On Plane Bipartite Graphs without Fixed Edges

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Abstract---An edge of a graph *H* with a perfect matching is a fixed edge if it either belongs to none or to all of the perfect matchings of *H*. It is shown that a connected plane bipartite graph has no fixed edges if and only if the boundary of every face is an alternating cycle. Moreover, a polyhex fragment has no fixed edges if and only if the boundaries of its infinite face and the non-hexagonal finite faces are alternating cycles. These results extend results on generalized hexagonal systems from [1].

Keywords---Perfect matching, Fixed edge, Alternating cycle, Plane bipartite graph, Polyhex fragment, Generalized hexagonal system.

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1 Introduction

Benzenoid hydrocarbons constitute a class of conjugated hydrocarbons. For many aspects of these compounds, the reader is invited to consider the recent extensive survey of Randić [2]. Benzenoid hydrocarbons can be represented by graphs, known as hexagonal systems, and so they lend themselves to graph-theoretic analysis.

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A fascinating amount of theoretical work has been done on hexagonal systems, but here we only briefly mention some areas of this research. Two of the central problems are to find the number of perfect matchings (or Kekulé structures) of a hexagonal system and to try to relate this number to physico-chemical properties of the underlying compound [3, 4]. Interactions among the Kekulé structures of a given benzenoid hydrocarbon turned out to be important as well. One way to model these interactions is by means of the so called resonance graph (or *Z*-transformation graph). These resonance graphs have a nice structure and interesting properties [5-9] and their definition offers several possibilities for generalizations [10, 11].

An edge is fixed if it belongs to all or none of the perfect matchings. Hence, an edge is not fixed if and only if it belongs to an alternating cycle. Randić [12, 13] used alternating cycles (or conjugated circuits) to estimate resonance energies of benzenoid hydrocarbons. In 1991, Zhang and Chen [14] characterized hexagonal systems without fixed edges. They proved:

Theorem 1.1 [14] Let *H* be a Kekuléan hexagonal system. Then the following statements are equivalent.

(i) *H* has no fixed edges.
(ii) Every hexagon of *H* is alternating.
(iii) The infinite face is alternating.

A year later, Zhang and Zheng [15] characterized generalized hexagonal systems without fixed edges. They proved:

Theorem 1.2 [15] Let *G* be a Kekuléan generalized hexagonal system. Then the following statements are equivalent.

(i) *G* has no fixed edges.
(ii) Every face of *G* is alternating.
(iii) Every non-hexagonal face is alternating.

The main goal of this note is to extend results from [15] on generalized hexagonal systems to polyhex fragments or to plane bipartite graphs. The proofs of the extensions are analogous or similar to the proofs by Zhang and Zheng and are therefore omitted or outlined, but they can be found in [16].

In the rest of this section, we define the concepts used while in the next section the results are presented.

All graphs considered are finite and simple. A *plane* graph is a planar graph together with a particular embedding in the plane.

A vertex and an edge are said to *cover* each other if they are incident. A *matching* in a graph is a set of edges no two of which have shared end vertices. A *perfect matching* or a *Kekulé structure* is a matching *M* such that each vertex of the graph is covered by some edge in *M*. A graph is called *Kekuléan* if it contains at least one perfect matching.

Let *C* be a cycle of a graph *H*. *C* is called an *alternating cycle* of *H* if there exists a perfect matching *M* of *H* such that the edges of *C* are alternately in *M* and its complement. We will say that C is *M-alternating*. Note that an alternating cycle is of even length. The symmetric difference of two distinct perfect matchings *M* and *M'*, denoted

$M \oplus M'$, consists of disjoint (M, M')-alternating cycles. An alternating cycle of a plane graph is *maximal* if it is not contained in the region bounded by another alternating cycle.

An edge of a Kekuléan graph H is a *fixed single* (*fixed double*, resp.) *edge* if it belongs to none (all, resp.) of the perfect matchings of H. An edge is *fixed* if it is either a fixed single edge or a fixed double edge.

A *hexagonal system* is a 2-connected subgraph of the hexagonal lattice without non-hexagonal finite faces. A *generalized hexagonal system* is a 2-connected subgraph of the hexagonal lattice, while a *polyhex fragment* is a connected subgraph of the hexagonal lattice. Clearly, hexagonal systems form a proper subset of generalized hexagonal systems which, in turn, form a proper subset of polyhex fragments. The *boundary* of a polyhex fragment is defined as the union of the boundaries of its infinite face and the non-hexagonal finite faces.

2 Results

All the results in this note are stated for Kekuléan graphs.

Lemma 2.1. Let H be a bipartite graph, M a perfect matching of H, C an M-alternating cycle, and P an M-alternating path. If the intersection of P and C consists of the two end vertices of P, then the edges of P and C are not fixed in H.

Before stating the next lemma, we need to define a technical notation. Let H be a polyhex fragment, e an edge of H and s a hexagon that contains e (s may or may not belong to H). By $L_{s,e}$ we denote the segment of the perpendicular bisector of e such that it starts from the midpoint of e and if s is not a hexagon of H it ends at the central point of s, otherwise it passes through s and ends at the boundary of H and is totally contained in some hexagons of H.

Lemma 2.2. Let H be a polyhex fragment, M a perfect matching of H, and e be a fixed single edge of H. If the edges e_1 and e_2 of M which cover the end vertices of e belong to a hexagon s (s may or may not belong to H), then the edges of H which intersect $L_{s,e}$ are all fixed single edges.

Lemma 2.3. Let H be a Kekuléan polyhex fragment which has both fixed edges and non-fixed edges. Then there exist a fixed single edge e and a perfect matching of H such that the edges of the perfect matching which cover the end vertices of e belong to a hexagon (not necessarily of H).

Lemma 2.4. Let H be a Kekuléan polyhex fragment which has both fixed edges and non-fixed edges. Then H has a fixed single edge in its boundary.

Lemma 2.5. Let C be a maximal alternating cycle of a plane bipartite graph H. Then the edges incident with the vertices of C in the outside of C are fixed single edges.

Theorem 2.6. Let H be a Kekuléan connected plane bipartite graph. H has no fixed edges if and only if the boundary of every face of H (including the infinite face) is an alternating cycle of H.

Proof. The "if part" is trivial and we outline the proof of the "only if" part. First, we prove that the boundary of the infinite face is an alternating cycle. *H* has an alternating cycle since it has no fixed edges. Let *C* be a maximal alternating cycle. By Lemma 2.5, *H* has no edges incident with the vertices of *C* in the outside of *C*. Since *H* is connected, *H* has neither vertices nor edges in the outside of *C*. Hence, *C* is the boundary of the infinite face.

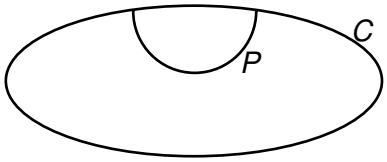

Figure 1. The path *P* divides the region bounded by *C*.

Let *F* be the boundary of a finite face of *H*. Let *C* be an alternating cycle with the property that *F* is contained in the region bounded by *C* and there is no other alternating cycle with this property contained in the region bounded by *C*. In other words, *C* is a *minimal* alternating cycle with this property. Assume that *F* is not equal to *C*. Since *H* is connected, there exists an edge *e* incident with a vertex of *C* in the inside of *C*. Let *M* be a perfect matching of *H* such that *C* is an *M*-alternating cycle. The edge *e* does not belong to *M* and since it is not fixed, it belongs to another perfect matching, *M'* say. Thus $e \in M \oplus M'$ and so it belongs to an *M*-alternating cycle, *C'* say.

If we move along the cycle *C'* starting from the end vertex of *e* on *C* and passing along *e* until we hit *C* again, we obtain a path, *P* say (not a cycle since both *C* and *C'* are *M*-alternating). This path is contained in the region bounded by *C* and it divides that region into two parts as shown in Fig. 1. It can be proved that the boundary of each of these two parts is an alternating cycle of *H*. Since *F* is the boundary of a face of *H*, *F* is contained in one of these two parts, a contradiction to the minimality of *C*. **Q.E.D.**

Remark. Theorem 2.6 also follows from a result in [17].

Theorem 2.7. A Kekuléan polyhex fragment has no fixed edges if and only if the boundaries of its infinite face and the non-hexagonal finite faces are alternating cycles.

Proof. The "only if" part follows from Theorem 2.6 and the "if part" follows from Lemma 2.4. **Q.E.D.**

As the final remark, let us add that we believe that the above results might be further extended to graphs embedded into surfaces of higher genus.

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