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ORIGINAL PAPER

Elementary components of essentially disconnected polyomino graphs

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Abstract An essentially disconnected polyomino graph is defined as a polyomino graph with some perfect matchings and forbidden edges. In this paper, we prove that the subgraph, obtained by deleting all the forbidden edges, is disconnected and has at least two elementary components, which generalizes the results for essentially disconnected benzenoid systems by Gutman et al. Furthermore, we show that if an essentially disconnected polyomino graph has an unit square as one of its elementary components, then it has at least three elementary components.

Keywords Polyomino graph · Elementary component · Perfect matching · Essentially disconnected · Forbidden edge

1 Introduction

Polyomino graphs [1], also called chessboards [2] or square-cell configurations [3], have attracted some mathematicians' considerable attention, for many interesting combinatorial subjects are yielded from them, such as hypergraphs [1], domination problem [2,4], rook polyominal [5], etc. Additionally, Motoyama and Hosoya obtained some interesting results by introducing king and domino polyomials, which can be applied in statistical physics and in modeling problems of surface chemistry [5,6].

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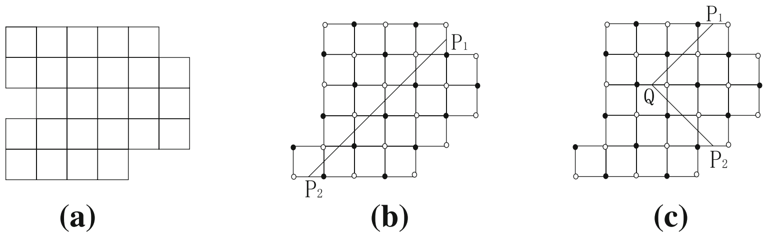

Fig. 1 **a** A polyomino graph G. **b** A cut segment. **c** A g-cut segment

A *polyomino graph* is a connected geometric graph obtained by arranging congruent regular squares of side length 1 (called a cell) in a plane such that two squares are either disjoint or have a common edge (see Fig. 1a). A *generalized polyomino* H is a subgraph of a polyomino graph G and has at least one edge which does not belong to any square of H. A *perfect matching of a graph* G is a set of independent edges of G covering all vertices of G. The perfect matching problem of polyomino graphs is closely related to the dimer problem in crystal physics [7,8]. An edge of a polyomino graph G with perfect matching is said to be a *forbidden single (double) edge* if it belongs to none (all) of the perfect matchings of G and allowed otherwise. An edge is said to be a *forbidden edge* if it is either a forbidden single edge or a forbidden double edge. A polyomino graph G is said to be *elementary* if it has no forbidden edge. Otherwise, it is said to be *essentially disconnected* (the term "essentially disconnected" is used to indicate those polyhexes with perfect matching and fixed bonds by Cyvin and Gutman [9]).

The structural features of essentially disconnected benzenoid systems are already known in [10,11]. In this paper, we concentrate ourselves on polyomino graphs and prove that their structural feature is similar to that of polyhex graphs.

2 Definitions and notations

Let G be a polyomino graph, C the outer perimeter of G. The following concept of special edge cut plays an important role in our investigations.

Definition 1 ([12]) A straight line segment P_1P_2 is called a *cut segment* of G if

(1) each of P_1 and P_2 is the center of an edge on the outer perimeter C;
(2) P_1P_2 and all edges of G form an angle of $\pi/4$;
(3) any point of P_1P_2 is either an interior or a boundary point of some square of G. (see Fig. 1b).

Definition 2 ([12]) A broken line segment P_1QP_2 is called a *generalized cut segment* (g-cut segment) of G if

(1) each of P_1 and P_2 is the center of an edge on the outer perimeter C;
(2) P_1Q and P_2Q form an angle of $\pi/2$, and Q is the center of some edge e which is the bisector of the right angle $\angle P_1QP_2$;

(3) any point of P_1QP_2 is either an interior or a boundary point of some square of G. (see Fig. 1c).

A *special cut segment* is either a cut segment or a g-cut segment. A *special edge cut* R is the set of edges of G intersected by a special cut segment. Obviously, two special edge cuts are disjoint if their corresponding special cut segments are disjoint.

By the definition of polyomino graphs, it is easy to check that a polyomino graph G is a bipartite graph. Thus polyomino graphs are 2-colorable. In the following, we assume that all the vertices of G are colored black or white such that any two adjacent vertices of G are differently colored. We denote the sets of white and black vertices of G by $W(G)$ and $B(G)$, respectively. Let E be a special edge cut of G. $G - E$ is the subgraph of G obtained by deleting all the edges of E.

In [13], a necessary and sufficient condition for a polyomino graph with perfect matchings to be essentially disconnected was given.

Theorem 2.1 ([13]) *Let G be a polyomino graph with the perfect matching, C the outer perimeter of G. Then G is essentially disconnected if and only if G possesses a cut or g-cut R, satisfying*

(1) $|B(G_1)| = |W(G_1)|$ *and* $|B(G_2)| = |W(G_2)|$, *where* $G_i(i = 1, 2)$ *are the two components of* $G - R$;
(2) all the edges of R are forbidden single edges.

The above theorem implies that for an essentially disconnected polyomino graph G, deleting the forbidden edges which form a special edge cut, the subgraph $G - R$ is not connected and has at least two connected components.

3 Elementary components

In this section we prove that for each component $G_i(i = 1, 2)$ of $G - R$, there exist some allowed edges, which implies that G_i is elementary or contains an elementary subgraph.

Let G be a polyomino graph, A be a set of vertices of G. $G- < A >$ designates the subgraph obtained by deleting all the vertices of A together with their incident edges. For a perfect matching M of G, an *M-alternating cycle* is a cycle whose edges are alternate in M and $E(G) - M$, where $E(G)$ is the edge set of G.

Lemma 3.1 *Let G be a polyomino graph, C the perimeter of G, $v_1, \ldots, v_t$ be t vertices on the perimeter C of G, $A = \{v_1, \ldots, v_t\}$. Suppose that in $G - <A>$, the perimeter C of G is broken into t segments with even lengths (i.e. odd vertices). If $G - <A>$ has a perfect matching M, then $G - <A>$ has an M-alternating cycle.*

Proof Let G be a graph with n vertices, m edges, s squares and p external edges (i.e. the edges lying on the perimeter of G). Then G has $m - p$ internal edges (i.e. the edges not lying on the perimeter of G). Since each internal edge belongs to two squares, we have $4s = 2(m - p) + p$, i.e.

$$m = 2s + p/2. \quad (1)$$

By Euler's formula which says that for a connected plane graph, the number of vertices plus the number of faces is equal to the number of edges plus two [14], we have $n + (s + 1) = m + 2$, i.e.

$$n - m + s = 1. \tag{2}$$

which together with (1) yields

$$n - s - p/2 = 1. \tag{3}$$

On the other hand, suppose that the perfect matching M of $G - <A>$ contains r external edges of G and hence has $(n - t)/2 - r$ internal edges of G. If none of the squares of $G - <A>$ is an M-alternating cycle, then at most one edge of each square of G belongs to M. Hence we have $s \geq r + 2((n - t)/2 - r)$, i.e.

$$s \geq n - r - t. \tag{4}$$

In $G - <A>$ the perimeter C of G is broken into t segments, and each of which contains an even number of edges. Therefore, we have: $r \leq (p - 2t)/2$, i.e.

$$r \leq p/2 - t. \tag{5}$$

Substituting (5) back into (4) we obtain: $s \geqslant n - p/2$ i.e.

$$n - s - p/2 \leqslant 0. \tag{6}$$

Formula (6) is evidently in contradiction with formula (3). The contradiction means that the assumption about the non-existence of M-alternating cycle which is a square is false. The proof is completed. □

Theorem 3.2 *If G is an essentially disconnected polyomino graph, then the subgraph obtained from G by deleting all the forbidden single edges and all the end vertices of the forbidden double edges is disconnected.*

Proof By Theorem 2.1, G has a special edge cut R such that the edges of R are forbidden single edges. Then after deleting all the forbidden single edges of R, G has at least two connected components G_1 and G_2. Each of them may be a component with or without some pendent edges. In the following, we prove that each component G_i has some allowed edges, i.e. G_i has an elementary component which is also an elementary component of G. We distinguish two cases:

Case 1 Suppose that G_i has no pendent edge. Then G_i is itself a polyomino graph. Thus by Lemma 3.1, G_i has some allowed edges (note that all the edges on an M-alternating cycle are allowed edges). Thus, after deleting all the forbidden single edges and all the end vertices of the forbidden double edges, G_i has a component consisting of allowed edges, i.e. an elementary component. It is clear that this elementary component is also an elementary component of G and is an elementary polyomino graph.

Case 2 Suppose that G_i has some pendent edges, say $u_{ij}v_{ij}(j = 1, 2, \ldots, s)$, where u_{ij} is a vertex of degree 1 in G_i. Since G is a polyomino graph with perfect matchings and all the edges of R are forbidden single edges, all the pendent edges $u_{ij}v_{ij}$ $(j = 1, 2, \ldots, s)$ of G_i are forbidden double edges. By deleting all the pendent edges $u_{ij}v_{ij}$ $(j = 1, 2, \ldots, s)$ together with the end vertices u_{ij}, we obtain a polyomino graph G_i^*. Put $A_i = \{v_{i1}, v_{i2}, \ldots, v_{is}\}$. Then $G_i^* - A_i$ has a perfect matching $M_i - \{u_{ij}, v_{ij}\}$, where M_i is a perfect matching of G_i. Keep in mind the definition of special edge cut, one can check that A_i satisfies the condition in Lemma 3.1. Therefore, $G_i^* - A_i$ has some allowed edges. Consequently, $G_i^* - A_i$ has at least an elementary component which is also an elementary component of G and is an elementary polyomino graph.

Therefore, we come to the conclusion that G has at least two elementary components, one from G_1, and the other from G_2. Each of them is an elementary polyomino graph. □

4 Small elementary components

The size of the elementary components may influence their numbers of elementary components. We will show it in this section. We need the following two lemmas.

Lemma 4.1 *Let G be a generalized polyomino graph with at most one pendent edge, M be a perfect matching of G.Then G has a square containing two double edges in M.*

Proof Assume that G has n vertices, m edges, and s squares. Further, assume that G has p external edges, then G has $m - p$ internal edges. By the assumption, we distinguish two cases.

Case 1 G has no pendent edge. Then G is a polyomino graph with perfect matchings. Since each internal edge belongs to two squares, we have: $4s = 2(m - p) + p$, i.e.

$$m = 2s + p/2. \tag{7}$$

By Euler's formula, we have $n + (s + 1) = m + 2$, i.e.

$$n - m + s = 1. \tag{8}$$

which together with (7) yields

$$n - s - p/2 = 1. \tag{9}$$

On the other hand, suppose that the perfect matching M of G contains r external edges of G and hence has $n/2 - r$ internal edges of G. If none of the squares of G is an M-alternating cycle, then at most one edge of each square of G belongs to M. Hence we have $s \geq r + 2(n/2 - r)$, i.e.

$$n - r - s \leqslant 0. \tag{10}$$

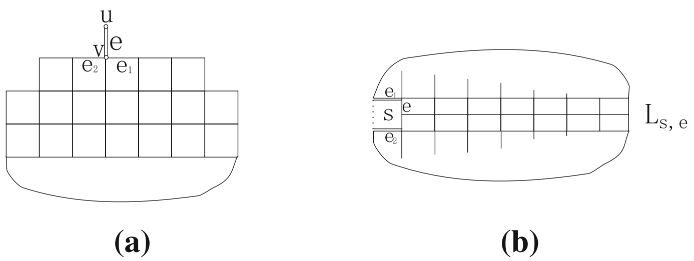

Fig. 2 **a** Illustration for the proof of Lemma 4.1 **b** Illustration for Lemma 4.2

It is evident that we have $r \leq p/2$. Hence $n - s - p/2 \leqslant 0$, which contradicts with formula (9). This contradiction implies that G has a square which is an M-alternating cycle.This square contains two double edges in M.

Case 2 G has one pendent edge e (see Fig. 2a). Then the edge e is a forbidden double edge, and both e_1 and e_2 are forbidden single edges. Hence we have $4s + 1 = 2(m - p) + p$, i.e.

$$m = 2s + p/2 + 1/2. \tag{11}$$

By Euler's formula, we have

$$n - m + s = 1. \tag{12}$$

which together with (11) yields

$$n - s - p/2 = 3/2. \tag{13}$$

On the other hand, suppose that the perfect matching M of G contains r external edges of G. Since both e_1 and e_2 are forbidden single edges, G has $n/2 - r$ internal edges. If none of the squares of G is an M-alternating cycle, then at most one edges of each square of G belongs to M. Hence we have: $s \geq r + 2(n/2 - r)$, i.e.

$$n - r - s \leqslant 0. \tag{14}$$

It is evident that we have: $r \leq (p - 3)/2 + 1$ i.e.

$$r \leqslant p/2 - 1/2. \tag{15}$$

which together with (14) yields

$$n - s - p/2 \leqslant -1/2. \tag{16}$$

Formula (16) is evidently in contradiction with formula (13). Hence G has a square which is an M-alternating cycle. This square contains two double edges in M. Therefore, the lemma is completely proved. □

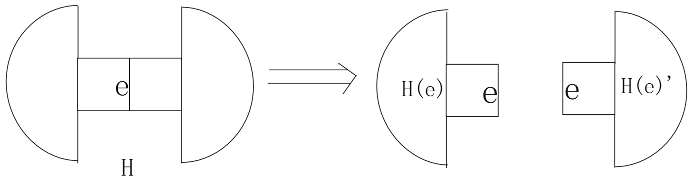

Fig. 3 Illustration for the separating edge e

Before continuing we introduce some notations. Let G be a polyomino graph, e an edge of G, e_1 and e_2 the edges of G which are parallel to each other and adjacent to the edge e, s the square which contains the edges e, e_1 and e_2 (note that s may or may not be a square of G). Let $L_{s,e}$ denote the segment of the perpendicular bisector of e which starts from the midpoint of e and ends at the central point of s if s does not belong to G, and otherwise passes through s, ends at the perimeter of G and is totally contained in the interior region of G (see Fig. 2b).

Similar to the proof of Lemma 3 of [15], we have the following conclusion.

Lemma 4.2 *Let G be a polyomino graph, M be a perfect matching of G and e be a forbidden single edge of G. If the edges e_1 and e_2 of M which cover the end vertices of e belong to a square s (s may or may not belong to G), then the edges of G intersecting $L_{s,e}$ are all forbidden single edges (see Fig. 2 b).*

Definition 3 An edge of a polyomino graph G is said to be a *separating edge* if the removal of its end vertices disconnects G.

If e is a separating edge, let $H(e)$ and $H(e)'$ denote the polyomino graph obtained by splitting G at the separating edge e such that $H(e)$ and $H(e)'$ only have one common edge e (see Fig. 3).

Theorem 4.3 *If a polyomino graph H with more than one square has an elementary component which is an unit square, then H has at least three elementary connected components, each of which is an elementary polyomino graph.*

Proof Let s be the square which is an elementary component. Then all edges are forbidden single edges. Let M_1 be a perfect matching of H in which the vertices of s are matched themselves. Let M_2 be the perfect matching obtained by rotating M_1 along s. We distinguish two cases:

Case 1 There is an edge e which is a separating edge of H in the square s. Without loss of generality, let $H(e)$ contain s, and e belong to M_1. Evidently $M_1 \cap H(e)'$ is a perfect matching of $H(e)'$. Moreover, the two edges of $H(e)'$ which are adjacent to e are forbidden single edges of $H(e)'$. Otherwise, they are not forbidden single edges in H, which contradicts with the assumption. Thus, $H(e)'$ is an essentially disconnected polyomino graph and $H(e)'$ has at least two elementary components by Theorem 3.2. It can be checked that each of the elementary components of $H(e)'$ is also an elementary component of H. So H has at least three elementary connected components, one from H_2, one from H_3, and another is just the unit square s. Each of them is an elementary polyomino graph.

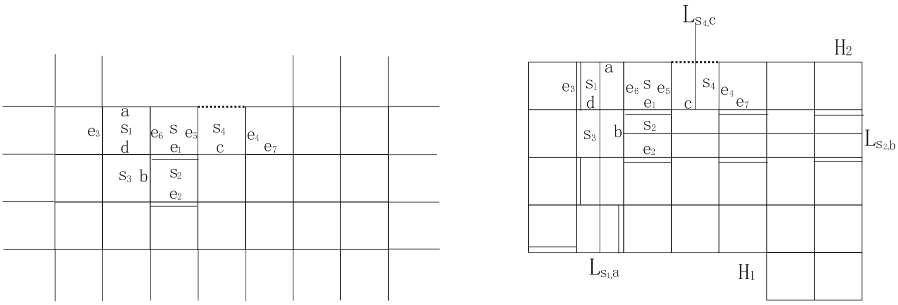

Fig. 4 **a** Illustration for Theorem 4.3. **b** Illustration for subcase 1 of Theorem 4.3

Case 2 None of the edges in s is separating edge of G. So there are at least two squares s_1, s_2 which are adjacent to s (two squares are adjacent if they share a common edge). Furthermore, there is a square s_3 which is simultaneously adjacent to s_1 and s_2 (see Fig. 4a). Let $e_1, e_2, e_3, e_4, e_5, e_6, e_7, a, b, c$ and d be the edges as shown in Fig. 4a. Also let s_4 (which may or may not belong to H) denote the square shown in Fig. 4a. Without loss of generality, let e_1 and e_2 belong to K_1(see Fig. 4a). There are two subcases:

Subcase 1 Suppose that e_3 belongs to K_1 (see Fig. 4b). It is in K_2 as well. Considering K_2, all edges intersecting $L_{s_1,a}$ and $L_{s_4,c}$ are forbidden single edges by Lemma 4.2. Similarly, considering K_1, the edges intersecting $L_{s_2,b}$ are forbidden single edges by Lemma 4.2. Let H' be the subgraph obtained by deleting the forbidden single edges which intersect $L_{s_1,a}$, $L_{s_4,c}$ and $L_{s_2,b}$ from H, but not their end vertices. Let H_1 and H_2 be the two connected components of H' which contain e_2 and e_7, respectively (see Fig. 4b). Both of them are polyomino graphs. Considering K_1, both H_1 and H_2 contain an elementary component of H by Lemma 4.1. Thus H has at least three elementary components, one from H_2, one from H_3, and another is just the unit square s. Each of them is an elementary polyomino graph.

Subcase 2 Suppose e_3 does not belong to K_1. Obviously, the two edges a and d are forbidden single edges. Considering K_1, b and s_2, the edges intersecting $L_{s_2,b}$ and $L_{s_4,c}$ are forbidden single edges (see Fig. 5). Let H_3 be the subgraph obtained by deleting the two forbidden single edges a, d (but not their end vertices) and all the forbidden single edges intersecting $L_{s_2,b}$ from H (see Fig. 5). And H_3 which contains e_2 is a polyomino graph with a perfect matching $H_3 \cap K_1$. Then H_3 contains an elementary component of H by Lemma 4.1. Also as in subcase 1, H_2 contains anther elementary component of H. So H has at least three elementary connected components, one from H_2, one from H_3, and another is just the unit square s. Each of them is an elementary polyomino graph. The theorem is completely proved. □

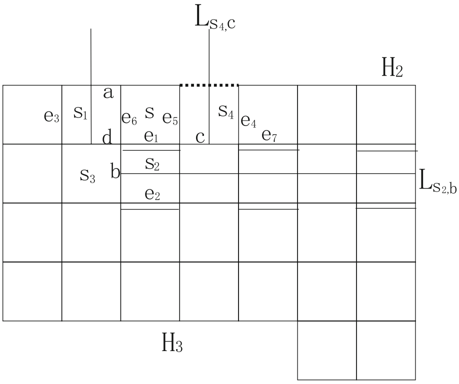

Fig. 5 Illustration for subcase 2 of Theorem 4.3

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