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A complete characterization for k-resonant Klein-bottle polyhexes

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A hexagonal tessellation $K(p, q, t)$ on Klein bottle, a non-orientable surface with cross-cap number 2, is a finite-sized elemental benzenoid which can be produced from a $p \times q$-parallelogram of hexagonal lattice with usual identifications of sides and with torsion t. Unlike torus, Klein bottle polyhex $K(p, q, t)$ is not transitive except for some degenerated cases. We shall show, however, that $K(p, q, t)$ does not depend on t. Accordingly, criteria for $K(p, q, t)$ to be k-resonant for every positive integer k will be given. Moreover, we shall show that $K(3, q, t)$ of 3-resonance are fully-benzenoid.

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

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

1. Introduction

There are precisely two closed surfaces, namely torus and Klein bottle on which a purely hexagonal tessellation can be given [1, 2]. From a graph-theoretical point of view, a toroidal polyhex (toroidal graphitoid, or torene) is a 3-regular (cubic or trivalent) bipartite graph embedded in the torus each face of which is a hexagon. Mathematical foundation on toroidal polyhexes can be found in [3–5]. As early as in 1970s Altschuler [3] showed that toroidal polyhex construction can be determined by a unique string of three integers. Detailed classifications of such hexagonal tilings (dually, triangulations) on the torus and the Klein bottle can be found in [4, 5]. Some features of toroidal polyhexes with chemical relevance were mainly discussed on the following topics: the enumerations of

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connectional isomers [6, 7], spanning trees [6, 8], Kekulé structures [6, 9–11], and chirality and symmetry [12, 13], as well as calculation for the spectrum [11, 14]. A survey is referred to [2].

To date there are few studies on Klein bottle polyhexes. Because of "self-intersection" in three dimensional space Klein bottle polyhexes might not exist in chemical world. D.J. Klein, however, proposed [2] possible schemes for the "self-avoiding" intersection. Klein bottle polyhex $K(p, q, t)$ considered here is an analogue of toroidal polyhex $H(p, q, t)$ in [13] and can be obtained from a $p\times q$-parallelogram of hexagonal lattice with usual identifications of sides and with torsion t. Klein and Zhu [11] extended their transfer-matrix enumeration of Kekulé structures from toroidal polyhexes to Klein bottles. In applying the techniques used for encoding toroidal polyhex, Kirby [15] found that a detailed formulation of rules to Klein bottle is much complicated and only got partial results. Other forms of hexagonal tessellations on Klein bottle exist [5].

In this article we first show that $K(p, q, t)$ is independent of the third parameter t, that is, all Klein bottle polyhexes $K(p, q, t)$ are equivalent for all $0 \leqslant t \leqslant p-1$ by establishing two shift operations which are hexagon-preserving isomorphisms. In this respect, it is indeed different from toroidal polyhexes. Then, as a continuation of researches on the k-resonance of planar [16–23], cylindrical [24] and toroidal polyhexes [25], we consider the k-resonance of Klein bottle polyhexes. Recall that a polyhex is *k-resonant* if for $1 \leqslant i \leqslant k$, any i disjoint hexagons are mutually resonant, i.e., they are alternating or conjugated hexagons with respect to a certain Kekulé structure. The concept of k-resonance originates from Clar's aromatic sextet theory [26] and Randić's conjugated circuit model [27–29].

For a planar polyhex (or even more generally, a plane bipartite graph) with normal or elementary property will be 1-resonant, i.e., each face is resonant. The problem whether a planar polyhex is 2-resonance still remains open. The cases for toroidal polyhex [25] and Klein bottle polyhex, however, are rather different from that of planar. Although, they are all elementary bipartite, $H(p, q, t)$ ($p, q \geq 2$) is 1-resonant except for $H(2, 2, 0)$ [25] and $K(p, q, t)$ is 1-resonant if and only if $p \geq 2$ and $q \geq 2$ but $(p, q) \neq (2, 2)$. Unlike torus, both resonant and non-resonant hexagons of $K(2, 2)$ exist simultaneously. Furthermore we obtain criteria for $K(p, q, t)$ to be k-resonant for every positive integer k. In particular, for each $k \geq 3$, $K(p, q, t)$ is k-resonant if and only if $(p, q) = (2, 3)$ or $(4, 3)$, or $p = 3$ and $q \geq 2$. Besides, all 3-resonant Klein bottle polyhexes $K(3, q, t)$ are fully-benzenoid.

2. Klein bottle polyhexes $K(p, q, t)$

Like toroidal polyhexes, a *Klein bottle polyhex* $K(p, q, t)$ is produced from a $p\times q$-parallelogram P on the hexagonal lattice L with the usual boundary identification [5, 13]: each side of P connects the centers of two hexagons, and is perpendicular to an edge-direction of L, both top and bottom sides of P intersect p vertical edges of L; while two lateral sides intersect q edges. First we identify its two lateral sides. Then rotating the top cycle t hexagons and identify the top and bottom at their corresponding points, we get a toroidal polyhex $H(p, q, t)$ [10, 13]. If in the last stage we identify top and bottom circle along their reversed corresponding points, we get a Klein bottle polyhex $K(p, q, t)$ with the torsion $t(0 \leqslant t \leqslant p-1)$. Two representations of Klein bottle polyhex $K(7, 5, 2)$ are shown in figure 1. Usually we use the left representation. It is obvious that both $H(p, q, t)$ and $K(p, q, t)$ are 3-regular bipartite graphs with pq hexagons, $2pq$ vertices and $3pq$ edges.

For convenience, we establish an affine coordinate system XOY of $K(p, q, t)$ as in [25] (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 the non-negative region. The distance between a pair of parallel edges in a hexagon is of unit length. For any positive integer n, we use $\mathbb{Z}_n$ to denote the set $\{0, 1, \ldots, n-1\}$ with arithmetic modulo n. Each hexagon is named by the coordinates (x, y) of its center, where $x \in \mathbb{Z}_p$ and $y \in \mathbb{Z}_q$. This hexagon is thus denoted by (x, y) (h_{xy} or $h_{x,y}$). For each hexagon (x, y), the top vertex is colored black and named b_{xy} (or $b_{x,y}$). The lower-right neighbor of b_{xy} is colored white and named w_{xy} (or $w_{x,y}$) and the lower-left neighbor of b_{xy} is colored white and named by $w_{x-1,y}$ (a *neighbor* of a vertex means another vertex adjacent to it).

In this notation, each w_{0y} is adjacent to b_{0y} and each w_{x0} adjacent to $b_{p-x+t+1,q-1}$. If we define a mapping f_t from $\mathbb{Z}_p$ onto itself as

$$f_t(x) = p - x + t + 1, \qquad \text{for each } x \in \mathbb{Z}_p, \tag{1}$$

then $b_{f_t(x),q-1}$ is always adjacent to $w_{x,0}$. One can easily check that

$$f_t = f_t^{-1} \text{ and } f_t(x+s) = f_t(x) - s. \tag{2}$$

Sometimes, the subscript t may be omitted when t is specified.

The y-th *layer* of $K(p, q, t)$ is the even cycle $w_{0y}b_{1y}w_{1y}b_{2y}\cdots w_{p-1,y}b_{0y}w_{0y}$, where $0 \leqslant y \leqslant q-1$. The region enclosed by the yth and $(y+1)$th layers of

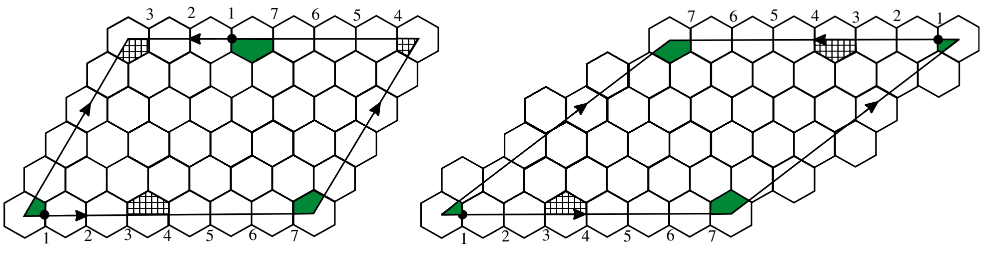

Figure 1. The Klein bottle polyhex $K(7, 5, 2)$.

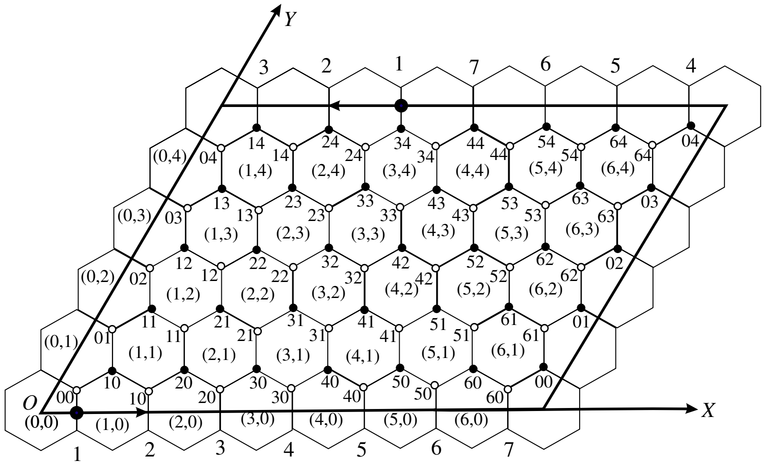

Figure 2. Labeling for the hexagons and vertices of Klein bottle polyhex $K(7, 5, 2)$.

$K(p, q, t)$ is called the *yth unit tube* (or zigzag nanotube), which is a closed hexagonal chain.

An *isomorphism* between two simple graphs G and H is a bijection $\pi : V(G) \to V(H)$ such that for $x, y \in V(G)$, x and y are adjacent in G if and only if $\pi(x)$ and $\pi(y)$ are adjacent in H.

We now establish two hexagon-preserving isomorphisms among Klein bottle polyhexes $K(p, q, t)$ for any fixed p and q as follows. The r-l shift ϕ_{rl} moves every vertex a unit horizontally backward, i.e.

$$\phi_{rl}(w_{x,y}) = w_{x-1,y} \quad \text{and } \phi_{rl}(b_{x,y}) = b_{x-1,y}, \quad \text{for every pair } (x, y) \tag{3}$$

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

$$\phi_{tb}(w_{x,y}) = w_{x,y-1}, \text{ and } \phi_{tb}(b_{x,y}) = b_{x,y-1} \text{ for } 1 \leqslant y \leqslant q - 1, \tag{4}$$

and

$$\phi_{tb}(w_{x,0}) = w_{f(x)-1,q-1} \quad \text{and } \phi_{tb}(b_{x,0}) = b_{f(x),q-1}. \tag{5}$$

Lemma 2.1. ϕ_{rl} is a hexagon-preserving isomorphism from $K(p, q, t)$ to $K(p, q, t - 2)$ for $t \geq 2$.

Proof. It is obvious that ϕ_{rl} is a bijection between $V(K(p, q, t))$ and $V(K(p, q, t - 2))$. Removing all edges $w_{x,0}b_{f_t(x),q-1}$ and $w_{x,0}b_{f_{t-2}(x),q-1}$ for x=0, 1, $\ldots, p - 1$ from $K(p, q, t)$ and $K(p, q, t - 2)$ respectively, we get two zigzag tubes. We can see that ϕ_{rl} is a hexagon-preserving isomorphism between the two tubes. So it suffices to show that ϕ_{rl} also preserves the adjacency and hexagonal faces between the $(q-1)$th and the 0th layers. For each such edge $w_{x,0}b_{f_t(x),q-1}$ of $K(p,q,t)$, $\phi_{rl}(w_{x,0})\phi_{rl}(b_{f_t(x),q-1}){=}w_{x-1,0}b_{f_t(x)-1,q-1}$ is an edge of $K(p,q,t-2)$ since $f_{t-2}(x-1){=}f_t(x)-1$ (see equation (1)). For each hexagon $h_{x,0}{=}w_{x-1,0}b_{x,0}w_{x,0}b_{f_t(x),q-1}w_{f_t(x),q-1}b_{f_t(x-1),q-1}$, it can be verified that the image of $h_{x,0}$ under the map ϕ_{rl} is

$$\phi_{rl}(h_{x,0}) = w_{x-2,0}b_{x-1,0}w_{x-1,0}b_{f_t(x)-1,q-1}w_{f_t(x)-1,q-1}b_{f_t(x),q-1},$$

which is the hexagon $h_{x-1,0}$ of $K(p,q,t-2)$, since $f_{t-2}(x-1) = f_t(x)-1$ and $f_{t-2}(x-2) = f_t(x)$. The converse can be seen analogously. □

Lemma 2.2. ϕ_{tb} is a hexagon-preserving isomorphism from $K(p,q,t)$ to $K(p,q,t-1)$, for $t \geq 1$.

Proof. It is obvious that ϕ_{tb} is a bijection between $V(K(p,q,t))$ and $V(K(p,q,t-1))$. It can be seen that ϕ_{tb} when restricted on the tube obtained from $K(p,q,t)$ by deleting the 0th layer is a hexagon-preserving isomorphism to the tube obtained from $K(p,q,t-1)$ by deleting $(q-1)$th layer. Similarly, the corresponding restricted ϕ_{tb} is also an isomorphism from 0th layer of $K(p,q,t)$ to the $(q-1)$th layer of $K(p,q,t-1)$. For any remaining vertical edges $w_{x,1}b_{x+1,0}$ and $w_{x,0}b_{f_t(x),q-1}$, $\phi_{tb}(w_{x,1})\phi_{tb}(b_{x+1,0}){=}w_{x,0}b_{f_t(x+1),q-1}$ and $\phi_{tb}(w_{x,0})\phi_{tb}(b_{f_t(x),q-1}){=}w_{f_t(x)-1,q-1}b_{f_t(x),q-2}$ are edges of $K(p,q,t-1)$, since $f_{t-1}(x){=}f_t(x)-1{=}f_t(x+1)$. For any remaining hexagons $h_{x,1}{=}w_{x-1,1}b_{x,1}w_{x,1}b_{x+1,0}w_{x,0}b_{x,0}$ and $h_{x,0}{=}w_{x1,0}b_{x,0}w_{x,0}b_{f_t(x),q-1}w_{f_t(x),q-1}b_{f_t(x-1)q-1}$ of $K(p,q,t)$, by definitions (4) and (5) we have

$$\begin{aligned}\phi_{tb}(h_{x,1}) &= w_{x-1,0}b_{x,0}w_{x,0}b_{f_t(x+1),q-1}w_{f_t(x)-1,q-1}b_{f_t(x),q-1}\\ &= w_{x-1,0}b_{x,0}w_{x,0}b_{f_{t-1}(x),q-1}w_{f_{t-1}(x),q-1}b_{f_{t-1}(x)+1,q-1}\end{aligned}$$

and

$$\begin{aligned}\phi_{tb}(h_{x,0}) &= w_{f_t(x-1)-1,q-1}b_{f_t(x),q-1}w_{f_t(x)-1,q-1}b_{f_t(x),q-2}w_{f_t(x),q-2}b_{f_t(x-1),q-2}\\ &= w_{f_{t-1}(x)+1,q-1}b_{f_{t-1}(x)+1,q-1}w_{f_{t-1}(x),q-1}b_{f_{t-1}(x)+1,q-2}w_{f_{t-1}(x)+1,q-2}\\ &\quad b_{f_{t-1}(x)+2,q-2},\end{aligned}$$

which are hexagons $h_{x,0}$ and $h_{f_{t-1}(x)+1,q-1}$ of $K(p,q,t-1)$, respectively. The converse can be proved in a similar way. □

Note that the above discussions include the degenerated cases when $q=1$ or $p=1$. If two graphs on a surface has a face-preserving isomorphism, we say that such two graphs are *equivalent*. From lemmas 2.1 and 2.2, at once we have the following important result, which says that Klein bottle polyhexes $K(p,q,t)$

defined previously rely only on (p, q), and can be abbreviated as $K(p, q)$. So for any non-negative integer t, $K(p, q, t)$ may be regarded as a *representation* of $K(p, q)$.

Theorem 2.3. All Klein bottle polyhexes $K(p, q, t)$, $t = 0, 1, \ldots, p-1$, are equivalent.

3. Concepts for resonance

In this section, we extend the concept of resonance from planar molecular graphs to any plane graphs, graphs embedded cellularly in some surfaces. We first recall some useful concepts. A *perfect matching* or 1-*factor* F (called 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 F. Furthermore, a cycle of G is called F-*alternating* or *conjugated* if its edges appear alternately in and off F. A bipartite graph is called *elementary* [30] or *normal* if it is connected and each edge is contained in a perfect matching. Both $H(p, q, t)$ and $K(p, q)$ are elementary and bipartite since they are cubic. In fact their edge-set can be decomposed into three perfect matchings so that each consists of all edges with the same edge-direction [10].

For a map M, a set of disjoint (bounded) faces of M is said to form a *resonant pattern* if their boundaries are alternating cycles with respect to a perfect matching. The faces in a resonant pattern are often referred to "*mutually resonant*". In the case each face is bounded by a cycle with even edges, equivalently, some disjoint faces form a resonant pattern if the subgraph obtained from M by deleting the vertices of the faces either has a perfect matching or is empty. Trivially, an empty set is allowed to form a resonant pattern if M has a perfect matching. In particular, a resonant pattern is a *sextet* pattern if it consists only of hexagons (cycles with six edges). So resonant patterns in hexagonal systems, toroidal and Klein bottle polyhexes are sextet patterns. So we can give a unified definition for k-resonance:

Definition 3.1. For a given positive integer k, a map M is called k-*resonant* if any i ($\leqslant k$) disjoint faces form a resonant pattern.

For example, $K(2, 2)$, the cube drawn on the Klein bottle, is not 1-resonant (figure 3 (a) and (b)). In fact, for $K(2, 2, 0)$ hexagons $(0, 0)$ and $(1, 0)$ are both resonant; whereas neither $(1, 1)$ nor $(0, 1)$ is resonant. However $H(2, 2, 1)$ is 1-resonant (figure 3 (c)). Since, $K(1, q)$ and $K(p, 1)$ contain a hexagonal face which is not bounded by a cycle. So we restrict our consideration to Klein bottle polyhexes $K(p, q, t)$ with $p \geq 2$ and $q \geq 2$.

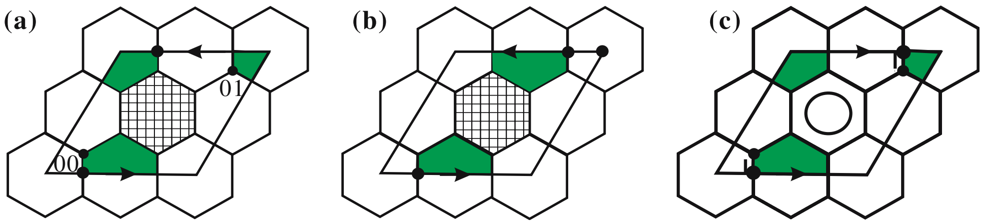

Figure 3. (a) $K(2, 2, 0)$, (b) $K(2, 2, 1)$, and (c) $H(2, 2, 1)$.

Next, we mainly give criteria for k-resonant Klein bottle polyhexes $K(p, q, t)$. We first introduce the so-called Clar cover and ideal configuration used in [25], which play a crucial role in our approach. Let $\mathcal{S}$ be a subgraph of $K(p, q, t)$ for which each component is either a hexagon or a path of length one. Then $\mathcal{S}$ is called an *ideal configuration* if $\mathcal{S}$ is alternately incident with white and black vertices along any direction of each layer; $\mathcal{S}$ is called a *Clar cover* [31] if $\mathcal{S}$ includes all vertices of $K(p, q, t)$. Similar to lemma 3.12 of Ref. [25] we have the following important result.

Lemma 3.2. Any ideal configuration $\mathcal{S}$ of a Klein bottle polyhex $K(p, q, t)$ can be extended to a Clar cover, and the hexagons in $\mathcal{S}$ are thus mutually resonant.

We now give a characterization for 1-resonant Klein bottle polyhexes as follows.

Theorem 3.3. $K(p, q)$ is 1-resonant if and only if $(p, q) \neq (2, 2)$.

Proof. As $K(2, 2)$ is not 1-resonant, it is sufficient to show that all $K(p, q)$ are 1-resonant for $(p, q) \neq (2, 2)$, i.e., every hexagon is resonant. For any hexagon $h_{m,n}$ of $K(p, q, 0)$, $0 \leqslant m \leqslant p - 1$, $0 \leqslant n \leqslant q - 1$, by applying the t-b shift

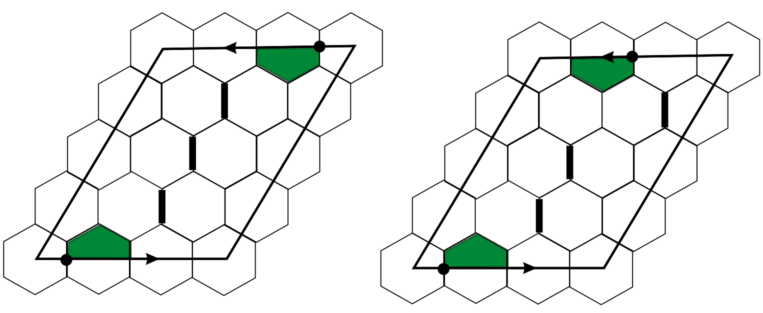

Figure 4. Illustration for the proof of theorem 3.3.

operations to $K(p,q,0)$ and $h_{m,n}$ n times we obtain $K(p,q,p-n)$ and hexagon $h_{m',0}$ for some m', respectively. By lemma 2.2, we only need to show that every hexagon $h_{m,0}$ of $K(p,q,t)$ for all $m,t \in \mathbb{Z}_p$ is resonant.

Let $h_{m,0} = w_{m-1,0}b_{m,0}w_{m,0}b_{f(m),q-1}w_{f(m),q-1}b_{f(m)+1,q-1}$. Let $\mathcal{S}$ consist of $h_{m,0}$ and the vertical edges $w_{m,1}b_{m+1,0}, w_{m,2}b_{m+1,1}, \ldots, w_{m,q-1}b_{m+1,q-2}$ (indicated by thick lines in figure 4). Suppose, $f(m) \neq m$. $\mathcal{S}$ forms an ideal configuration of $K(p,q,t)$ since it is incident with vertices $w_{m-1,0}, b_{m,0}, w_{m,0}$ and $b_{m+1,0}$ in the 0th layer; $w_{m,y}$ and $b_{m+1,y}$ in the yth layers, $1 \leqslant y \leqslant q-2$; and $b_{f(m),q-1}, w_{f(m),q-1}, b_{f(m)+1,q-1}$ and $w_{m,q-1}$ in the $(q-1)$th layer. Hence by lemma 3.2 $h_{m,0}$ is a resonant hexagon. Suppose $f(m) = m$. The last edge $w_{m,q-1}b_{m+1,q-2}$ intersects hexagon $h_{m,0}$ at vertex $w_{m,q-1}$. Replacing it with another vertical edge $w_{m+1,q-1}b_{m+2,q-2}$, then the new $\mathcal{S}$ is also an ideal configuration since $f(m) \neq m+1$ and $(m,0) \neq (m+2,q-2)$. The latter follows from the fact that $(p,q) \neq (2,2)$. □

4. 2-resonance

By applying lemma 3.2, in this section we characterize 2-resonant Klein bottle polyhexes (see Theorem 4.3).

Lemma 4.1. For $p \geq 4$, $K(p,2)$ is not 2-resonant.

Proof. We only need to consider $K(p,2,0)$. It suffices to find a pair of disjoint hexagons h and h' so that $K(p,2,0) - h - h'$ has no 1-factors.

The three neighbors of the vertex w_{10} are b_{10}, b_{20}, and $b_{f_0(1),1} = b_{01}$. They lie on $h_{01} \cup h_{21}$. Then w_{10} is an isolated vertex of $K(p,2,0) - h_{01} - h_{21}$. Hence $K(p,2,0) - h_{01} - h_{21}$ does not contain a 1-factor. □

Lemma 4.2. For $q \geq 4$, $K(2,q)$ is not 2-resonant.

Proof. For disjoint hexagons h_{11} and h_{13}, the vertex w_{02} has all neighbors b_{11}, b_{12}, and b_{02} belonging to the chosen hexagons. Hence w_{02} is an isolated vertex of $H(2,q,t) - h_{11} - h_{13}$, i.e., h_{11} and h_{13} cannot form a sextet pattern. □

Lemma 4.3. For $p \geq 3$ and $q \geq 3$, $K(p,q)$ is 2-resonant.

Proof. By theorem 3.3 $K(p,q)$ is 1-resonant. From theorem 2.3 it suffices to prove that any pair of disjoint hexagons of $K(p,q,0)$ are mutually resonant. Analogous to [25], by applying repeatedly the shifts ϕ_{rl} and ϕ_{tb} if necessary, the chosen hexagons of $K(p,q,0)$ can be transformed equivalently into (x_1,y_1) and

(x_2, y_2) ($x_i \in \mathbb{Z}_p$ and $y_i \in \mathbb{Z}_q$, $i = 1, 2$) of $K(p, q, t)$ for some $t \in \mathbb{Z}_p$ satisfying the following two conditions:

(i) $1 = y_1 \leqslant y_2 \leqslant \frac{q}{2} + 1$ ($\leqslant q - 1$), and
(ii) $1 = \min(x_1, x_2) \leqslant \max(x_1, x_2) \leqslant \frac{p}{2} + 1$ ($\leqslant p - 1$).

So we need to show that such two hexagons (x_1, y_1) and (x_2, y_2) are mutually resonant for any t. To this end, we will apply mainly the technique appeared in lemma 3.2: to construct an ideal configuration containing such two hexagons by choosing a series of additional edges. We consider the following four cases.

Case 1. $x_1 = y_1 = x_2 = 1$ and $3 \leqslant y_2 \leqslant \frac{q}{2}+1$. We choose vertical edges $w_{2,i}b_{3,i-1}$ ($i = 2, \ldots, y_2 - 1, y_2 + 1, \ldots, q - 1$), and the edge $w_{2,0}b_{f(2),q-1}$ (indicated by thick lines, see figure 5 (left)). When $y_2 = q - 1$ and $f(2) = 1$, the edge $w_{2,0}b_{f(2),q-1}$ is replaced by $w_{0,0}b_{f(0),q-1}$ and the others are unchanged (see figure 5 (right)). For this case, since $f(0) = 3 \not\equiv 1 \pmod{p}$, the chosen hexagons and vertical edges form an ideal configuration. Otherwise the previous chosen edges together with the chosen hexagons form an ideal configuration.

Case 2. $1 = x_1 < x_2 \leqslant \frac{p}{2} + 1$ and $1 = y_1 < y_2 \leqslant \frac{q}{2} + 1$. We choose a series of vertical edges $w_{x_2-1,i}b_{x_2,i-1}$ ($i = 2, \ldots, y_2 - 1$), $w_{x_2,j}b_{x_2+1,j-1}$ ($j = y_2 + 1, \ldots, q - 1$) and $w_{00}b_{f(0),q-1}$, which are indicated by thick lines in figure 6 (left). When $y_2 = q - 1$ and $f(0) = x_2$, the edge $w_{00}b_{f(0),q-1}$ is replaced by $w_{2,0}b_{f(2),q-1}$ and we obtain an ideal configuration since $f(2) = f(0) - 2 = x_2 - 2 \neq x_2$. Otherwise the previous chosen edges together with hexagons (x_1, y_1) and (x_2, y_2) form an ideal configuration.

Case 3. $1 = x_2 < x_1 \leqslant \frac{p}{2} + 1$ and $1 = y_1 < y_2 \leqslant \frac{q}{2} + 1$. We choose vertical edges $w_{x_1,i}b_{x_1+1,i-1}$ ($i = 2, \ldots, y_2 - 1, y_2 + 1, \ldots, q - 1$), and $w_{00}b_{f(0),q-1}$ (indicated by thick lines, see figure 6 (right)). When $y_2 = q - 1$ and $f(0) = 1$,

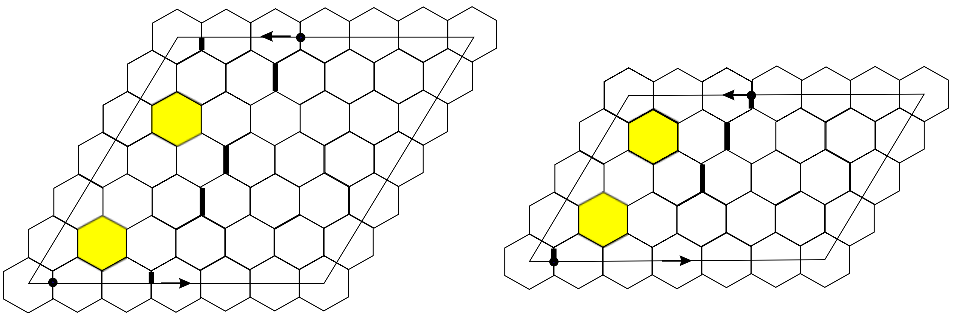

Figure 5. Illustration for case 1 in the proof of lemma 4.3.

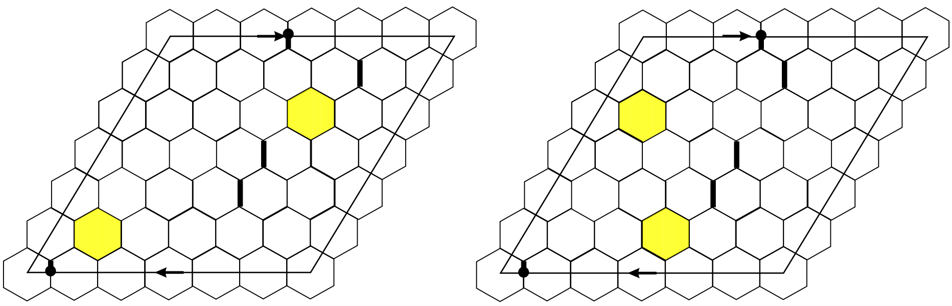

Figure 6. Illustration for cases 2 and 3 in the proof of lemma 4.3.

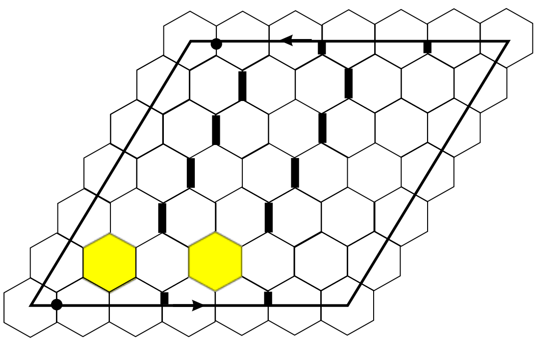

Figure 7. Illustration for case 4 in the proof of lemma 4.3.

the chosen edge $w_{00}b_{f(0),q-1}$ is replaced by $w_{10}b_{f(1),q-1}$ and we obtain an ideal configuration since $f(1) \neq 1$. Otherwise, the previous chosen edges together with hexagons (x_1, y_1) and (x_2, y_2) form an ideal configuration.

Case 4. $x_1 = y_1 = y_2 = 1$ and $3 \leqslant x_2 \leqslant \frac{p}{2} + 1$. Obviously, $p \geq 4$ and $q \geq 3$. We choose vertical edges $w_{1,i+1}b_{2,i}$ and $w_{x_2,i+1}b_{x_2+1,i}$ $(1 \leqslant i \leqslant q-2)$ (indicated by thick lines, see figure 7). We also choose additional vertical edges $w_{2,0}b_{f(2),q-1}$ and $w_{x_2+1,0}b_{f(x_2+1),q-1}$.
For convenience, we introduce further notations as follows. For $a, b \in \mathbb{Z}_p$ and $a < b$ (viewing as integers), let $[a, b] = \{a, a+1, a+2, \ldots, b\}$ denote the interval between a and b in an increasing way and let $[b, a] = \{b+1, b+2, \ldots, a\} = \mathbb{Z}_p \backslash \{a+1, \ldots, b-1\}$. Their lengths are $b-a$ and $p+a-b+1$, respectively.
Then $[f(x_2+1), f(2)] = [p+t-x_2, p+t-1]$ has the same length as $[1, x_2]$. If $f(2) \in [2, x_2]$, then $f(x_2+1) \in [3-x_2, 1] \subseteq [x_2+1, 1]$, since $[x_2, 1]$ is not shorter than $[1, x_2]$. Hence, the chosen edges are in turn incident with vertices $w_{1,q-1}, b_{f(2),q-1}, w_{x_2,q-1}$ and $b_{f(x_2+1),q-1}$ in the $(q-1)$-layer's direction. If $f(2) \in [x_2+1, p]$, then replaced the chosen edge $w_{x_2+1,0}b_{f(x_2+1),q-1}$ by $w_{f(2),0}b_{2,q-1}$ and the others are unchanged.

Since $f(f(2)) = 2$ from equation (2), the chosen edges are in turn incident with vertices $b_{f(2),q-1}, w_{1,q-1}, b_{2,q-1}$ and $w_{x_2,q-1}$ in $(q-1)$-layer's direction. Otherwise, $f(2) = 1$. Then replace the chosen edge $w_{x_2+1,0}b_{f(x_2+1),q-1}$ by $w_{0,0}b_{3,q-1}$. Since $f(0) = 3$, the chosen edges are in turn incident with vertices $b_{1,q-1}, w_{1,q-1}, b_{3,q-1}$ and $w_{x_2,q-1}$ in $(q-1)$-layer's direction. It can be seen for each subcase as mentioned above the chosen vertical edges together with given hexagons (x_1, y_1) and (x_2, y_2) have similar facts for other layers and form an ideal configuration. □

Since $K(2,3)$ and $K(3,2)$ do not contain two disjoint hexagons, automatically they are 2-resonant. Combining this fact with lemmas 4.1–4.3, we arrive at the following criterion for the 2-resonance of Klein bottle polyhexes.

Theorem 4.4. $K(p,q,t)$ is 2-resonant if and only if $\min\{p,q\} \geq 3$, or $(p,q) = (2,3)$ or $(3,2)$.

5. k-resonance ($k \geq 3$)

We are in the position to discuss general k-resonance ($k \geq 3$) in Klein bottle polyhexes. Like benzenoid systems, coronoid systems, and open-ended carbon nanotubes, our results show that any 3-resonant Klein bottle polyhexes $K(p,q)$ are also k-resonant for any k.

Since $K(2,3)$ and $K(3,2)$ are 2-resonant and have no three disjoint hexagons, they are automatically k-resonant for any integer $k \geq 3$. Other possible 3-resonant Klein bottle polyhexes must be among $K(p,q,t)$ for $p \geq 3$ and $q \geq 3$ by theorem 4.4. Like toroidal polyhexes, we first have the following lemma.

Lemma 5.1. For $p, q \geq 4$, $K(p,q)$ is not 3-resonant.

Proof. All neighbors of b_{21}, namely w_{11}, w_{12}, and w_{21}, are contained in three disjoint hexagons h_{11}, h_{13}, and h_{31} (see figure 2), 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. □

Lemma 5.2. For $p \geq 4$, $K(p,3)$ is 3-resonant if and only if $p = 4$.

Proof. For $p \geq 5$, we only need to consider $K(p,3,1)$. All neighbors of the vertex w_{00} are $b_{10}, b_{f(0),2} = b_{22}$ and b_{00}. They lie on three disjoint hexagons $h_{1,1}, h_{2,2}$, and $h_{p-1,1}$, respectively. Hence $h_{1,1}, h_{2,2}$, and $h_{p-1,1}$ are not mutually resonant. Hence, for $p \geq 5$, $K(p,3,t)$ is not 3-resonant.

We now show that $K(4,3)$ is 3-resonant. For any three disjoint hexagons of $K(4,3)$, it follows that different hexagon contains in different unit tube. Hence the chosen hexagons are incident alternately white and black vertices along each layer. So they are mutually resonant by Lemma 3.2. □

Lemma 5.3. For $q \geq 3$, $K(3,q)$ is k-resonant for every positive integer k.

Proof. By lemma 4.3 or theorem 4.4, $K(3,q)$ is 2-resonant. So it suffices to show that for each integer $k \geq 3$, any k disjoint hexagons $(x_i, y_i), x_i \in \mathbb{Z}_3$ and $y_i \in \mathbb{Z}_q, i = 1, 2, \ldots, k$, of $K(3,q,t)$ are mutually resonant.

Since each unit tube contains at most one of these hexagons, $k \leqslant q$ and we may assume that $0 \leqslant y_1 < y_2 < \cdots < y_k \leqslant q-1$ (see figure 8). To that end, by lemma 3.2 we construct an ideal configuration containing these hexagons by choosing a sequence of vertical edges.

For each $1 \leqslant i \leqslant k-1$, we consider two consecutive hexagons (x_i, y_i) and (x_{i+1}, y_{i+1}), as well as the tube T between y_ith and y_{i+1}th layers. If $y_{i+1} = y_i+1$, then these two hexagons occupy all vertices of the i-layer. Otherwise, $y_{i+1} \geq y_i + 2$. We choose a sequence of vertical edges $w_{x_i,j+1}b_{x_i+1,j}$ $(j = y_i, y_i+1, \ldots, y_{i+1}-2)$ if $x_i \neq x_{i+1}$; and $w_{x_i+1,j+1}b_{x_i+2,j}$ $(j = y_i, y_i+1, \ldots, y_{i+1}-2)$, if $x_i = x_{i+1}$. Then the chosen edges together with hexagons (x_i, y_i) and (x_{i+1}, y_{i+1}) are pairwise disjoint. Let $\mathcal{S}_0$ be the set of these edges and hexagons. Then $\mathcal{S}_0$ is alternatively incident with white and black vertices along any direction of each layer in T.

By similar argument, we consider the remaining cases: (x_1, y_1) and (x_k, y_k) and the tube from the y_kth, (y_k+1)th to (y_1-1)th layers. If $y_1 = 0$, then the hexagon (x_1, y_1) contains a white vertex $w_{f(x_1),q-1}$. We choose a sequence of vertical edges $w_{x_k,j+1}b_{x_k+1,j}$ $(j = y_k, y_k+1, \ldots, q-2)$, if $x_k \neq f(x_1)$; and

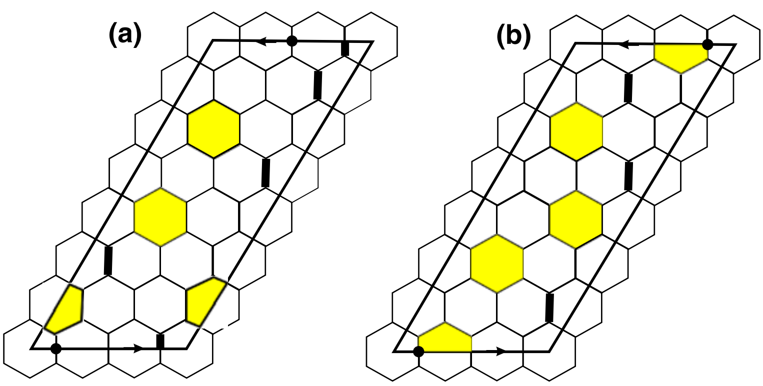

Figure 8. Illustration to the proof of lemma 5.3, (a)$K(3,7,1)$ with hexagons h_{01}, h_{13}, and h_{15}, (b)$K(3,7,2)$ with hexagons h_{10}, h_{12}, h_{23}, and h_{15}.

$w_{x_k+1,j+1}b_{x_k+2,j}$ ($j = y_k, y_k + 1, \ldots, q - 2$), otherwise. If $y_1 \geq 1$, then the hexagon (x_1, y_1) contains a white vertex w_{x_1,y_1-1}. We choose a sequence of vertical edges $w_{x_k,j+1}b_{x_k+1,j}$ ($j = y_k, y_k + 1, \ldots, q - 2$), $w_{f(x_k+1),0}b_{x_k+1,q-1}$, and $w_{f(x_k+1),j+1}b_{f(x_k),j}$ ($j = 0, 1, \ldots, y_1 - 2$). If $f(x_k + 1) = x_1$, the last edge $w_{x_1,y_1-1}b_{f(x_k),y_1-2}$ is replaced by $w_{x_1+1,y_1-1}b_{x_1+2,y_1-2}$.

For all cases, the previous chosen edges together with the given k hexagons form an ideal configuration. Hence such k hexagons are mutually resonant. □

Combining lemmas 5.1–5.3, we obtain the following criterion for the k-resonance of toroidal polyhexes for any $k \geq 3$.

Theorem 5.4. A Klein bottle polyhex $K(p, q)$ is k-resonant for any integer $k \geq 3$ if and only if either $q = 3$ and $2 \leq p \leq 4$, or $p = 3$ and $q \geq 2$.

For a given polyhex G, a sextet pattern of G is 'proper' *Clar formula* [17] if it contains the maximum number of hexagons; this maximum number is called the *Clar number* of G; G is said to be *fully-benzenoid* [26] if it has a sextet pattern including all vertices.

Theorem 5.5. All Klein bottle polyhex $K(3, q)$ with $q \geq 2$ are fully-benzenoid, and the Clar number of $K(3, q)$ is equal to q.

Proof. It suffices to construct a sextet pattern of $K(3, q, t)$ for some t ($0 \leq t \leq 2$) containing exactly one hexagon on each unit tube. Choose q hexagons, (i, i) $0 \leq i \leq q - 1$, the first coordinate taken in module 3 (see figure 9). Choose the value t such that $t \equiv q - 1 \pmod 3$. We first show that any two consecutive chosen hexagons are disjoint. For any $0 \leqslant i \leqslant q - 2$, hexagons (i, i) and $(i + 1, i + 1)$ contain paths $w_{i-1,i}b_{i,i}w_{i,i}$ and $b_{i+1,i}w_{i+1,i}b_{i+2,i}$ in the

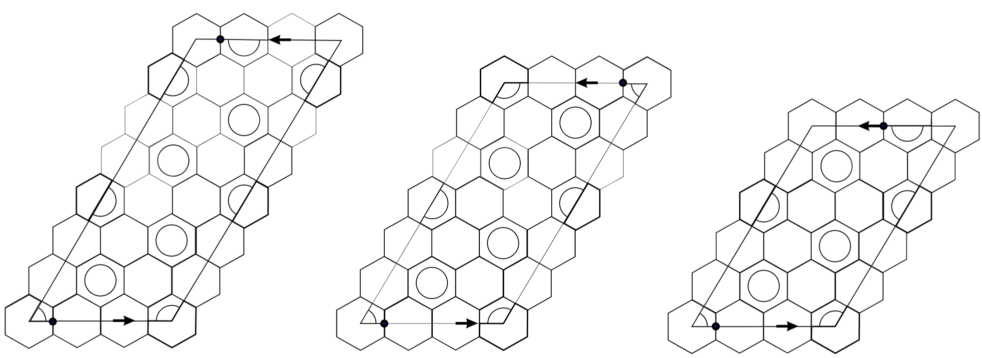

Figure 9. Three types of Clar formulas for $K(3, q)$: examples for $K(3, 7, 0)$, $K(3, 6, 2)$ and $K(3, 5, 1)$.

ith layer, respectively. Obviously they are disjoint and each vertex of the ith layer are contained in one of the paths. It remains to show that hexagons $(0, 0)$ and $(q-1, q-1)$ possess the same property on the $(q-1)$th layer. Hexagon $(q-1, q-1)$ contains the path $w_{q-2,q-1}b_{q-1,q-1}w_{q-1,q-1}$ in the $(q-1)$th layer; however, hexagon $(0, 0)$ contains the path $b_{f(0),q-1}w_{f(0),q-1}b_{f(2),q-1}$ in the $(q-1)$th layer. Since $q-1 \equiv t \pmod 3$, we have that $w_{q-2,q-1}b_{q-1,q-1}w_{q-1,q-1} = w_{t-1,q-1}b_{t,q-1}w_{t,q-1}$ and $b_{f(0),q-1}w_{f(0),q-1}b_{f(2),q-1} = b_{t+1,q-1}w_{t+1,q-1}b_{t-1,q-1}$. Hence hexagons $(0, 0)$ and $(q-1, q-1)$ are also disjoint. So the chosen hexagons $(0, 0)$, $(1, 1)$, ..., $(q-1, q-1)$ form a maximum sextet pattern containing all vertices of $K(3, q, t)$. □

Since neither $K(4, 3)$ nor $K(2, 3)$ are fully-benzenoid, the theorem shows that 3-resonant Klein bottle polyhexes $H(p, q)$ is fully-benzenoid if and only if $p = 3$ and $q \geq 2$.

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