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ORIGINAL PAPER

The number of Kekulé structures of polyominos on the torus

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Abstract Let G be a (molecule) graph. A perfect matching, or Kekulé structure of G is a set of independent edges covering every vertex exactly once. Enumeration of Kekulé structures of a (molecule) graph is interest in chemistry, physics and mathematics. In this paper, we focus on some polyominos on the torus and obtain the explicit expressions on the number of the Kekulé structures of them.

Keywords Kekulé structure · Polyomino · Torus · Pfaffian orientation

1 Introduction

A general problem of interest in chemistry, physics and mathematics is the enumeration of perfect matchings, on lattices and (molecule) graphs. A *perfect matching* of a graph is a set of independent edges covering every vertex exactly once, which is called *Kekulé structure* in organic chemistry and *closed-packed dimer* in statistical physics. The number of perfect matchings of a graph G is denoted by $\Phi(G)$. In organic chemistry, there are strong connections between the number of the Kekulé structures and chemical properties for many molecules such as benzenoid hydrocarbons. For instance, those edges which are present in comparatively few of the Kekulé structures of a (molecule) graph turn out to correspond to the bonds that are least stable, and the more Kekulé structures a (molecule) graph possesses the more stable

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is the corresponding benzenoid molecule [24]. Additionally, the number of Kekulé structures is an important topological index which had been applied for estimation of the resonant energy and total π-electron energy [3,8], calculation of pauling bond order [22] and Clar aromatic sextet [4].

A *polyomino* [1], also called quadrilateral lattice or chessboards [2] or square-cell configurations or lattice animals [9,10,29], is a finite 2-connected geometric graph in which every interior face is bounded by a regular square of side length 1 (i.e. called a cell). Historically, polyominos have attracted many mathematicians' and chemists' considerable attentions, for many interesting combinatorial subjects are yielded from them, such as domination problem [2,6] and rook polyominal [19], etc.. Berge et al. [1] studied the generalized covering problem for polyominos by introducing hypergraphs. Zhang [32] gave the necessary and sufficient conditions to have a Kekulé structure. Wei and Ke [28] and Liu and Chen [13] gave two different bounds on the number of elementary components of essentially disconnected polyominos.

The problems involving enumeration of Kekulé structures of a graph were firstly examined by chemists and physicists in the 1930s [3,16], for two different and unrelated purposes: the study of aromatic hydrocarbons in molecular chemistry and the attempt to create a theory of the liquid state in statistical physics. The first exact solutions to the problem of enumeration of Kekulé structures were due to Temperley and Fisher [27], Kasteleyn [12] and Fisher [5] in 1961. They gave formulas of Kekulé structures for a finite polyomino of size $m \times n$ with free boundary condition by different methods, where m and n are arbitrary positive integers. John et al. [11] and Sachs [23] also considered enumeration of Kekulé structures of them, respectively. It is well known that the boundary conditions play a crucial role in the enumeration of Kekulé structures of polyomino of size $m \times n$. Later, McCoy and Wu [20] and Lu and Wu [17,18] extended the enumeration of Kekulé structures for a polyomino of size $m \times n$ to cylindrical boundary condition, the Möbius strip and the Klein bottle, respectively. Following this, Lu et al. [15] presented the explicit expressions for the number of Kekulé structures of other four kinds of polyominos on a Klein bottle.

Since there are more than one embedded modes of polyominos on a Klein bottle or on a torus, Thomassen [25] characterized six embedding modes on a Klein bottle. Lu et al. [15] proved that those embedding modes are equivalent to two embedding modes denoted by $Q_{m,n,a}$ and $Q_{m,n,b}$. The number of Kekulé structures of $Q_{m,n,a}$ has been exactly solved by Lu and Wu [17,18]. Lu et al. [15] exactly solved the number of Kekulé structures of $Q_{m,n,b}$. Meanwhile, Thomassen also characterized that there are exact two embedded modes on a torus denoted by $Q_{m,n,r}$ and $Q_{k,l}$ in [25]. A *quadrilateral cylinder* of length m and breadth n is the Cartesian products of an m-cycle (with m vertices) and an n-path (with n vertices). Let $x_1, x_2, \ldots, x_m$ and $y_1, y_2, \ldots, y_m$ denote the vertices of the two cycles on the boundary of the quadrilateral cylinder, respectively, where x_i corresponds to y_i, $i = 1, 2, \ldots, m$ (refer to Fig. 1a). The graphs $Q_{m,n,r}$, $0 \leq r \leq \lfloor m/2 \rfloor$ and $n > 0$, are obtained from a quadrilateral cylinder of length m and breadth n by adding all edges $x_i y_{i+r}$, where $i = 1, 2, \ldots, m$ and $i + r$ is modulo m. Clearly, the cylinder shown in Fig. 1a is a plane spanning subgraph of $Q_{m,n,r}$, where a spanning subgraph means a subgraph with all vertices. The graphs $Q_{k,l}$, $2 < l \leq k/2$, are obtained from a k-cycle $x_1 x_2 \ldots x_k x_1$ by adding all edges

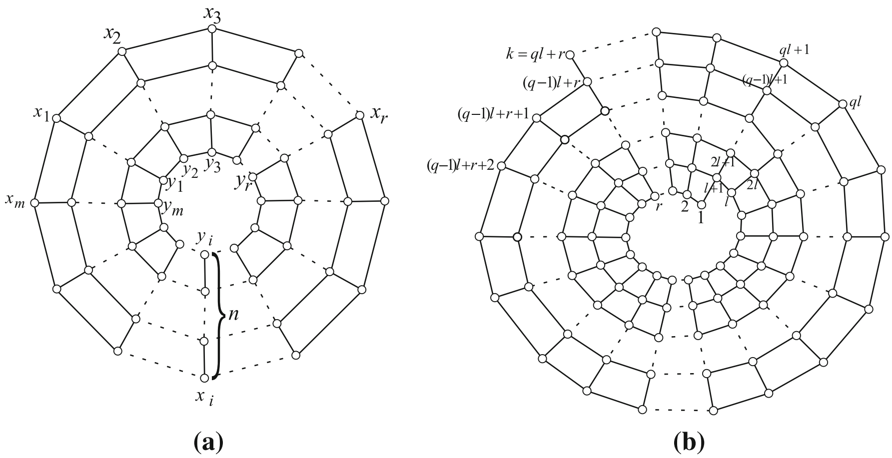


Fig. 1 Plane spanning subgraphs of $Q_{m,n,r}$ and $Q_{k,l}$

Table 1 Polyominos on a torus in different embedded forms with 22 vertices and their corresponding numbers of Kekulé structures

Q	$Q_{11,2,0}$	$Q_{11,2,1}$	$Q_{11,2,2}$	$Q_{11,2,3}$	$Q_{11,2,4}$	$Q_{11,2,5}$	$Q_{22,8}$
Φ	16,328	398	2,048	2,048	1,058	838	794

$x_i x_{i+l}$, where $i = 1, 2, \ldots, k$ and $i + l$ is modulo k. A plane spanning subgraph of $Q_{k,l}$ is shown in Fig. 1b. Clearly, both $Q_{m,n,r}$ and $Q_{k,l}$ have a natural embedding on a torus.

Table 1 shows a polyomino with 22 vertices embedded on a torus by different modes and their corresponding numbers of Kekulé structures. From Table 1, we see that, for the polyominos on a torus with the same number of vertices, they may have the different number of Kekulé structures if embedded in different modes.

Kasteleyn [12] had discussed the number of Kekulé structures of $Q_{m,n,0}$ and deduced an explicit expression. Lu, Zhang and Lin [14] generalized the results of Kasteleyn. In this paper, we consider the problem of enumerating Kekulé structures of $Q_{k,l}$. We prove that $Q_{k,l}$ is Pfaffian if l is even. Then we give some Pfaffian orientations on $Q_{k,l}$ and the explicit formulas of Kekulé structures of $Q_{k,l}$ are obtained by enumerating Pfaffians.

2 Pfaffian orientation

Given an undirected graph $G = (V(G), E(G))$ with vertex set $V(G) = \{1, 2, \ldots, 2p\}$, we allow each edge $\{i, j\}$ to have a weight w_{ij}. To unweighted graphs, we define the weight to be 1 for all edges. Let $\overrightarrow{G}$ be an arbitrary orientation of G. Denote the arc of $\overrightarrow{G}$ by (i, j) if the direction of it is from the vertex i to the vertex j. The *skew adjacency matrix* of $\overrightarrow{G}$, denoted by $A(\overrightarrow{G})$, is defined as

$$A(\overrightarrow{G}) = (a_{ij})_{2p\times 2p},$$

where

$$a_{ij} = \begin{cases} w_{ij}, & \text{if } (i,j) \text{ is an arc of } \overrightarrow{G}; \\ -w_{ij}, & \text{if } (j,i) \text{ is an arc of } \overrightarrow{G}; \\ 0, & \text{otherwise.} \end{cases}$$

Let $\mathbf{M} = \{\{i_1, i_1^{'}\}, \ldots, \{i_p, i_p^{'}\}\}$ be a perfect matching, or Kekulé structure. The signed weight of $\mathbf{M}$ is defined as

$$w_{\mathbf{M}} = \operatorname{sgn}\begin{pmatrix} 1 & 2 & \cdots & 2p-1 & 2p \\ i_1 & i_1^{'} & \cdots & i_p & i_p^{'} \end{pmatrix} \cdot a_{i_1 i_1^{'}} \cdots a_{i_p i_p^{'}},$$

where

$$\operatorname{sgn}\begin{pmatrix} 1 & 2 & \cdots & 2p-1 & 2p \\ i_1 & i_1^{'} & \cdots & i_p & i_p^{'} \end{pmatrix} = \begin{cases} 1, & \text{if the permutation is even;} \\ -1, & \text{if the permutation is odd.} \end{cases}$$

The Pfaffian of the matrix A is defined as

$$\mathrm{Pf}A = \sum_{\mathbf{M}} w_{\mathbf{M}}.$$

Muir [21] gave a relation between the determinant of A and the Pfaffian of A as follows.

Theorem 2.1 ([21]) *Let $A = (a_{ij})_{2p\times 2p}$ be a skew symmetric matrix of the order of $2p$. Then the determinant of A, $\det(A) = (\mathrm{Pf}A)^2$.*

We call $w_{\mathbf{M}}$ the *signed weight* of the perfect matching $\mathbf{M}$ and define *the sign of the perfect matching* $\mathbf{M}$ to be the sign of $w_{\mathbf{M}}$. If the signs of all perfect matchings of G are the same, we say that the orientation $\overrightarrow{G}$ is a *Pfaffian orientation* of G. A graph is *Pfaffian* if it has a Pfaffian orientation. The significance of Pfaffian orientations stems from the fact that if a graph G has one, then the number of the perfect matchings of G (as well as other related problems) can be computed in polynomial time and we have

Theorem 2.2 ([16]) *If a graph G is Pfaffian and $\overrightarrow{G}$ is a Pfaffian orientation of G, then the number of perfect matchings of G,*

$$\Phi(G) = |PfA(\overrightarrow{G})| = \sqrt{\det(A(\overrightarrow{G}))}.$$

Pfaffian orientations for planar graphs [12]: every planar graph G is Pfaffian and an orientation of a plane graph G such that its each face is clockwise odd, i. e. an odd number of edges pointing along its boundary when traversed clockwise, is a Pfaffian orientation.

Kasteleyn [12] also stated that perfect matchings in a graph embedded on a surface of genus g could be enumerated as a linear combination of 4^g Pfaffians of modified adjacency matrices of the graph, which was proved by Galllucio and Loebl [7], and Tesler [26], independently.

The number of perfect matchings of a given Pfaffian graph is easily obtained in a mathematical sense by Theorem 2.2 and Kasteleyn's methods, but it is not efficient for computation since not all of the determinants of adjacency matrices of a Pfaffian graph G has an explicit expression. It is therefore reasonable to find a Pfaffian orientation in a plane model of $Q_{k,l}$ such that we can obtain the explicit expressions of the number of perfect matchings of G. The Pfaffian method was frequently used to enumerate perfect matchings of the graphs. Some related results can be found in [14,30,31] and in the references cited therein.

3 Plane model and crossing orientations on $Q_{k,l}$

Suppose that P is a 4-polygon with four sides p_1, p_2, p'_1, p'_2 and G is a graph embedded on a torus. *A plane model* of the graph G is a drawing such that if the edges of G can be separated into three parts E_0, E_1 and E_2 and the subgraph induced by the edges of E_0 is a spanning plane graph, which wholly contained inside the polygon P, and the edges in E_j $(j = 1, 2)$ going through the sides p_j and p'_j of P do not cross.

Suppose that $1, 2, \ldots, k$ are k vertices of $Q_{k,l}$ and $k = ql + r$, $0 \leq r < l$. For each vertex i of $Q_{k,l}$, there are exactly four vertices $i-1$, $i+1$, $i-l$ and $i+l$ which are adjacent to it, where $i-1$, $i+1$, $i-l$ and $i+l$ are modulo k. Let $E(Q_{k,l})$ be the edge set of $Q_{k.l}$. Referring to Fig. 2a, we separate the edges of $Q_{k,l}$ into three parts E_0, E_1 and E_2 such that E_2 is the set of those edges, one end in $\{1, 2, \ldots, l\}$ and the other end in $\{(q-1)l + r + 1, (q-1)l + r + 2, \ldots, k\}$; E_1 is the set of those edges

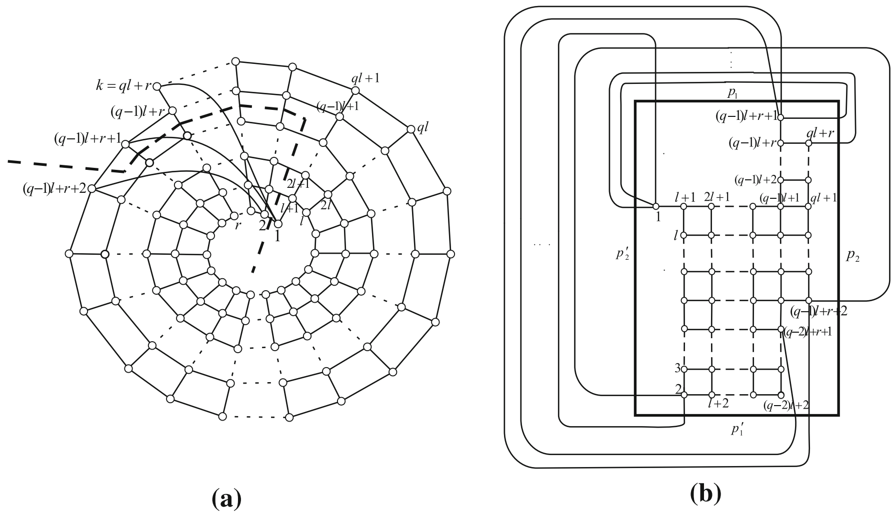


Fig. 2 $Q_{k,l}$ on a torus and its plane model

crossing the curve, drawn in heavy broken lines, crossing some edges but no vertices and $E_0 = E(Q_{k,l})\backslash(E_1 \cup E_2)$. That is

$$\begin{aligned}
E_0 = \{&\{(t-1)l+h, tl+h\} \mid t = 1, 2, \ldots, q-2; h = 2, 3, \ldots, r+1\} \\
&\cup\{\{(t-1)l+h, tl+h\} \mid t = 1, 2, \ldots, q; h = 1, r+2, r+3, \ldots, l\} \\
&\cup\{\{(q-1)l+h, ql+h\} \mid h = 2, 3, \ldots, r\} \\
&\cup\{\{(t-1)l+h, tl+h+1\} \mid t = 1, 2, \ldots, q-1; h = 2, 3, \ldots, l\} \\
&\cup\{\{(q-1)l+h, (q-1)l+h+1\} \mid h = 1, \ldots, r, r+2, r+3, \ldots, r+l-1\}; \\
E_1 = \{&\{(t-1)l+1, (t-1)l+2\} \mid t = 1, 2, \ldots, q-1\} \\
&\cup\{\{(q-2)l+h, (q-1)l+h\} \mid h = 2, 3, \ldots, r+1\} \\
&\cup\{\{(q-1)l+r+1, (q-1)l+r+2\}\}; \\
E_2 = \{&\{h, (q-1)l+r+h\} \mid h = 1, 2, \ldots, l\} \cup \{\{1, ql+r\}\}.
\end{aligned}$$

Now, we give a plane model of a polyomino $Q_{k,l}$ on a torus such that the subgraph induced by the edges of E_0 is a spanning plane graph, which wholly contained inside the polygon P, and the edges in E_j $(j = 1, 2)$ going through sides p_j and p'_j of P do not cross. The plane model of $Q_{k,l}$ is shown in Fig. 2b. Clearly, each edge in E_1 crosses each edge in E_2 once.

The crossing orientation in a plane model [26]: an orientation of a graph on a torus in a plane model is the crossing orientation if the edges in E_0 are oriented such that all faces in the 4-polygon are oriented clockwise odd, and each edge e in $E_1 \cup E_2$, ignoring all other edges in $E_1 \cup E_2$, is orientated such that the face formed by e and certain edges in E_0, is clockwise odd.

Tesler [26] characterized a relation of signs among perfect matchings on a crossing orientation.

Theorem 3.1 ([26]) *(a) A graph may be oriented so that every perfect matching* $\mathbf{M}$ *has sign*

$$\omega_{\mathbf{M}} = \omega_0(-1)^{\kappa(\mathbf{M})},$$

where $\omega_0 = \pm 1$ *is constant that may be interpreted as the sign of a perfect matching with no crossing edges when such exists, and* $\kappa(\mathbf{M})$ *is the number of times edges in* $\mathbf{M}$ *cross.*

(b) An orientation of a graph satisfies (a) if, and only if, it is a crossing orientation.

A crossing orientation of $Q_{k,l}$ for $k \equiv 2 \pmod 4$ and l is even is indicated in Fig. 3. Figure 3a gives the orientations of the edges $E_0 \cup E_1$ and Fig. 3b gives the orientations of the edges $E_0 \cup E_2$.

Let $\overrightarrow{G}_{k,l}$ be the crossing orientation of $Q_{k,l}$ in the plane model above. In order to prove that $\overrightarrow{G}_{k,l}$ is a Pfaffian orientation, we distinguish the Kekulé structures of $Q_{k.l}$ into four classes. The Kekulé structures belonging to class 1 are those that have odd number of edges of E_1 and odd number of edges of E_2. The Kekulé structures in class 2 have odd number of edges of E_1 and even number of edges of E_2. The Kekulé structures in class 3 have even number of edges of E_1 and odd number of edges of

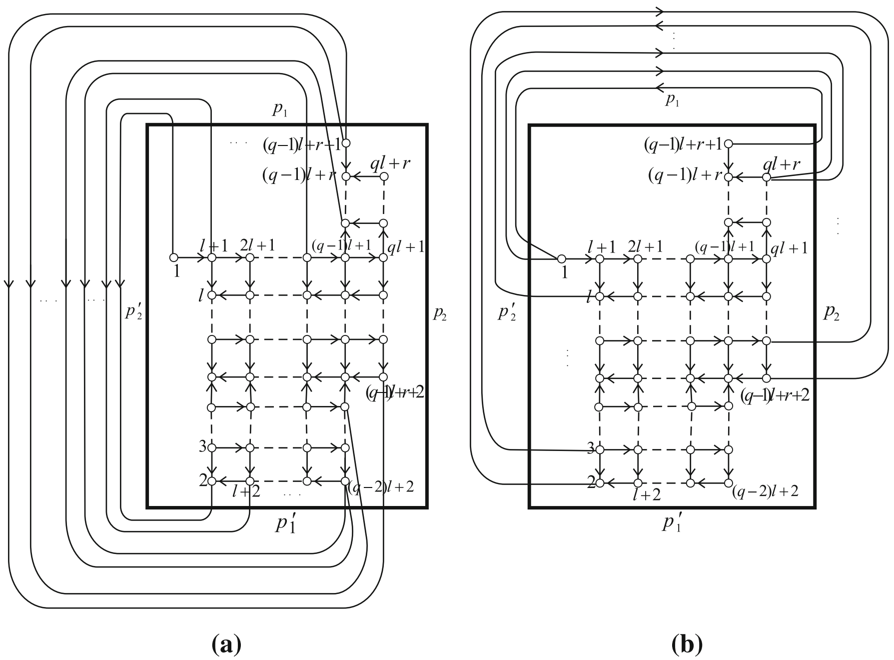


Fig. 3 A crossing orientation of $Q_{k,l}$, where l is even and $k \equiv 2 \pmod 4$

E_2 and the ones have even number of edges of E_1 and even number of edges of E_2 in class 4.

Theorem 3.2 *If l is even, then $\overrightarrow{G}_{k,l}$ is a Pfaffian orientation.*

Proof It is enough to prove that all Kekulé structures in the crossing orientation above have the same sign.

Denoted by $\mathcal{M}$ the set of all Kekulé structures of class 1 in $Q_{k,l}$. By Theorem 3.1, the sign of any Kekulé structure in $\mathcal{M}$ is different from all the other Kekulé structures of $Q_{k,l}$ related to $\overrightarrow{Q}_{k,l}$ for $\kappa(\mathbf{M})$ ($\mathbf{M} \in \mathcal{M}$) is odd. Following we show that $\mathcal{M}$ is empty. If it is true, then all the Kekulé structures have the same sign under $\overrightarrow{Q}_{k,l}$, so $\overrightarrow{Q}_{k,l}$ is a Pfaffian orientation.

Note that the plane spanning subgraph consisting of all the edges of E_0, denoted by $H(X, Y)$, is a bipartite graph. Since l is even, the two end vertices of any edge of E_1 are in the same color class of $H(X, Y)$. According to the parity of q, we have the following discussions. If q is even, then $|X| = |Y|$. After removing the vertices incident to the edges of E_1 in $\mathbf{M}$ ($\mathbf{M} \in \mathcal{M}$), the left edges of E_0 and E_2 constitute of a bipartite graph H_2 in $\mathbf{M}$. If q is odd, then $\||X| - |Y|\| = 2$. After removing the vertices incident to the edges of E_1 and E_2 in $\mathbf{M}$ ($\mathbf{M} \in \mathcal{M}$), the left edges of E_0 constitute of a bipartite graph H_2 in $\mathbf{M}$. Then the number of vertices in the two color classes of the bipartite graphs H_1 or H_2 in $\mathbf{M}$ is different, contradicting the fact that $\mathbf{M}$ is a Kekulé structure.

Thus $\mathcal{M}$ is empty, and the proof is completed. □

4 Enumeration of Kekulé structures of $Q_{k,l}$

It is well known that for a block circulant matrix

$$V = \begin{pmatrix} V_0 & V_1 & \cdots & V_{m-1} \\ V_{m-1} & V_0 & \cdots & V_{m-2} \\ \vdots & \vdots & \ddots & \vdots \\ V_1 & V_2 & \cdots & V_0 \end{pmatrix}$$

or a skew block circulant matrix

$$V = \begin{pmatrix} V_0 & V_1 & \cdots & V_{m-1} \\ -V_{m-1} & V_0 & \cdots & V_{m-2} \\ \vdots & \vdots & \ddots & \vdots \\ -V_1 & -V_2 & \cdots & V_0 \end{pmatrix},$$

its determinant

$$\det(V) = \prod_{t=0}^{m-1} \det(J_t), \tag{1}$$

where $J_t = V_0 + \omega_t V_1 + \omega_t^2 V_2 + \cdots + \omega_t^{m-1} V_{m-1}$ and

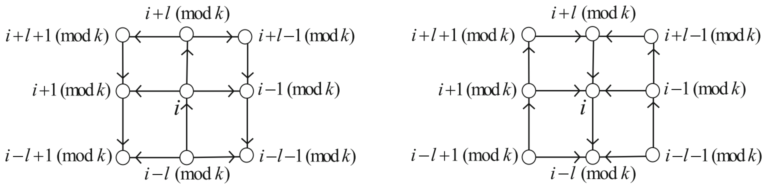
$$\omega_t = \begin{cases} \cos\frac{2t\pi}{m} + i\sin\frac{2t\pi}{m}, & \text{if } V \text{ is a block circulant matrix;} \\ \cos\frac{(2t+1)\pi}{m} + i\sin\frac{(2t+1)\pi}{m}, & \text{if } V \text{ is a skew block circulant matrix.} \end{cases}$$

4.1 l is even and $k \equiv 2 \pmod 4$

For a vertex i in $Q_{k,l}$, $i = 1, 2, \ldots, k$, there are four edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ incident to the vertex i, where $i-1$, $i+1$, $i-l$ and $i+l$ are modulo k. For convenience, write $i \to j$ for the orientation of the edge $\{i, j\}$ from i to j, and $j \to i$ for the orientation from j to i. We orient the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ as follows:

(a) if i is odd, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $i \to (i-1)$, $i \to (i+1)$, $(i-l) \to i$ and $i \to (i+l)$, respectively (see Fig. 4a);
(b) if i is even, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $(i-1) \to i$, $(i+1) \to i$, $i \to (i-l)$ and $(i+l) \to i$, respectively (see Fig. 4b).

It is not difficult to check that the orientation is a crossing orientation shown in Fig. 4. Suppose the skew adjacency matrix of the crossing orientation $\overrightarrow{Q}_{k,l}$ of $Q_{k,l}$ is denoted



(a) **(b)**

Fig. 4 The orientations of the edges incident to the vertex i, where l is even and $k \equiv 2 \pmod 4$

by $A(\overrightarrow{Q}_{k,l})$. Then $A(\overrightarrow{Q}_{k,l})$ is a 2×2 block circulant matrix. For example, the skew adjacency matrix of the crossing orientation $\overrightarrow{Q}_{10,4}$ of $Q_{10,4}$,

$$A(\overrightarrow{Q}_{10,4}) = \left(\begin{array}{cc|cc|cc|cc|cc} 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & -1 \\ -1 & 0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ \hline 0 & -1 & 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 & 0 & 1 \\ \hline -1 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 \\ \hline 1 & 0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & -1 & 0 & -1 & 0 \\ \hline -1 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & -1 \\ \hline 0 & 0 & 1 & 0 & -1 & 0 & 0 & -1 & 0 & 1 \\ -1 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & -1 & 0 \end{array}\right),$$

is a 2×2 block circulant matrix. Generally, the skew adjacency matrix of the crossing orientation $\overrightarrow{Q}_{k,l}$ is a block circulant matrix

$$A(\overrightarrow{Q}_{k,l}) = \begin{pmatrix} A_0 & A_1 & A_2 & \cdots & A_{\frac{k-2}{2}} \\ A_{\frac{k-2}{2}} & A_0 & A_1 & \cdots & A_{\frac{k-4}{2}} \\ A_{\frac{k-4}{2}} & A_{\frac{k-2}{2}} & A_0 & \cdots & A_{\frac{k-6}{2}} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ A_1 & A_2 & A_3 & \cdots & A_0 \end{pmatrix},$$

where

$$A_0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad A_1 = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \quad A_{\frac{l}{2}} = -A_{\frac{k-l}{2}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$A_{\frac{k-2}{2}} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad A_i = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, i \neq 0, 1, l/2, (k-l)/2, (k-2)/2.$$

Since $A(\overrightarrow{Q}_{k,l})$ is a block circulant matrix and by formula (1), we have the determinant of $A(\overrightarrow{Q}_{k,l})$,

$$\begin{aligned}
\det(A(\overrightarrow{Q}_{k,l})) &= \prod_{t=0}^{\frac{k-2}{2}} \det\left(A_0 + \omega_t A_1 + \omega_t^2 A_2 + \cdots + \omega_t^{\frac{k-2}{2}} A_{\frac{k-2}{2}}\right)\\
&= \prod_{t=0}^{\frac{k-2}{2}} \det\left(A_0 + \omega_t A_1 + \omega_t^{\frac{l}{2}} A_{\frac{l}{2}} + \omega_t^{\frac{k-l}{2}} A_{\frac{k-l}{2}} + \omega_t^{\frac{k-2}{2}} A_{\frac{k-2}{2}}\right)\\
&= \prod_{t=0}^{\frac{k-2}{2}} \det\left[\begin{pmatrix} 0 & 1\\ -1 & 0\end{pmatrix} + \omega_t \begin{pmatrix} 0 & 0\\ -1 & 0\end{pmatrix} + \omega_t^{\frac{l}{2}} \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}\right.\\
&\qquad \left. + \omega_t \begin{pmatrix} 0 & 0\\ -1 & 0\end{pmatrix} + \omega_t^{\frac{l}{2}} \begin{pmatrix} 1 & 0\\ 0 & -1\end{pmatrix}\right]\\
&= \prod_{t=0}^{\frac{k-2}{2}} \left\{-\left[\omega_t^{\frac{l}{2}} - (\omega_t^{\frac{l}{2}})^{-1}\right]^2 + (1+\omega_t)(1+\omega_t^{-1})\right\}\\
&= \prod_{t=0}^{\frac{k-2}{2}} \left(4 - \omega_t^{l} - \omega_t^{-l} + \omega_t + \omega_t^{-1}\right)\\
&= \prod_{t=0}^{\frac{k-2}{2}} \left(4 + 2\cos\frac{4t\pi}{k} - 2\cos\frac{4lt\pi}{k}\right)\\
&= 2^{\frac{k}{2}} \prod_{t=0}^{\frac{k-2}{2}} \left(2 + \cos\frac{4t\pi}{k} - \cos\frac{4lt\pi}{k}\right).
\end{aligned}$$

Since $\overrightarrow{Q}_{k,l}$ is a crossing orientation of $Q_{k,l}$ and l is even, the orientation is a Pfaffian orientation by Theorem 3.2. Consequently, by Theorem 2.2, the number of Kekulé structures of $Q_{k,l}$ is

$$\Phi(Q_{k,l}) = [\det(A(\overrightarrow{Q}_{k,l})]^{\frac{1}{2}} = 2^{\frac{k}{4}} \prod_{t=0}^{\frac{k-2}{2}} \left(2 + \cos\frac{4t\pi}{k} - \cos\frac{4lt\pi}{k}\right)^{\frac{1}{2}}. \tag{2}$$

4.2 l is even and $k \equiv 0 \pmod 4$

For a vertex i of $Q_{k,l}$, we orient the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ incident to the vertex i as follows:

(a) for $i = 1$, the orientations of the edges $\{1, k\}$, $\{1, 2\}$, $\{1, 1-l\}$ and $\{1, 1+l\}$ are $k \to 1$, $1 \to 2$, $1 \to (1-l)$ and $1 \to (1+l)$, respectively (see Fig. 5a);

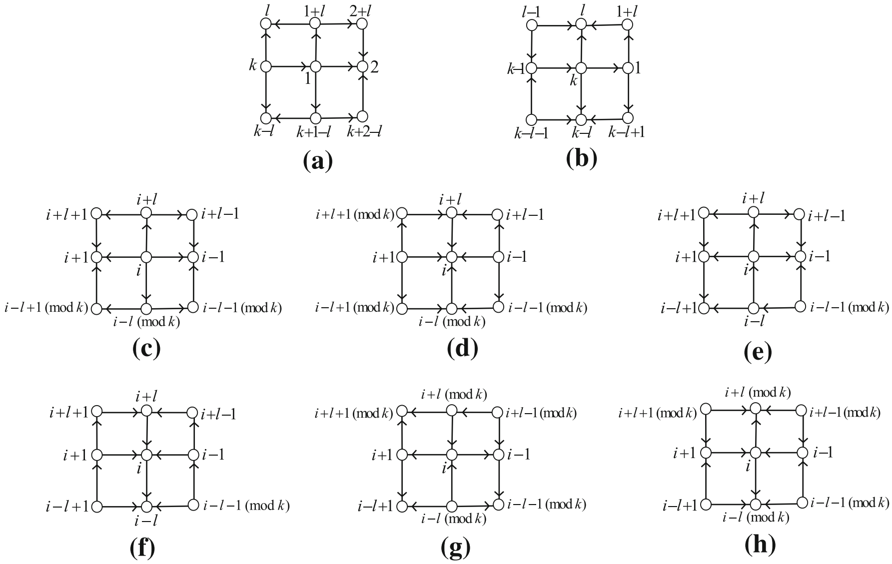


Fig. 5 The orientations of the edges incident to the vertex i, where l is even and $k \equiv 0 \pmod 4$

(b) for $i = k$, the orientations of the edges $\{k, k-1\}$, $\{k, 1\}$, $\{k, k-l\}$ and $\{k, k+l\}$ are $(k-1) \rightarrow k$, $k \rightarrow l$, $k \rightarrow (k-l)$ and $k \rightarrow (k+l)$, respectively (see Fig. 5b);

(c) if $2 \le i \le l$ and i is odd, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $i \rightarrow (i-1)$, $i \rightarrow (i+1)$, $i \rightarrow (i-l)$ and $i \rightarrow (i+l)$, respectively (see Fig. 5c);

(d) if $2 \le i \le l$ and i is even, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $(i-1) \rightarrow i$, $(i+1) \rightarrow i$, $(i-l) \rightarrow i$ and $(i+l) \rightarrow i$, respectively (see Fig. 5d);

(e) if $l+1 \le i \le k-l-1$ and i is odd, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $i \rightarrow (i-1)$, $i \rightarrow (i+1)$, $(i-l) \rightarrow i$ and $i \rightarrow (i+l)$, respectively (see Fig. 5e);

(f) if $l+1 \le i \le k-l-1$ and i is even, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $(i-1) \rightarrow i$, $(i+1) \rightarrow i$, $i \rightarrow (i-l)$ and $(i+l) \rightarrow i$, respectively (see Fig. 5f);

(g) if $k-l \le i \le k-1$ and i is odd, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $i \rightarrow (i-1)$, $i \rightarrow (i+1)$, $(i-l) \rightarrow i$ and $(i+l) \rightarrow i$, respectively (see Fig. 5g);

(h) if $k-l \le i \le k-1$ and i is even, then the orientations of the edges $\{i, i-1\}$, $\{i, i+1\}$, $\{i, i-l\}$ and $\{i, i+l\}$ are $(i-1) \rightarrow i$, $(i+1) \rightarrow i$, $i \rightarrow (i-l)$ and $i \rightarrow (i+l)$, respectively (see Fig. 5h).

The orientation above is equivalent to the crossing orientation shown in Fig. 6. Suppose that the skew adjacency matrix of the crossing orientation $\overrightarrow{Q}_{k,l}$ of $Q_{k,l}$ is denoted by $B(\overrightarrow{Q}_{k,l})$. Then $B(\overrightarrow{Q}_{k,l})$ is a skew 2×2 block circulant matrix.

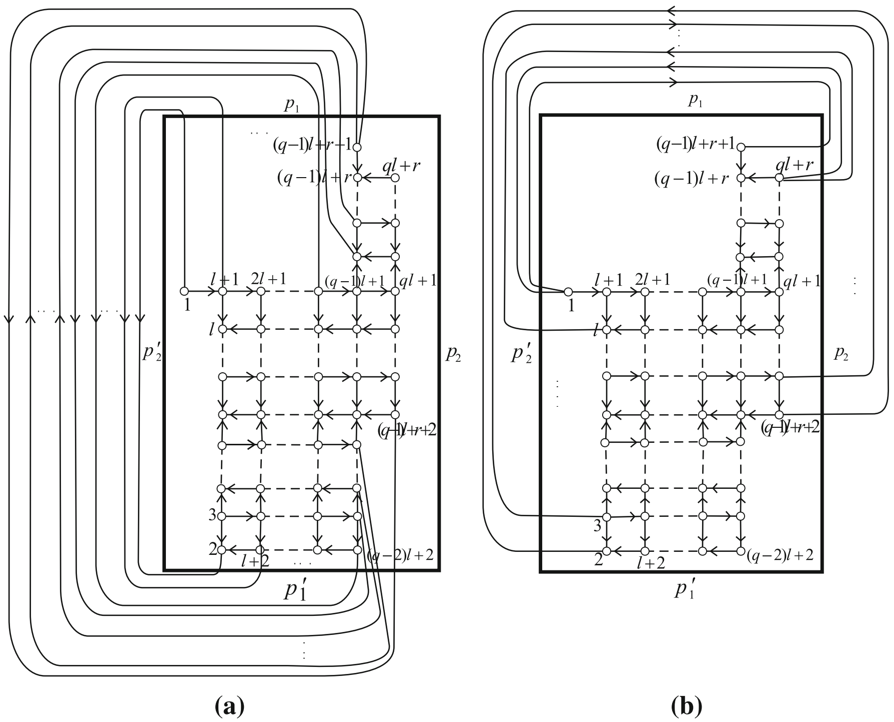


Fig. 6 A crossing orientation of $Q_{k,l}$, where l is even and $k \equiv 0$ (mod k)

For example, the skew adjacency matrix of the crossing orientation $\overrightarrow{Q}_{16,6}$ of $Q_{16,6}$,

$$B(\overrightarrow{Q}_{16,6}) = \left(\begin{array}{cc|cc|cc|cc|cc|cc|cc|cc}
0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\
-1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
\hline
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 \\
\hline
0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 \\
\hline
-1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
\hline
0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & -1 \\
\hline
-1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 0 & 0 \\
\hline
0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\
\hline
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0
\end{array}\right),$$

is a skew 2×2 block circulant matrix. Generally, the skew adjacency matrix $B(\overrightarrow{Q}_{k,l})$ of $\overrightarrow{Q}_{k,l}$ is a skew block circulant matrix

$$B(\overrightarrow{Q}_{k,l}) = \begin{pmatrix} B_0 & B_1 & B_2 & \cdots & B_{\frac{k-2}{2}} \\ -B_{\frac{k-2}{2}} & B_0 & B_1 & \cdots & B_{\frac{k-4}{2}} \\ -B_{\frac{k-4}{2}} & -B_{\frac{k-2}{2}} & B_0 & \cdots & B_{\frac{k-6}{2}} \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ -B_1 & -B_2 & -B_3 & \cdots & B_0 \end{pmatrix},$$

where

$$B_0 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}, \quad B_{\frac{l}{2}} = B_{\frac{k-l}{2}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$B_{\frac{k-2}{2}} = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B_j = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \, j \neq 0, 1, l/2, (k-l)/2, (k-2)/2.$$

Since $B(\overrightarrow{Q}_{k,l})$ is a skew circulant matrix and by formula (1), we have the determinant of $B(\overrightarrow{Q}_{k,l})$,

$$\begin{aligned}
\det(\overrightarrow{B}(Q_{k,l})) &= \prod_{t=0}^{\frac{k-2}{2}} \det\left(B_0 + \omega_t B_1 + \omega_t^2 B_2 + \cdots + \omega_t^{\frac{k-2}{2}} B_{\frac{k-2}{2}}\right) \\
&= \prod_{t=0}^{\frac{k-2}{2}} \det\left(B_0 + \omega_t B_1 + \omega_t^{\frac{l}{2}} B_{\frac{l}{2}} + \omega_t^{\frac{k-l}{2}} B_{\frac{k-l}{2}} + \omega_t^{\frac{k-2}{2}} B_{\frac{k-2}{2}}\right) \\
&= \prod_{t=0}^{\frac{k-2}{2}} \det\left[\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \omega_t \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix} + \omega_t^{\frac{l}{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\right. \\
&\quad \left. + \omega_t^{\frac{k-l}{2}} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \omega_t^{\frac{k-2}{2}} \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}\right] \\
&= \prod_{t=0}^{\frac{k-2}{2}} \det\begin{pmatrix} \omega_t^{\frac{l}{2}} + \omega_t^{\frac{k-l}{2}} & 1 - \omega_t^{\frac{k-2}{2}} \\ -1 - \omega_t & -\omega_t^{\frac{l}{2}} - \omega_t^{\frac{k-l}{2}} \end{pmatrix} \\
&= \prod_{t=0}^{\frac{k-2}{2}} \left(4 - \omega_t^{l} - \omega_t^{-l} + \omega_t + \omega_t^{-1}\right) \\
&= \prod_{t=0}^{\frac{k-2}{2}} \left\{-\left[\omega_t^{\frac{l}{2}} - (\omega_t^{\frac{l}{2}})^{-1}\right]^2 + (1 + \omega_t)(1 + \omega_t^{-1})\right\}
\end{aligned}$$

$$= \prod_{t=0}^{\frac{k-2}{2}} \left[4 + 2\cos\frac{2(2t+1)\pi}{k} - 2\cos\frac{2l(2t+1)\pi}{k} \right]$$

$$= 2^{\frac{k}{2}} \prod_{t=0}^{\frac{k-2}{2}} \left[2 + \cos\frac{2(2t+1)\pi}{k} - \cos\frac{2l(2t+1)\pi}{k} \right].$$

By Theorem 3.2, the crossing orientation $\overrightarrow{Q}_{k,l}$ of $Q_{k,l}$ is a Pfaffian orientation when l is even. Hence, by Theorem 2.2, the number of Kekulé structures of $Q_{k,l}$ is

$$\Phi(Q_{k,l}) = [\det(B(\overrightarrow{Q}_{k,l})]^{\frac{1}{2}} = 2^{\frac{k}{4}} \prod_{t=0}^{\frac{k-2}{2}} \left[2 + \cos\frac{2(2t+1)\pi}{k} - \cos\frac{2l(2t+1)\pi}{k} \right]^{\frac{1}{2}}. \tag{3}$$

Combining formulas (2) and (3), we have the following main result.

Theorem 4.1 *If l is even, then the number of Kekulé structures of $Q_{k,l}$ can be expressed by*

$$\Phi(\overrightarrow{Q}_{k,l}) = \begin{cases} 2^{\frac{k}{4}} \prod_{t=0}^{\frac{k-2}{2}} \left(2 + \cos\frac{4t\pi}{k} - \cos\frac{4lt\pi}{k}\right)^{\frac{1}{2}}, & \text{if} \quad k \equiv 2 \pmod 4; \\ 2^{\frac{k}{4}} \prod_{t=0}^{\frac{k-2}{2}} \left[2 + \cos\frac{2(2t+1)\pi}{k} - \cos\frac{2l(2t+1)\pi}{k}\right]^{\frac{1}{2}}, & \text{if} \quad k \equiv 0 \pmod 4). \end{cases}$$

5 Concluding remarks

Thomassen characterized that there are exactly two types of embedded modes on a torus of polyominos which are $Q_{m,n,r}$ and $Q_{k,l}$. Lu et al. investigated the type $Q_{m,n,r}$ and gave two explicit expressions for the number of Kekulé structures when n is even or both m and r are even. Two explicit expressions for the number of Kekulé structures of $Q_{k,l}$ when both k and l are even are deduced in the present paper. A question remains here: whether there also exists an explicit expression for the number of Kekulé structures of $Q_{k,l}$ when l is odd?

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