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Maximum Forcing Number of Hexagonal Systems[1]

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Abtract. The forcing number of a perfect matching M of a graph G is the cardinality of the smallest subset of M that is contained in no other perfect matching of G. A spanning subgraph C of a hexagonal system H is said to be a Clar cover of H if each of its components is either a hexagon or an edge, the maximum number of hexagons in Clar covers of H is called the Clar number of H. In this paper, we show that the maximum forcing number of a hexagonal system is equal to its Clar numbers, based on this result, we have that the maximum forcing number of the hexagonal systems can be computed in polynomial time, which answers the open question proposed by Afshani etal.[1] when G is a hexagonal system. Moreover, we obtain the maximum forcing number of some special classes of hexagonal systems.

1 Introduction

Let G be a graph that admits 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 matching of G. The cardinality of a forcing set of M with the smallest size is called the forcing number of M, and is denoted by $f(G; M)$. The minimum and maximum of $f(G; M)$ over the set of all perfect matchings M of G is denoted by $f(G)$ and $F(G)$, respectively. A hexagonal system is a finite connected plane graph with no cut vertex in which every interior region

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is surrounded by a regular hexagon of side length 1. Let H be a hexagonal system. A spanning subgraph C of H is said to be a Clar cover of H if each of its components is either a hexagon or an edge[2]. The maximum number of hexagons in Clar covers of H is called Clar number of H, and denoted by $C(H)$[3-7].

The idea of a forcing number was inspired by practical chemistry problems. It is for this reason that hexagonal systems were the first to be studied. This concept was proposed by Harary et al.[8]. The same idea appeared in earlier papers by Randić and Klein[9, 10] using instead the nomenclature of innate degree of freedom of a Kekulé structure. The forcing numbers of bipartite graphs, in particular, for square grids, stop signs, torus, and hypercube, have been considered[1,11-14]. Recently, spectra of forcing numbers for some special fullerene graphs C_{20}, C_{60}, C_{70} and C_{72} have been established[15-18]. Adams et al.[11] proved it is NP-complete to find the smallest forcing set of a bipartite graph with maximum degree 3. Later, Afshani etal.[1] proved it is NP-complete to find the smallest forcing number of a bipartite graph with maximum degree 4, and proposed the following question: Given a graph G, what is the computational complexity of finding the maximum forcing number of G.

In this paper, we show that the maximum forcing number of hexagonal systems are equal to their Clar numbers. Based on this result, we have that the maximum forcing number of hexagonal systems can be computed in polynomial time, which answer the above question proposed by Afshani etal.[1] when G is hexagonal systems. Moreover, we obtain the maximum forcing number of some special classes of hexagonal systems.

2 Preliminaries

In this section we give some definitions and Theorems which will be used in the proof of the main result.

Definition 1 *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 not in M. The maximum number of disjoint M-alternating cycles in G is denoted by $c(M)$.*

Theorem 2 ([12, 19]) *If G is a planar bipartite graph and M is a perfect matching in G, then the forcing number of M is equal to the maximum number of disjoint M-alternating cycles, that is $f(G, M) = c(M)$.*

Theorem 3 ([20]) *Let H be a hexagonal system with a perfect matching M and C' be a set of hexagons in a Clar cover of H. Then $H - C'$ has a unique 1-factor.*

In [21], Hansen and Zheng formulate the Clar number problem as an interger program. Later, Abeledo and Atkinson[22] generalized the concept of Clar number to bipartite and 2-connected plane graphs, and prove that:

Theorem 4 ([22]) *The Clar number can be computed in polynomial time using linear programming methods.*

Definition 5 *A connected bipartite graph is called elementary (or normal) if its every edge is contained in some perfect matching. Let G be a plane bipartite graph, a face of G is called resonant if its boundary is an alternating cycle with respect to some perfect matching of G.*

Theorem 6 ([23]) *Let G be a plane bipartite graph with more than two vertices. Then each face of G is resonant if and only if G is elementary.*

Corollary 7 ([23]) *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.*

3 Main result

Theorem 8 *Let G be a plane elementary bipartite graph. Then $F(G) \geq C(G)$.*

Proof: Let C be a Clar cover of G with precisely $C(G)$ faces and M be a perfect matching of G corresponding to a Clar cover C, then $c(M) \geq C(G)$. By Theorem 2, $f(G, M) = c(M)$, thus, $F(G) \geq f(G, M) = c(M) \geq C(G)$.

Theorem 9 *Let H be an elementary hexagonal system. Then F(H)=C(H).*

Proof: By Theorem 8, we have $F(H) \geq C(H)$. Now we show that $F(H) \leq C(H)$ in the following.

Let M be a perfect matching of H such that $f(H, M) = F(H)$. According to Theorem 2, there exist $F(H)$ disjoint M-alternating cycles, say as $C_1, C_2, \ldots, C_{F(H)}$. Let C^* denote the subgraph of H such that the outer boundary of C^* is the M-alternating cycle C. If no C_i^* is a subgraph of any other C_j^*, then by Corollary 7, C_i^* has a resonant hexagon

K_i^*, for $i = 1, 2, \cdots, F(H)$, and so there exist at least $F(H)$ pairwise disjoint resonant hexagons in H, by the definition of Clar number, we have $F(H) \leq C(H)$.

Otherwise, there exists C_i^*, which is subgraph of C_j^*, $i \neq j$. Without loss of generality, we can select C_i^* such that as many as possible subgraphs C_j^* containing C_i^*. Take the minimum subgraph C_j^* containing C_i^*. If C_j^* contain m disjoint M-alternating cycles, being the selection of C_i^*, we have that these m M-alternating cycles are not pairwise containing. According to Corollary 7, every M-alternating cycle contains an M-alternating hexagon, and these m M-alternating hexagons are pairwise disjoint. Hence, C_j^* contain m disjoint M-alternating hexagons, it is clear that the perfect matching of the resulting graph obtained by deleting m M-alternating hexagons from C_j^* is not unique and then by Theorem 3 we have $C(C_j^*) > m$. There exists a Clar cover of C_j^* such that $C(C_j^*) \geq m+1$, let M' be a perfect matching of C_j^* corresponding to the Clar cover. Then C_j^* contains at least $m+1$ disjoint M'-alternating hexagons, let $M_1 = M - M|_{C_j^*} + M'$, then $c(M_1) \geq c(M)$, and these disjoint M'-alternating hexagons are also disjoint M_1-alternating hexagons. If these disjoint M_1-alternating hexagons of C_j^* still contain in some subgraph C_k^*, by the similar method, we can find a perfect matching M_2 of H such that $c(M_2) \geq c(M_1)$, and all M_2-alternating cycles in C_k^* are disjoint M_2-alternating hexagons. Repeated in this way, we can finally obtain a perfect matching M_t of H such that $c(M_t) \geq c(M_{t-1}) \geq \cdots \geq c(M)$, and all these disjoint M_t-alternating cycles are M_t-alternating hexagons. So there is a Clar cover of H containing $c(M_t)$ hexagons, then $C(H) \geq c(M_t) \geq c(M) = F(H)$. This complete the proof.

By Theorem 4 and Theorem 9, we have the following:

Theorem 10 *Let H be an elementary hexagonal system. Then the maximum forcing number of H can be computed in polynomial time.*

From the proof of Theorem 9, it can be seen that, if the result in Theorem 3 can be generalized to a polyomino, then the conclusion in the following conjecture would hold.

Conjecture 11 Let G be an elementary polyomino. Then the maximum forcing number of G can be computed in polynomial time.

Now we consider the maximum forcing number of some special classes of hexagonal systems in the following.

Let M be a perfect matching of hexagonal system H, $E(M)$ denote the set of those edges of M. The set of $E(M)$ can be partitioned into three subsets, $E_1(M)$, $E_2(M)$ and $E_3(M)$, such that all edges from $E_i(M)$ are mutually parallel, $i = 1, 2, 3$. The number of elements $E_1(M)$, $E_2(M)$ and $E_3(M)$ will be denoted by x, y and z, respectively, and by convention $x \le y \le z$. Use the abbreviate notation T for the triple (x, y, z). The following result was given by Zhang et al.

Theorem 12 (**[24]**) *For a hexagonal system H with a perfect matching M, then the triple T is independent of M, namely, T is an invariant of H.*

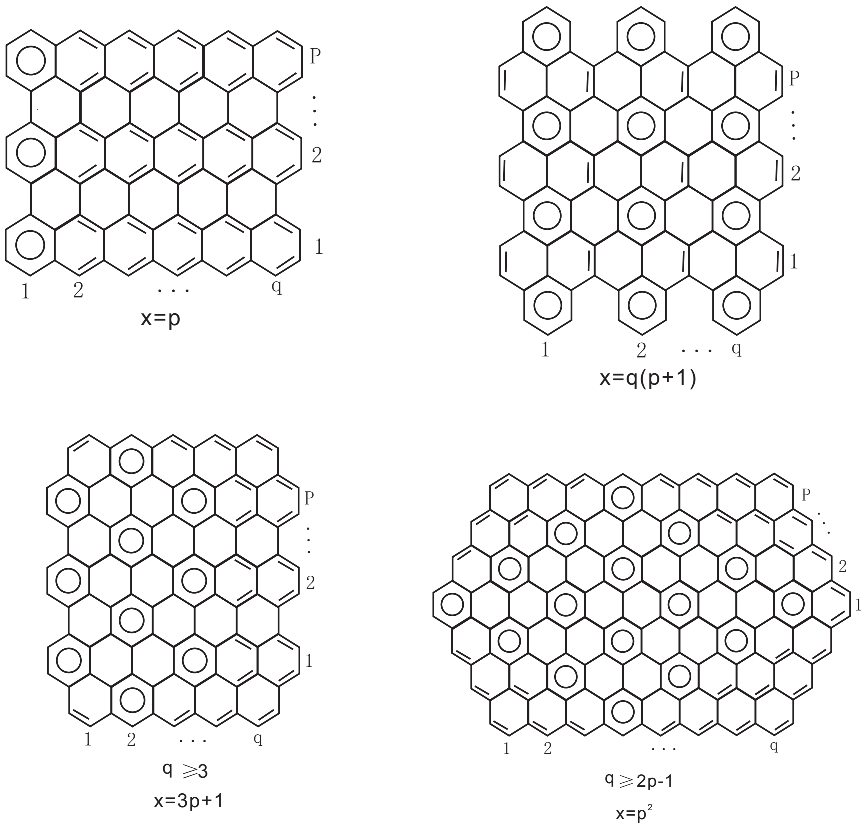

Figure 1

Theorem 13 (**[24]**) *Let H be a hexagonal system in Fig.1 with $T = (x, y, z)$. Then $C(H) = x$.*

According to the Theorem 9, we have the following result.

Theorem 14 *Let H be a hexagonal system in Fig.1 with $T = (x, y, z)$. Then $F(H) = x$.*

A hexagonal system is said to be a CHS (see Fig. 2) if it can be dissected by parallel horizontal lines $L_i (i = 1, 2, \cdots, t)$ such that it decomposes into $t + 1$ paths, the one top and the one bottom must be of even length. Zhang and Li[25] discuss some topological properties of CHS and obtain a fast algorithm for finding its Clar number. According to the Theorem 9, we can also obtain a fast algorithm for finding the maximum forcing number of CHS.

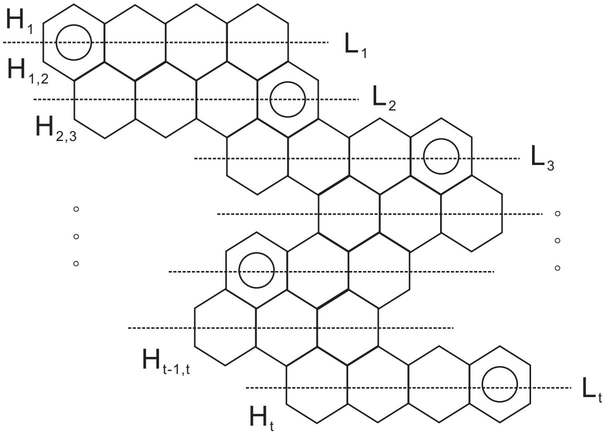

Figure 2

Many classes of HS are CHS, for example, Single chains, Multiple chains, Ribbon, Chevron[26] etc. According to the Theorem 9, we can easily give their maximum forcing number.

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