MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 721-732

ISSN 0340 - 6253

Conjugated Circuits and Forcing Edges

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(Received February 27, 2012)

Abstract

An even cycle C in a graph G is called a *conjugated circuit* if a perfect matching of C can be extended to a perfect matching of G. An edge of a graph G is called a *forcing edge* if it is contained in exactly one perfect matching of G. The two concepts have played important roles in the studies of Kekulé structures of benzenoid hydrocarbon molecules. In this paper, we first present a different proof for a result just published in the 2012 article [9] by Klavžar and Salem, that is, all circuits of a 2-connected outerplanar bipartite graph are conjugated. Then we further give a characterization for the conjugated circuits in any 2-connected (no matter whether bipartite or not) outerplanar graph with an even number of vertices. We also show that each edge of a connected bipartite graph G is a forcing edge if and only if G is an even cycle or an edge, which generalizes a main result in the 1991 paper [6] on polyhexes by Harary, Klein, and Živković. Finally we present miscellaneous related results on perfect matching forcings, one of which asserts that a bipartite graph G with $2n$ vertices has its forcing number attaining the largest possible value $n-1$ if and only if G is the complete bipartite graph $K_{n,n}$.

1 Introduction

An edge of a graph G is called a *forcing edge* if it is contained in exactly one perfect matching of G. This notion first appeared in a 1991 paper [6] by Harary, Klein, and Živković on polyhexes. Since then, problems related to forcing edges have been investigated intensively for benzenoid systems (also called hexagonal systems, or polyhexes), because they are closely related to the study of molecule resonance structures in chemistry. In fact, the root of the concept of forcing edges can be traced to the works ([8] and [12]) by Randić and Klein during 1985-1987. Most known results on forcing perfect matchings can be seen in the 2011 survey [2].

A *benzenoid system* is a finite 2-connected subgraph of a plane hexagonal lattice whose finite faces are regular hexagons, which is often used to represent a benzenoid hydrocarbon in chemistry. In 1991, Harary et al. [6] proved that the single hexagon is the only benzenoid system each edge of which is a forcing edge.

A benzenoid system H is called *catacondensed* if every vertex of H is on the boundary of H. Clearly, a catacondensed benzenoid system is a special 2-connected outerplanar bipartite graph. An even cycle C in a graph G is called a *conjugated circuit* if a perfect matching of C can be extended to a perfect matching of G.

In 2006 Salem [13] proved that all circuits of a catacondensed benzenoid system are conjugated, which is a generalization of a 1983 result by Gutman [3], and a rediscovery of a 1994 result by Guo and Zhang [5]. In the just published paper [9], Klavžar and Salem extended it further to all 2-connected outerplanar bipartite graphs. In fact they derived the result from a more general theorem which is proved by utilizing several results in Zhang and Zhang's 2000 paper [15] including the tool of reducible face decomposition.

Here we make a note that before the publication of [9], we had independently discovered the same result that all circuits in a 2-connected outerplanar bipartite graph are conjugated. In this paper, after presenting our different proof (which may be easier to follow by readers) for this result, we further give a characterization for the conjugated circuits in any 2-connected (no matter whether bipartite or not) outerplanar graph with an even number of vertices. We also show that each edge of a connected bipartite graph G is a forcing edge if and only if G is an even cycle or an edge, which generalizes a main result in the 1991 paper [6] on polyhexes by Harary, Klein, and Živković. Finally we present miscellaneous related results on perfect matching forcings.

2 Preliminaries

For the related mathematical concepts in chemistry, we refer to the book [4] by Gutman and Polansky (1986). For details of the related study in chemistry, the reader is referred to the survey [11] by Randić (2003).

Throughout the paper, G always denotes a finite graph that is connected and simple. A *perfect matching* (or, 1-*factor*) of G is a set of disjoint edges that covers all vertices of G. Perfect matchings of a molecule graph are also called *Kekulé structures* in chemistry, which play a key role in the molecule resonance energy and aromaticity of organic molecules. An edge of G is called *allowed* if it is contained in a perfect matching of G, and *forbidden* otherwise. A graph G is called *elementary* if the union of all perfect matchings of G forms a connected subgraph. So any elementary graph with more than two vertices has at least two perfect matchings. In particular, a connected bipartite graph G is elementary if and only if each edge of G is contained in some perfect matching of G, see [10].

Let M be a perfect matching of a graph G. A cycle C of G is called an *M-alternating cycle* if its edges are alternately in M and $E(G) - M$, and we call C an *alternating cycle* briefly if there is no need to specify the perfect matching M. An alternating cycle is also called a *conjugated circuit* in literature. The *symmetric difference* of two perfect matchings M and N of G, denoted by $M \oplus N$, is the set of edges contained in either M or N, but not in both. An *(M, N)-alternating cycle* of G is a cycle whose edges are in M and N alternately. It is well known [10] that the symmetric difference of two perfect matchings M and N of G is a disjoint union of (M, N)-alternating cycles. By definition, we can see that M is the unique perfect matching of G if and only if G has no M-alternating cycles. Kotzig [7] showed that if a connected graph G has a unique perfect matching M, then G has a bridge in M. Therefore, any 2-connected graph with a perfect matching has at least two perfect matchings.

A *forcing set* of a perfect matching M is a subset $S \subseteq M$ such that S is not contained in any other perfect matching of G. The empty set is a forcing set of M if and only if M is the unique perfect matching of G. A *forcing edge* of a graph G is an edge contained in exactly one perfect matching of G. So a forcing edge of a graph G constitutes a forcing set with cardinality 1. The *forcing number* (or, *degree of freedom*) of a perfect matching M, denoted by $f(G, M)$, is the cardinality of a smallest forcing set of M. The *forcing number* of a graph G, denoted as $f(G)$, is the smallest forcing number of all perfect matchings of G. The *spectrum of forcing numbers* of a graph G, denoted by *Spec*(G), is the set of forcing numbers $f(G, M)$ of all perfect matchings M of G.

Let $G = (B, W)$ be a bipartite graph with two color classes B and W. In the book by Lovász and Plummer ([10], p. 139), a necessary condition is given for $G = (B, W)$ to have a unique perfect matching, that is, the vertices of G can be labeled as $B = \{b_1, b_2, \cdots, b_m\}$ and $W = \{w_1, w_2, \cdots, w_m\}$ such that for every edge $b_i w_j$, $i \geq j$. It follows that for each $1 \leq i \leq m$, $\deg_G(b_i) \leq i$ and $\deg_G(w_i) \leq m - i + 1$. In particular, b_1 and w_m must be degree-1 vertices in G. Therefore, the following theorem comes immediately.

Theorem 2.1 [10] Any bipartite graph with a unique perfect matching must contain a degree-1 vertex in each color class.

Clearly, Theorem 2.1 can also be stated as follows:

Theorem 2.1* If a bipartite graph G does not have a degree-1 vertex in a color class, then G has either no perfect matchings or at least two perfect matchings.

A graph is called a *planar graph* if it can be embedded in the plane so that its edges intersect only at their end vertices. A *plane graph* is a planar graph which is already drawn on the plane in such a way. A plane graph divides the plane into regions which are called faces. Each bounded region is called a *finite face*, and the unbounded region is called the *infinite face*.

An *outerplanar graph* is a graph that can be embedded in the plane so that all its vertices lie on the boundary of the graph. There is a Kuratowski-type characterization of outerplanar graphs (refer to Theorem 7.18 in [1]) stated as follows: a graph is outerplanar if and only if it contains no subgraphs homeomorphic to the complete graph K_4 or complete bipartite graph $K_{2,3}$, with one exception that is the graph obtained from K_4 by deleting one edge. (Here we make a note by passing that this characterization was stated with errors in some recent references, such as the book [14] (page 251) published in 1990.)

A face s (finite or infinite) of a plane graph G is said to be *M-resonant* if the boundary of s is an M-alternating cycle with respect to some perfect matching M of G. An M-resonant face is briefly said to be *resonant* when there is no need to specify the perfect matching M. The following characterization of a plane elementary bipartite graph in terms of resonant faces was given by H. Zhang and F. Zhang [15] in 2000.

Theorem 2.2 [15] Let G be a plane bipartite graph with more than two vertices. Then each face of G (including the infinite face) is resonant if and only if G is elementary.

Theorems 2.1 and 2.2 will be utilized to obtain our main results in the paper.

3 Main Results

3.1 Conjugated Circuits

First, we present a different proof for the following result just published in [9] by Klavžar and Salem, which had also been independently discovered by us before the publication of [9].

Theorem 3.1 All circuits in a 2-connected outerplanar bipartite graph are conjugated.

Proof. Let G be a 2-connected outerplanar bipartite graph. Since G is outerplanar, it can be embedded in the plane so that all vertices lie on the boundary B of G. Note that B must be an even cycle since G is bipartite. Then B is the union of two perfect matchings of G. It follows that the union of all perfect matchings of G is connected since it contains B. Therefore, G is elementary.

Let C be a circuit of G. If C is the boundary of a face of G, then C is conjugated since each face of a plane elementary bipartite graph is resonant by Theorem 2.2. If C is not the boundary of any face of G, then we can construct a spanning subgraph H of G by removing all edges of G that do not belong to C but have both end vertices on C. Then C is the boundary of a face of H. It is clear that H contains B. So H is also a plane elementary bipartite graph. Then C is conjugated in H with respect to some perfect matching M of H by Theorem 2.2. Note that any perfect matching of H is also a perfect matching of G. Hence, C is conjugated in G. ■

Note that in the above proof we also proved the following proposition.

Proposition 3.2 Any 2-connected outplanar graph with an even number of vertices is elementary.

It is natural to further consider the conjugated circuits in non-bipartite 2-connected outerplanar graphs. We obtain a characterization of the conjugated circuits in the following theorem.

Theorem 3.3 Let G be a 2-connected outerplanar graph with an even number of vertices. Then a circuit C of G is conjugated if and only if C does not contain any forbidden edges of G.

Proof. The necessity is obvious. It remains to prove the sufficiency. Assume that G is embedded in the plane with the hamiltonian even cycle B as the boundary. Let H be the spanning subgraph of G obtained by removing all forbidden edges of G. We first show that H is a 2-connected outerplanar bipartite graph. It is clear that H is 2-connected since it contains the hamiltonian even cycle B. Suppose that H is not bipartite. Then H has an odd cycle C. Color the vertices of H in two colors so that the boundary cycle B is properly 2-colored. Hence, C must have an edge uv whose two end vertices have received the same color. It is clear that uv cannot be an edge of B. Recall that G is a plane graph whose boundary is the hamiltonian even cycle B. Then $G - \{u, v\}$ is disconnected with two components S_1 and S_2. Because vertices u and v have the same color on the properly 2-colored even cycle B, each of S_1 and S_2 must have an odd number of vertices. Then $G - \{u, v\}$ has no perfect matchings. It follows that uv is a forbidden edge of G and so cannot be an edge of H. This is a contradiction. Therefore, H is a bipartite graph.

By Theorem 3.1, all circuits of H are conjugated since H is a 2-connected outerplanar bipartite graph. Let C be an arbitrary circuit of G that does not contain any forbidden edges of G. Then C is a circuit of H and so is conjugated in H with respect to some perfect matching M of H. It follows that C is also a conjugated circuit of G since any perfect matching of H is a also a perfect matching of G. ■

Now we can give the following corollary.

Corollary 3.4 Let G be a 2-connected outerplanar graph with an even number of vertices. Then

(i) the spanning subgraph of G obtained by removing all forbidden edges (if any) of G is a 2-connected outerplanar elementary bipartite graph and it is the maximum spanning subgraph of G that is 2-connected, bipartite, and elementary;

(ii) the number of forbidden edges of G is at least the maximum number of edge disjoint odd cycles in G.

Proof. As in the proof of Theorem 3.3, we may assume that G is embedded in the plane with the hamiltonian even cycle B as the boundary, and let H be the spanning subgraph of G obtained by removing all forbidden edges of G.

(i) By the proof of Theorem 3.3, H is a 2-connected outerplanar bipartite graph. Moreover, H is elementary by Proposition 3.2. So we only need show the extremeness of H. Let K be a 2-connected spanning subgraph of G that is bipartite and elementary. It is known (see [8], p.122) that a connected bipartite graph is elementary if and only if each edge is allowed. Then each edge of K is allowed and so is contained in a perfect matching of K. It follows that any edge of G contained in K is also contained in a perfect matching of G, since any perfect matching of K is also a perfect matching of G. Hence, K does not contain any forbidden edges of G. Thus, K is a subgraph of H. That is, H is the maximum spanning subgraph of G that is 2-connected and elementary bipartite.

(ii) Let m be the maximum number of edge disjoint odd cycles in G. By part (i), we can see that each of the m edge disjoint odd cycles of G contains a forbidden edge. This proves that the number of forbidden edges of G is greater than or equal to m. ■

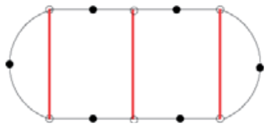

Figure 1: An outerplanar graph with 2 edge disjoint odd cycles and 3 forbidden edges.

Note that in Corollary 3.4, the number of forbidden edges of a 2-connected outerplanar graph G may be equal to or strictly greater than the maximum number of edge disjoint odd cycles in G. The first case can be seen from the examples when G is bipartite or $G = K_4 - e$ where e is an edge of the complete graph K_4. The second case can be seen from Fig. 1.

3.2 Forcing edges

Theorem A in [6] by Harary et al. states that a single-hexagon is the only polyhex in which every edge is a forcing edge. In this section, we first establish the following proposition which will enable us to generalize the theorem of Harary et al. from polyhexes to all connected bipartite graphs.

Proposition 3.5 Let G be a bipartite graph with minimum degree > 1. If uv is a forcing edge of G, then each end vertex of uv is adjacent to a degree-2 vertex of G that is different from u and v.

Proof. Without loss of generality, we may assume that G is connected in the proof. If uv is a forcing edge of G, then the subgraph $H = G - \{u, v\}$ has a unique perfect matching. By Theorem 2.1, H has two degree-1 vertices x and y contained in different color classes of $H \subseteq G$. Since G is a connected bipartite graph with minimum degree > 1, x must be adjacent to exactly one vertex of u and v in G, say, x is adjacent to u in G. Then, by the same reason, y must be adjacent to v in G. It follows that both x and y have degree 2 in G. This completes the proof. ■

Remark 3.6 We have the following observations for Proposition 3.5.

1. None of the following two conditions can be omitted in Proposition 3.5.

   (a) The condition that G is a bipartite graph cannot be omitted, see Fig. 2 (a).

(b) The condition that G has minimum degree > 1 cannot be omitted, see Fig. 2 (b).

In both examples, uv is a forcing edge of a graph G missing one of the two conditions, but each end vertex of uv is adjacent to a degree-3 vertex of G different from u and v.

2. The necessary condition for a forcing edge given in Proposition 3.5 is also sufficient if the graph G in consideration is a linear hexagonal chain (i.e., G is a catacondensed benzenoid system in which the geometric centers of all hexagons are on the same straight line.), see Fig. 3.

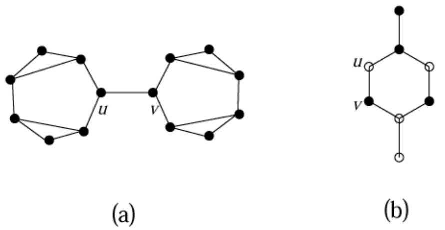

Figure 2: A forcing edge each end vertex of which is adjacent to a degree-3 vertex.

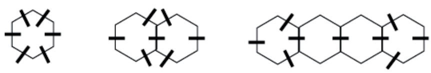

Figure 3: Forcing edges (marked by small bars) in linear hexagonal chains.

By Proposition 3.5, we can get the following theorem, which generalizes the Theorem A in [6] by Harary et al. from polyhexes to connected bipartite graphs.

Theorem 3.7 Let G be a connected bipartite graph. Then each edge of G is forcing if and only if G is an even cycle or an edge.

Proof. The sufficiency is obvious. We only need prove the necessity. Let G be a connected bipartite graph each edge of which is forcing. If G has only two vertices, then G is K_2. So we may assume that G has more than two vertices. We will show that G is an even cycle as follows.

First, we claim that each vertex of G has degree > 1. Otherwise, G must have an edge adjacent to a pendant edge and so G has a forbidden edge, which contradicts the condition that each edge of G is forcing.

Next, for any vertex v of G, we show that $\deg_G(v) = 2$. Let uv be an edge incident to the vertex v. By the given condition on G, uv is a forcing edge. So by Proposition 3.5, v is adjacent to a degree-2 vertex y of G in $V(G) \setminus \{u, v\}$. Since $\deg_G(y) > 1$ and G is bipartite, y must be adjacent to a vertex $w \in V(G) \setminus \{u, v, y\}$. Now, since the edge yw is also a forcing edge by the given condition on G, y must be adjacent to a degree-2 vertex z of G in $V(G) \setminus \{y, w\}$ by Proposition 3.5. Recall that $\deg_G(y) = 2$ and both v, w are adjacent to y. Then we must have $v = z$ and so $\deg_G(v) = 2$.

Therefore, all vertices of G have degree two. So, G must be an even cycle as a connected bipartite graph. ■

By Proposition 3.5, we have the following two corollaries, which give a lower bound on the forcing number of a bipartite graph involving vertex degrees.

Corollary 3.8 Let G be a bipartite graph with a perfect matching. If G has the minimum degree > 2, then G has no forcing edges and its forcing number $f(G) > 1$.

It is well known that any regular bipartite graph has a perfect matching. From the above result we immediately see the following.

Corollary 3.9 Let G be an r-regular bipartite graph with $r > 2$. Then G has no forcing edges and its forcing number $f(G) > 1$.

4 Miscellaneous

The classical Kotzig's theorem (1959) asserts that if a connected graph G has a unique perfect matching M, then G has a bridge in M [7]. So Kotzig's theorem implies that any 2-connected graph with a perfect matching has at least two perfect matchings. By the definition of a forcing set, a set S of independent edges of a graph G is forcing if and only if $G - V(S)$ has a unique perfect matching (including the case when $G - V(S)$ is empty). Then Kotzig's theorem implies the following result.

Theorem 4.1 Let G be a connected graph with a perfect matching M. If $S \subset M$ $(S \neq M)$ is a forcing set of M, then $G - V(S)$ must have a bridge which belongs to M.

The following lower bound on the forcing number of all k-connected graphs comes as a corollary of Theorem 4.1.

Corollary 4.2 Let G be a k-connected graph with a perfect matching. Then its forcing number $f(G) \geq \lfloor \frac{k}{2} \rfloor$.

Proof. Let G be a k-connected graph. Then removing any $\lfloor \frac{k}{2} \rfloor - 1$ disjoint edges together with their vertices, the resultant graph can not have a bridge. By Theorem 4.1, any forcing set of G has at least $\lfloor \frac{k}{2} \rfloor$ edges. ■

It is well known (see, for example, [1]) that any regular bipartite graph has a perfect matching. So the following result can be obtained from Theorem 2.1* or from the above corollary since any connected regular bipartite graph with more than two vertices is 2-connected.

Corollary 4.3 Any connected regular bipartite graph with more than two vertices has at least two perfect matchings.

Corollary 4.4 If a bipartite graph G is k-extendable (i.e., any k-matching is contained in a perfect matching) and for any k-matching S, $G - V(S)$ does not have a degree-1 vertex in one color class, then its forcing number $f(G) > k$.

Note that $0 \leq f(G) \leq f(G, M) < \frac{|V(G)|}{2}$ for any perfect matching M of G. For a graph G with a perfect matching M, $f(G, M) = 0$ if and only if M is the unique perfect matching of G if and only if $f(G) = 0$. A graph G has a forcing edge if and only if $f(G) = 0$ or 1. If G has at least two perfect matchings, then G has a forcing edge if and only if $f(G) = 1$. The following properties for a graph G whose $Spec(G)$ only has a small forcing number 0 or 1 comes immediately from definitions.

Proposition 4.5 Let G be a graph with a perfect matching. Then

(i) $Spec(G) = \{0\}$ if and only if $0 \in Spec(G)$ if and only if $f(G) = 0$ if and only if G has a unique perfect matching.

(ii) $Spec(G) = \{1\}$ if and only if G has more than one perfect matching and every perfect matching M has $f(G, M) = 1$, i.e., every perfect matching of G contains a forcing edge.

Proposition 4.6 Let G be a graph with a perfect matching. Then $Spec(G) = \{0\}$ or $\{1\}$ if and only if after deleting all forcing edges of G the resultant graph has no perfect matchings.

Proof. Necessity: Assume that the resultant graph after the deletion has a perfect matching M. It is clear that M is also a perfect matching of G. Then M does not contain any forcing edge and so $f(G, M) > 1$. This contradicts the condition that $Spec(G) = \{0\}$ or $\{1\}$.

Sufficiency: Assume that $Spec(G) \neq \{0\}$ or $\{1\}$. Then G must have a perfect matching M such that $f(G, M) > 1$, that is, M does not contain any forcing edge of G, and so M is contained in the resultant graph after the deletion. This contradicts the assumption that the resultant graph has no perfect matchings. ■

The largest possible forcing number $f(G)$ for a graph G is $f(G) = \frac{1}{2}|V(G)| - 1$. Assume that $|V(G)| = 2n$. By definition, it is clear that $f(G) = n - 1$ if and only if $Spec(G) = \{n - 1\}$. All the bipartite graphs G with the largest possible forcing number can be determined as follows.

Proposition 4.7 Let G be a bipartite graph with $2n$ vertices. Then its forcing number $f(G) = n - 1$ if and only if G is the complete bipartite graph $K_{n,n}$.

Proof. The sufficiency is clear. We show the necessity by contradiction. Let G be a bipartite graph with $2n$ vertices and $f(G) = n - 1$. Assume that G is not the complete bipartite graph $K_{n,n}$. Let X and Y be two color classes of G. Then there are two vertices $x \in X$ and $y \in Y$ such that x and y are not adjacent. Hence, for any perfect matching M of G, there are vertices $x_1 \in X \setminus \{x\}$ and $y_1 \in Y \setminus \{y\}$ such that M contains the edges xy_1 and x_1y. The remaining vertices of G are covered by a set of $n - 2$ edges of M, which clearly forces M. Thus, $f(G) \leq n - 2$. This contradicts the assumption that $f(G) = n - 1$. ■

Acknowledgments We would like to thank the referees for their helpful comments, especially for their informing us that Theorem 3.1 already appeared in the just published article [9] by Klavžar and Salem.

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