, p-2, p-1\}$ for $p \geqslant 4$.

For $t \in \{0, p-3, p-2, p-1\}$, we now show that $H(p, 3, t)$ is 3-resonant. It suffices to show that any three disjoint hexagons (x_i, y_i), $x_i \in \mathbb{Z}_p$ and $y_i \in \mathbb{Z}_3$, $i = 1, 2, 3$, are mutually resonant. By l-r and t-b shift operations there are three cases to be considered.

Case 1. $y_1 = 0$, $y_2 = 1$ and $y_3 = 2$. Such three hexagons form an ideal configuration and are thus mutually resonant by Lemma 3.1.

Case 2. $y_1 = y_3 = 1$, $y_2 = 2$ and $1 = x_1 < x_2 < x_3 \leqslant p-1$. If $t = 0$ and $p-1$, we choose $w_{x_i-1,0}b_{x_i+t,2}$, $i = 1, 3$, and $w_{p-1,2}b_{01}$ as distinguished edges, see figure 11. We only list the incident vertices of the chosen hexagons and vertical edges on the 2nd layer as $b_{1+t,2}$, $w_{x_2-1,2}$, $b_{x_2,2}$, $w_{x_2,2}$, $b_{x_3+t,2}$, $w_{p-1,2}$ in one direction of the cycle. If $t = p-2$ and $p-3$, choose $w_{x_i+1,0}b_{x_i+t+2,2}$, $i = 1, 3$, and $w_{p-1,2}b_{0,1}$ as distinguished edges. The corresponding incident vertices are ordered as $b_{3+t,2}$, $w_{x_2-1,2}$, $b_{x_2,2}$, $w_{x_2,2}$, $b_{x_3+t+2,2}$, $w_{p-1,2}$ (note that $x_2 < x_3 - 1$). As for the 0th and 1st layers, the similar facts are obvious. Hence to each subcase the three hexagons and all chosen edges compose of an ideal configuration. By Lemma 3.1 such three hexagons are mutually resonant.

Case 3. $y_1 = y_2 = y_3 = 1$ and $1 = x_1 < x_2 < x_3 \leqslant p-1$. We choose vertical edges $w_{x_i,2}b_{x_i+1,1}$, $i = 1, 2, 3$. If $t = 0, p-1$, we further choose $w_{x_i-1,0}b_{x_i+t,2}$,

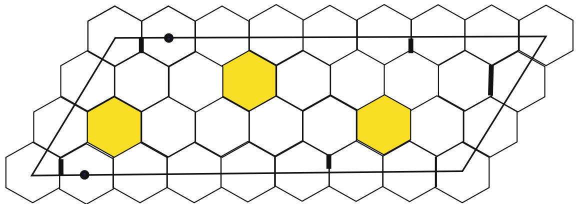

Figure 11. An ideal configuration of $H(8,3,0)$ for $x_2 = 3$, $x_3 = 6$ and $t = 0$.

$i = 1, 2, 3$. If $t = p-2, p-3$, we further choose $w_{x_i+1,0}b_{x_i+t+2,2}$, $i = 1, 2, 3$. To each subcase the three hexagons and all chosen edges compose of an ideal configuration. By Lemma 3.1 such three hexagons are mutually resonant. □

Lemma 4.4. For $p \geqslant 3$, $H(p, 2, t)$ is 3-resonant if and only if $t = 1, p-3$ or $p-1$.

Proof. For $t \in \mathbb{Z}_p \setminus \{1, p-3, p-1\}(p \geqslant 4)$, we choose disjoint hexagons $(1, 1)$, $(t+1, 1)$ and $(p-1, 1)$ of $H(p, 2, t)$ (note that if $t = 0$ and $t = p-2$, then two of them are coincidence). The vertex w_{00} has three neighbors: b_{10}, b_{00} and $b_{t+1,1}$, which are all included in the chosen hexagons. This implies that $H(p,2,t) - h_{1,1} - h_{t+1,1} - h_{p-1,1}$ has no perfect matching. Hence $H(p, 2, t)(p \geqslant 3)$ is not 3-resonant for $t \notin \{1, p-3, p-1\}$.

We now show that if $t \in \{1, p-1, p-3\}$, $H(p, 2, t)(p \geqslant 3)$ is 3-resonant. Since it is 2-resonant (Lemma 3.4 or Theorem 3.6), it suffices to show any three disjoint hexagons (x_i, y_i), $x_i \in \mathbb{Z}_p$ and $y_i \in \mathbb{Z}_2$, $i = 1, 2, 3$, are mutually resonant. By the l-r and t-b shift operations (equation (1) to (3)) there are two cases to be considered.

Case 1. $y_1 = y_2 = y_3 = 1$ and $1 = x_i < x_2 < x_3 \leqslant p-1$. If $t = 1$ or $p-1$, then we choose the edges $w_{x_i-1,0}b_{x_i+t,1}$, $i = 1, 2, 3$; if $t = p-3$, then we choose the edges $w_{x_i+1,0}b_{x_i+t+2,1}$ for $i = 1, 2, 3$. Then the chosen hexagons and edges form an ideal configuration and such three hexagons are thus mutually resonant by Lemma 3.1.

Case 2. $y_1 = y_3 = 1$, $y_2 = 0$ and $1 = x_1 < x_2 < x_3 \leqslant p-1$. If $t = p-1$, then we only choose the edge $w_{00}b_{01}$ (see figure 12 (right)). If $t = 1$, then $x_3 \geqslant x_2 + 3$. We choose edges $w_{x_i-1,0}b_{x_i+1,1}$, for $i = 1, 3$, and $w_{x_2,1}b_{x_2+1,0}$ (see figure 12 (left)). If $t = p-3$, then $x_2 - x_1 \geqslant 4$. We choose the edges $w_{x_i+1,0}b_{x_i-1,1}$ for $i = 1, 3$, and $w_{x_2-2,1}b_{x_2-1,0}$. In any subcase the chosen hexagons and vertical edges form an ideal configuration and such chosen hexagons are mutually resonant by Lemma 3.1. □

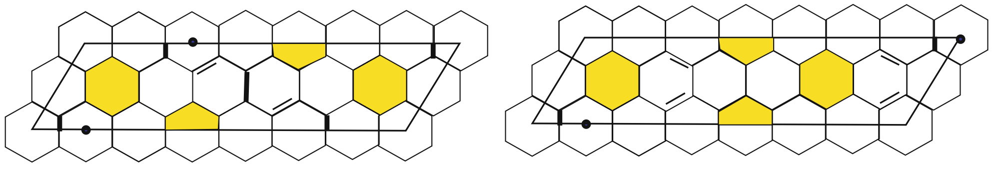

Figure 12. Illustration for Case 2 in the proof of Lemma 4.4 ($t = 1$ and $t = p - 1$).

Automatically $H(2, 3, t)$ and $H(2, 2, 1)$ are 3-resonant. Combining Lemmas 3.5 and 4.1–4.4, we obtain the following criterion for the 3-resonance of toroidal polyhexes.

Theorem 4.5. For $p \geqslant 2$ and $q \geqslant 2$, a toroidal polyhex $H(p, q, t)$ is 3-resonant if and only if one of the following cases appears

1. $(p, q, t) = (2, 2, 1)$,
2. $p = 2$ and $q = 3$,
3. $p = 3$ and $q \geqslant 2$,
4. $p \geqslant 4, q = 2$ and $t \in \{1, p - 3, p - 1\}$,
5. $p \geqslant 4, q = 3$ and $t \in \{0, p - 3, p - 2, p - 1\}$.

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