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The maximum forcing number of a polyomino*

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Dedicated to the memory of Mirka Miller

Abstract

In this paper, we show that a polyomino with perfect matchings has a unique perfect matching when removing the set of squares from its maximum Clar cover. Thus the maximum forcing number of the polyomino equals its Clar number and can be computed in polynomial time.

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1 Introduction

Let G be a graph that has a perfect matching. A *forcing set* for a perfect matching M of G is a subset S of M, such that S is contained in no other perfect matchings of G. The cardinality of a smallest forcing set of M is called the *forcing number* of M, and is denoted by $f(G; M)$. The minimum and maximum of $f(G; M)$ over all perfect matchings M of G is denoted by $f(G)$ and $F(G)$, respectively. Given a matching M in a graph G, an *M-alternating path (cycle)* is a path (cycle) in G whose edges are alternately in M and outside of M. Let e be an edge of G. If e is contained in all perfect matchings of G, or is not contained in any perfect matchings of G, then e is called a *fixed bond*. If e is contained in a perfect matching of G, then e is called a *double bond*.

A *square graph* is the cycle graph C_4, called *square* for short. A polyomino is a finite connected plane graph which has no cut vertex and every interior face is a square graph. A connected bipartite graph is called *elementary* (or *normal*) if every edge is contained in some perfect matchings. Let G be a plane bipartite graph, a face of G is called *resonant* if its boundary is an alternating cycle with respect to a perfect matching of G.

The Clar number was originally defined for hexagonal systems [1]. Later, Abeledo and Atkinson [1] generalized the concept of Clar number for bipartite and 2-connected plane graphs. For a planar embedding of a 2-connected bipartite planar G, a *Clar cover* of G is a spanning subgraph C such that each component is either a face or an edge, the maximum number of faces in Clar covers of G is called *Clar number* of G, and denoted by $C(G)$. We call a Clar cover with the maximum number of faces a maximum Clar cover.

The idea of forcing number was inspired by practical chemistry problems. This concept was first proposed by Harary et al. in [4]. The same idea appeared in earlier papers by Randić and Klein [5, 7] in terms of the innate degree of freedom of a Kekulé structure. An open problem has been proposed.

Open Problem. Given a graph G, what is the computational complexity of finding the maximum forcing number of G?

Recently, Xu, Bian and Zhang [8] showed that when G is an elementary hexagonal system, the maximum forcing number of G can be computed in polynomial time. In this paper, we showed the following.

Theorem 1. *If G is a polyomino with perfect matchings, then $F(G) = C(G)$ and $F(G)$ can be computed in polynomial time.*

2 The maximum forcing number of an elementary polyomino

In [3], Hansen and Zheng formulate the computation of Clar numbers as an integer programming problem. Later, Abeledo and Atkinson [1] proved the following result.

Theorem 2. *If G is a 2-connected bipartite planar graph with n vertices and m edges, then the Clar number of G can be computed in polynomial time by solving a linear program with $2m - n + 2$ variables and n constraints.*

Xu, Bian and Zhang [8] proved that the maximum forcing number of an elementary hexagonal system equals its Clar number. And using Theorem 2, they showed that the maximum forcing number of an elementary hexagonal system can be computed in polynomial time. They also proposed the following conjecture.

Conjecture. If G is an elementary polyomino, then the maximum forcing number of G can be computed in polynomial time.

We now prove that the conjecture is true. We will first prove the following theorem.

Theorem 3. *Let G be a polyomino with perfect matchings. Let K be a maximum Clar cover of G with $C(G)$ squares, and let K' be the set of squares in K. Then $G - K'$ has a unique perfect matching.*

Proof. Suppose that $G - K'$ has more than one perfect matching. The union of any two of the perfect matchings of $G - K'$ will give us a set of alternating cycles in the graph G. Let C be an alternating cycle in $G - K'$. Let G^* denote the subgraph of G such that the outer boundary of G^* is the alternating cycle C. Let $K'|_{G^*}$ denote the set of squares of K' in G^*. It is clear that C is a nice cycle of G (i.e., $G - C$ has a perfect matching) and $G^* - K'|_{G^*}$ has a perfect matching which is denoted by $M(G^*)$.

Now let us look at the graph G^*; we label the vertices of the graph G^* row by row, from top to bottom. The leftmost vertex in the top row is labelled as $v_{1,1}$, and the vertices in the same row will be labelled as $v_{1,i}$. The second row of vertices are labelled as $v_{2,i}$ and i could be 0 or a negative value if the vertex is on the left of the vertex $v_{2,1}$. The face with vertex $v_{i,j}$ on its left top is labelled as $f_{i,j}$ (see Fig. 1 for an example).

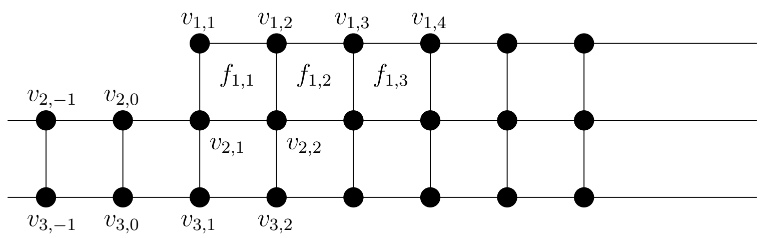

Figure 1: The labelling of a polyomino

By two parallel edges of a polyomino we mean two opposite edges of a face, either $v_{i,j}v_{i,j+1}$ and $v_{i+1,j}v_{i+1,j+1}$ or $v_{i,j}v_{i+1,j}$ and $v_{i+1,j}v_{i+1,j+1}$.

Observation 1. In $M(G^*)$, if there are two parallel edges, then K is not a maximum Clar cover.

Clearly, the square surrounded by these two parallel edges can be added to K' and then K is not a maximum Clar cover.

Along the same line of reasoning, we obtained the following two observations.

Observation 2. If there are two parallel edges on the boundary of G^*, then K is not a maximum Clar cover.

Suppose that the face $f_{i,j}$ is surrounded by these two parallel edges. Clearly, if $f_{i,j}$ is a pending face, then the corresponding square can be included in the K', a contradiction. In other cases, removing the square that corresponding to face $f_{i,j}$ does not disturb $M(G^*)$. Furthermore, the cycle C has been disconnected into two odd length paths with a unique perfect matching. Thus, we could include the square corresponding to face $f_{i,j}$ to increase K', a contradiction.

Observation 3. If there is an edge in $M(G^*)$ parallel to the boundary of G^*, then K is not a maximum Clar cover.

Now we shall prove that either there exists a pair of parallel edges in $M(G^*)$ or we could replace some squares of K' by a larger set, which leads to a contradiction.

Look at the consecutive faces $f_{1,1}, f_{1,2}, \ldots f_{1,i}$ in the first row of G^*. Because of Observation 2, we know that $i > 1$. Now we look at the faces $f_{2,1}, f_{2,2}, \ldots f_{2,i}$. Let us first see that these faces all belong to G^*. If one of the faces $f_{2,j}$, where $1 \leq j \leq i$, is not part of G^*, then G^* has two parallel edges on the boundary of G^*. Based on Observation 2, we know it is not possible (see Fig. 2 for an example).

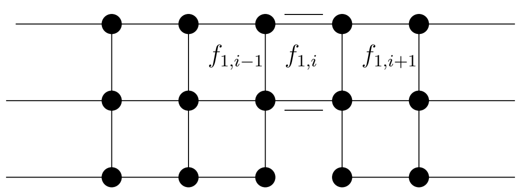

Figure 2: An illustration of the perfect matching in G^*

Now, we know that $f_{2,1}, f_{2,2}, \ldots f_{2,i}$ are faces of G^*. Firstly, it is clear that none of the edges $v_{2,1}v_{2,2}$, $v_{2,2}v_{2,3}, \ldots, v_{2,i-1}v_{2,i}$ are in $M(G^*)$ because of Observation 3. This implies that the edges $v_{2,2}v_{3,2}$, $v_{2,3}v_{3,3}$, $v_{2,i}v_{3,i}$ are either in the perfect matching $M(G^*)$ or in K'_{G^*}. And furthermore, due to Observation 2, there are no parallel edges in $M(G^*)$.

If i is odd, then we know that faces $f_{2,2}, f_{2,4}, \ldots, f_{2,i-1}$ should be in K'_{G^*}, otherwise, remove those faces in K' of the form $f_{2,t}$ where $1 \leq t \leq i-1$ and then take $f_{2,2}, f_{2,4}, \ldots, f_{2,i-1}$ with the remaining squares of K' to get a Clar cover of G with a larger number of squares, which is a contradiction.

Now we have $f_{2,2}, f_{2,4}, \ldots, f_{2,i-1} \in K'_{G^*}$, and we replace $f_{2,2}, f_{2,4}, \ldots, f_{2,i-1}$ with the faces $f_{1,1}, f_{1,3}, \ldots, f_{1,i}$ which gives us a Clar cover with one more square than K

(see Fig. 3 for an example), a contradiction.

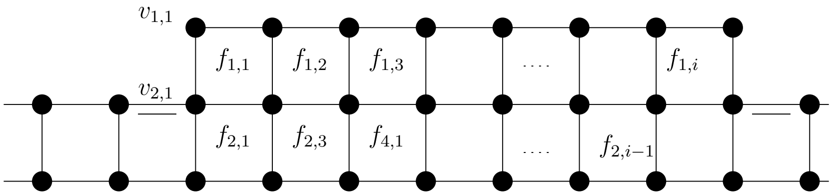

Figure 3: An illustration of the perfect matching in G^*

Now we look at the case when i is even, where the previous suggested approach does not work since it will not give us a new Clar cover with more squares. However, we could assume that edge $v_{2,2}v_{3,2}$ is in $M(G^*)$ and faces $f_{2,3}, f_{2,5}, \dots, f_{2,i-1}$ are in C', otherwise we could make a rearrangement for that configuration to happen. If the edge $v_{2,1}v_{3,1}$ is on the boundary of G^*, then by Observation 3, we know that K is not a maximum Clar cover of G. Now, we could assume that there are other faces on the left of $f_{2,1}$.

We know that the edge $v_{3,1}v_{4,1}$ is either in $M(G^*)$ or K'_{G^*} or else belongs to the boundary of G^*. First we see it is not possible for $v_{3,1}v_{4,1}$ to be on the boundary, since this implies that the edges $v_{2,0}v_{2,1}$ and $v_{3,0}v_{3,1}$ are on the cycle C, based on Observation 2. This is a contradiction. Thus we know that $v_{3,1}v_{4,1}$ must belong to $M(G^*)$ or K'_{G^*}.

Assume that the left most vertex on the second row of G^* is $v_{2,-j}$, i.e., there does not exist a vertex $v_{2,-t}$ where $t > j$. We could assume that $f_{2,0}, f_{2,-1}, \dots, f_{2,-j}$ all belong to G^*; otherwise, we relabel the graph and take the left-most $v_{2,-j}$ as $v_{1,1}$.

Now we also know that all faces $f_{3,0}, f_{3,-1}, \dots, f_{3,-j}$ belong to G^*; otherwise, based on Observation 2, we could show that one of the faces $f_{2,-t}$, where $1 < t < j$, could be included in K'_{G^*}. See Fig. 4 for details.

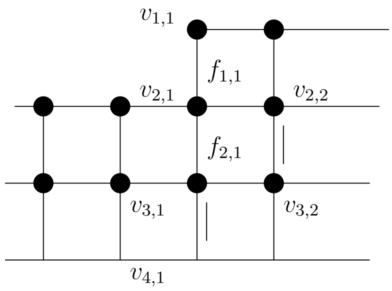

Figure 4: An illustration of the perfect matching in G^*

As in previous cases, we know that the edges $v_{3,0}v_{4,0}$, $v_{3,-1}v_{4,-1}$, $\dots$, $v_{3,-j+1}v_{4,-j+1}$ are either in the perfect matching $M(G^*)$ or in K'_{G^*}. If j is odd, then the faces $f_{3,0}, f_{3,-2}, \dots, f_{3,-j+1}$ must be in $C'|_{G^*}$.

If j is odd, we could then replace the faces $f_{3,0}, f_{3,-2}, \ldots, f_{3,-j+1}$ by $f_{2,1}, f_{2,-1}, \ldots, f_{2,-j}$, and clearly we have a larger Clar cover of G (see Fig. 5 for an example). Clearly the leftover graph has a perfect matching, i.e., a path of odd length has been removed from the boundary and no internal matchings have been disturbed.

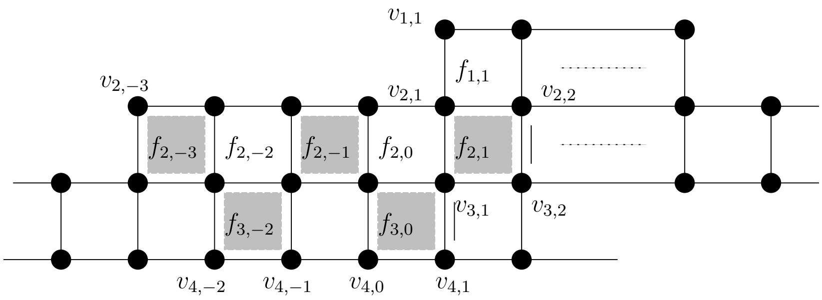

Figure 5: An illustration for getting a larger Clar cover

If j is even, then we could assume that the edge $v_{3,-j+1}v_{4,-j+1}$ is in the perfect matching $M(G^*)$. If $v_{3,-j}v_{4,-j}$ is on the boundary of G^*, then based on Observation 2, we know $K'(G^*)$ is not maximum (see Fig. 6 for an example). Now the leftover case is that there are more faces on the left of $f_{3,-j}$. Suppose that the left-most face in the third row is $f_{3,-t}$.

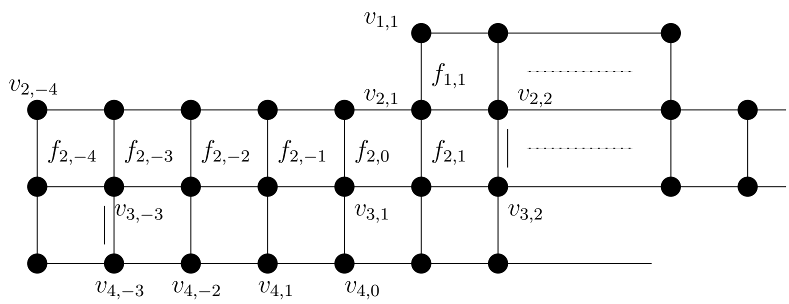

Figure 6: An illustration that $v_{3,-j}v_{4,-j}$ has to be in $M(G^*)$

In this case, we know that edge $v_{4,-j}v_{5,-j}$ is either in $M(G^*)$ or in K'_{G^*}, and along the same line of reasoning as for the second row of G^*, we could show that either we could get a larger Clar cover of G or $v_{4,-t+1}v_{5,-t+1}$ is in the perfect matching $M(G^*)$. The same argument terminates when the row containing the left-most bottom face is encountered, i.e. the row contains the face $f_{x,-y}$ and there are no faces with $f_{x,-w}$ where $w \geq y$. See Fig. 7 for details. In this case, we find a larger Clar cover which has more squares than $C(G)$, a contradiction. Consequently $G - C'$ has a unique perfect matching. □

The following theorem was proved in [6] and [8].

Theorem 4. *If G is a planar bipartite graph and M is a perfect matching in G,*

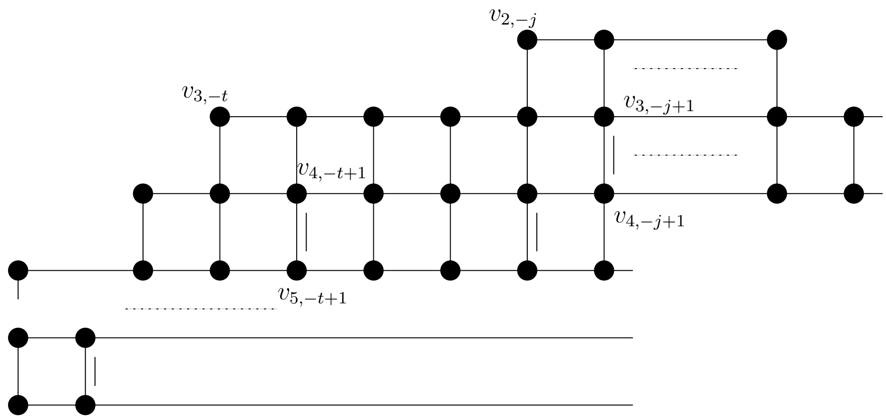

Figure 7: An illustration of termination case

then the forcing number of M equals the maximum number of disjoint M-alternating cycles.

Combining Theorems 3 and 4, it is clear that $F(G) \geq C(G)$. The following corollary was proved in [12].

Corollary 5. *Let G be a plane elementary bipartite graph with a perfect matching M and let C be an M-alternating cycle. Then there exists an M-resonant face in the interior of C.*

Similar to the proof of Theorem 9 in [8], taking each M-resonant face as a component of a Clar cover, the above corollary implies that the number of M-alternating cycles is no less than the Clar number, This implies that $F(G) \leq C(G)$. Now we can conclude with the following.

Theorem 6. *If G is an elementary polyomino, then $F(G) = C(G)$.*

Based on Theorem 2, we have the following theorem.

Theorem 7. *If G is an elementary polyomino, then the maximum forcing number of G can be computed in polynomial time.*

3 The maximum forcing number of a non-elementary polyomino

In this section we will consider the case of non-elementary polyominos. To find the Clar number and maximum forcing number of a non-elementary polyomino, we will consider decomposing a non-elementary polyomino into a number of elementary components.

In [9], Zhang et al. developed an $O(n^2)$ algorithm to decompose a hexagonal system into a number of regions consisting of fixed bonds and elementary components.

Later, Zhang [10, 11] developed a more efficient algorithm for the decomposition for more general cases; they showed that there is an algorithm of time complexity $O(|E| + |V|)$ to determine all elementary components and the fixed bonds of a bipartite graph G. The result is the following.

Theorem 8 ([10])**.** *Let G be a bipartite graph with a perfect matching M. There is an algorithm of $O(|E| + |V|)$ complexity to decompose G into a number of regions consisting of fixed bonds and a number of elementary components.*

Since a non-elementary polyomino with a perfect matching can be composed into a number of elementary components and fixed bonds, and the maximum forcing number of the non-elementary polyomino equals the sum of the maximum forcing number of those elementary components, it follows that the Clar number of the original non-elementary polyomino equals the sum of the Clar number of those elementary components. Thus we have the following result.

Theorem 9. *If G is a non-elementary polyomino with perfect matchings, then $F(G) = C(G)$.*

Since the complexity of decomposing a non-elementary polyomino with perfect matchings into a number of elementary components and fixed bonds is $O(|V|)$, and by Theorem 6, the maximum forcing number of every elementary component can be computed in polynomial time, it follows that the maximum forcing number of a non-elementary polyomino with perfect matchings can be computed in polynomial time. Thus we obtain the following result.

Theorem 10. *If G is a non-elementary polyomino with perfect matchings, then the maximum forcing number of G can be computed in polynomial time.*

Combining Theorems 7 and 10, we obtain the result stated in Theorem 1.

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