A characterization of 1-cycle resonant graphs among bipartite 2-connected plane graphs

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Abstract

It is proved that a bipartite 2-connected plane graph in which the common boundary of adjacent faces is a simple curve is 1-cycle resonant if and only if the outer face of G is alternating and each inner vertex has degree two. This extends a result from [X. Guo, F. Zhang, k-cycle resonant graphs, Discrete Math. 135 (1994) 113-120] that a hexagonal system is 1-cycle resonant if and only if it is catacondensed.

Keywords: bipartite plane graph, 1-cycle resonant graph, hexagonal system, alternating cycle

1. Introduction

The concept of resonance is an important topic in mathematical chemistry with a rapidly growing literature. Its origin lies in the work of Clar [1] on the aromatic sextet theory and the work of Randić on conjugated circuit model [2, 3]. Among recent related investigations let us mention the studies of resonance in toroidal polyhexes (alias toroidal graphitoids) [4, 5], in fullerene

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graphs [6], in cubic bipartite polyhedral graphs [7], and in boron-nitrogen fullerenes [8].

When dealing with chemical planar graphs it is implicitly assumed that they are plane, that is, equipped with a drawing in the plane. Many chemical planar graphs are 3-connected in which case their embedding into the plane is unique (with respect to the face structure) so the assumption of being plane is granted. On the other hand, several important chemical planar graphs are not 3-connected, for instance (chemical) trees, hexagonal graphs, and phenylenes. However, for such graphs most often a standard chemical representation in the plane is implicitly assumed. For instance, hexagonal graphs are usually defined as a class of subgraphs of a regular hexagonal lattice in the plane.

In this note we are interested in characterizing 1-cycle resonant graphs among bipartite 2-connected plane graphs. In 1994, Guo and Zhang [9] proved a characterization of k-cycle resonant graphs among 2-connected graphs. The following revised phrasing from 2003 of this latter characterization is due to the same authors [10]:

Theorem 1.1 ([9]). *Let G be a 2-connected graph containing (at least) k pairwise disjoint cycles. Then G is k-cycle resonant if and only if G is bipartite and for every $1 \leq t \leq k$ and for every set $\mathcal{C} = \{C_1, C_2, \ldots, C_t\}$ of t pairwise disjoint cycles in G, $G - \cup_{i=1}^{t} C_i$ has no odd component.*

Recall a folklore mathematical meta theorem "it is easy to generalize." On the other hand a specialization of a general result can bring additional insight into the problem considered. As we already said, we are interested in bipartite 2-connected plane graphs and our aim is to give a characterization of 1-cycle resonant graphs among them that is as simple as possible. In particular, this characterization should be simple enough to be used by working chemists.

The rest of the paper is organized as follows. In the rest of the section we define concepts needed in this note. In the subsequent section the main theorem is presented and some of its consequences discussed. The final section contains a proof of the main result (Theorem 2.1).

For basic graph theory terminology, the reader is referred to the books [11, 12].

A graph is *planar* if it can be embedded into the plane such that no two edges cross and is *plane* if it is planar and furthermore is equipped with a fixed embedding into the plane.

A *hexagonal system* is a 2-connected plane graph in which each inner face is a regular hexagon of side length 1. A hexagonal system is *catacondensed* if each vertex lies on the boundary of the outer face, i.e., if it has no inner vertices.

A set of cycles $\mathcal{C}$ in a graph G is said to be *resonant* if the cycles in $\mathcal{C}$ are pairwise disjoint and there exists a perfect matching M of G such that each cycle in $\mathcal{C}$ is M-alternating. Let k be a positive integer. A graph G is said to be *k-cycle resonant* or *k-cycle extendable* [9], if it contains (at least) k pairwise disjoint cycles and for every $1 \leq t \leq k$, and for every set $\mathcal{C}$ of t pairwise disjoint cycles in G, $\mathcal{C}$ is resonant.

2. Main result and its consequences

To formulate our result, we need the following technical definition. Let G be a 2-connected plane graph. Then we will say that the plane embedding of G is *simple* if for each inner faces $\mathcal{F}$ and $\mathcal{F}'$ of G the intersection graph $\mathcal{F} \cap \mathcal{F}'$ is either a path or is empty. In less formal words, in a simple embedding the common boundary of two adjacent faces is a simple curve. Now our main result reads as follows:

Theorem 2.1. *Let G be a bipartite 2-connected plane graph whose embedding is simple. Then G is 1-cycle resonant if and only if the outer face of G is alternating and each inner vertex of G has degree two.*

Note that the outer cycle of a catacondensed hexagonal system is a Hamilton cycle of even length, hence it is resonant. In 1994, Guo and Zhang [9] showed that a hexagonal system is 1-cycle resonant if and only if it is catacondensed [9], a result that was rediscovered by one of the present authors [13]. Hence, Theorem 2.1 can be seen as a generalization of this result.

Figure 1 illustrates the conditions of Theorem 2.1. All the four graphs are bipartite (their bipartitions are indicated with black and white vertices), 2-connected and plane. The abstract graphs from figures (a) and (b) are isomorphic as the figure indicate. The embedding of the plane graph from figure (a) is not simple. (On the other hand, the embedding of the plane graph from figure (b) is simple.) It is easy to see that the graph contains six cycles and that each of them is alternating, that is, the graph is 1-cycle resonant. However, not all inner vertices of the plane graph from figure (a) are of degree 2. This example shows that the assumption that G has a simple embedding cannot be dropped. The plane graph from figure (c) has a simple embedding, all inner vertices are of degree 2, but the outer cycle is not alternating. Finally, the graph from figure (d) has a simple embedding. Its outer cycle is alternating, but its inner vertices are not of degree 2. The graph is not 1-cycle resonant. For instance, the indicated cycle is not alternating.

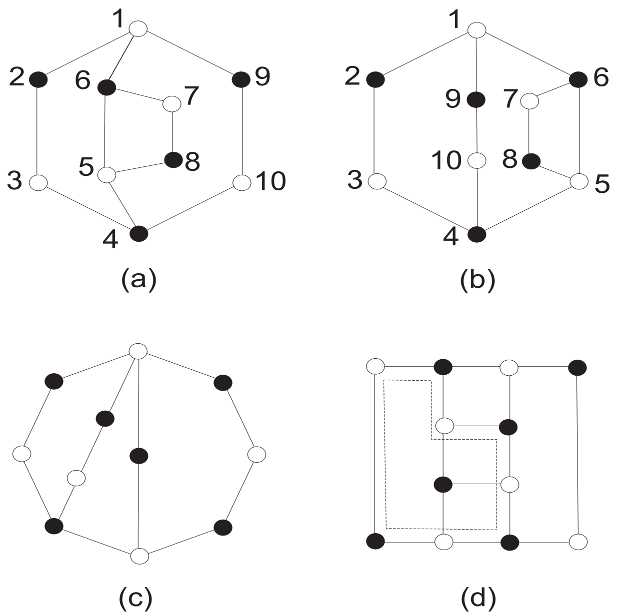

Figure 1: Bipartite, 2-connected, plane graphs

Theorem 2.1 has several consequences, the following is obvious:

Corollary 2.2. *Let G be a bipartite, 2-connected, outerplane graph. Then G is 1-cycle resonant.*

Now, let G be a bipartite, 3-connected, **planar** graph and consider its unique embedding in the plane. This embedding is simple. By 3-connectivity, G does not contain vertices of degree 2. This implies that G is not outerplane, but then it contains inner vertices (that are of degree at least 3). Hence, Theorem 2.1 implies that G is not 1-cycle resonant. Thus, we have:

Corollary 2.3. *Let G be a bipartite, 3-connected, planar graph. Then G is not 1-cycle resonant.*

In view of Corollary 2.3, it is natural to define a plane graph to be k-resonant if each set of at most k disjoint faces is resonant. For research in this direction see the work of H. Zhang and his co-workers [5, 6, 7, 8].

3. Proof of Theorem 2.1

For the proof of our main result we recall several concepts and known results.

Let e be an edge. Join the two vertices of e by an odd path P_1, the first *ear*. A sequence of bipartite graphs can be built as follows: For each $r \geq 1$, assume that $e+P_1+\cdots+P_r := G_r$ has already been constructed. Join any two vertices in different color classes of G_r by an odd path P_{r+1}, an *ear*, having no other vertex in common with G_r. The decomposition $e + P_1 + \cdots + P_r$ is called an *ear decomposition* of G_r [14, 15].

A graph is *elementary* if it is connected and the union of all its perfect matchings is a connected subgraph. It can be shown that a graph is elementary bipartite if and only if it has an ear decomposition [14, 15].

Let G be a plane elementary bipartite graph other than K_2. (It can be shown that an elementary bipartite graph other than K_2 is necessarily 2-connected [15].) An ear decomposition of G, say $e + P_1 + \cdots + P_r = G$, is called a *reducible face decomposition* if $e + P_1 := G_1$ is the boundary of an inner face of G and for each $1 \leq i \leq r-1$, P_{i+1} lies in the outer face of $e + P_1 + \cdots + P_i = G_i$. It is easy to see that the number of ears equals the number of inner faces of G.

We will apply the following results from [16]:

Theorem 3.1. *Let G be a bipartite 2-connected plane graph. Then G is elementary if and only if each face of G is alternating.*

Theorem 3.2. *Let G be a bipartite 2-connected plane graph. If G has a perfect matching and all the inner vertices of G have the same degree then the following statements are equivalent:*

(i) the graph G is elementary,
(ii) each inner face of G is alternating,
(iii) the outer face of G is alternating.

Theorem 3.3. *Let G be a plane elementary bipartite graph other than K_2. Then G has a reducible face decomposition.*

Now everything is ready for the proof of Theorem 2.1.

Let G be 1-cycle resonant. Then in particular the outer face is alternating. It remains to prove that each inner vertex of G has degree 2. Assume that there exists an inner vertex v_0 whose degree is not equal to 2. The degree of v_0 is at least 3 since G is 2-connected. Let $v_1, v_2, \ldots, v_k$ be the neighbors of v_0 in the clockwise order with respect to the embedding, where $k \geq 3$. For $i = 1, 2, \ldots, k$, let $\mathcal{F}_i$ be the face of G that contains the edges v_0v_i and v_0v_{i+1}, where the indices are taken modulo k throughout. For $i = 1, 2, \ldots, k$, let $P_{i+1} := \mathcal{F}_i \cap \mathcal{F}_{i+1}$. As the embedding is simple, P_{i+1} is a path.

Case 1: There exists $i \in \{1, 2, \ldots, k\}$ such that the number of inner vertices of P_{i+1} is odd.
Let C be the cycle of G obtained from $\mathcal{F}_i \cup \mathcal{F}_{i+1}$ by deleting the inner vertices of P_{i+1}. It is clear that $G - C$ has an odd component, the path obtained from P_{i+1} by deleting its ends. Hence, by Theorem 1.1, G is not 1-cycle resonant, a contradiction.

Case 2: *Case*: For each $i \in \{1, 2, \ldots, k\}$, the number of inner vertices of P_{i+1} is even.
Let C be the cycle obtained from $\mathcal{F}_1 \cup \mathcal{F}_2 \cup \cdots \cup \mathcal{F}_k$ by deleting v_0 and the inner vertices of $P_1, P_2, \ldots, P_k$. It is clear that $G - C$ has an odd component. Hence, by Theorem 1.1, G is not 1-cycle resonant, a contradiction.

For the converse let the outer face of G be alternating and let each inner vertex of G be of degree two. We proceed by induction on r, the number of inner faces of G, to show that G is 1-cycle resonant. The result is trivially true for $r = 1$.

Assume that the result is true for $r = s$, $s \geq 1$, and let $r = s+1$. By Theorem 3.2, G is elementary. Theorem 3.3 implies that G has a reducible face decomposition. Let $e + P_1 + \cdots + P_{s+1} = G$ be a reducible face decomposition of G. (Recall that G has $s+1$ inner faces.) Delete the inner vertices of P_{s+1} (and their incident edges) from G, thus, obtaining $e + P_1 + \cdots + P_s := G'$. This plane graph G' is an elementary bipartite graph (by the ear decomposition) other than K_2, hence, is 2-connected. The embedding of G' is simple. Theorem 3.1 implies that the outer face of G' is alternating and it is clear that each inner vertex of G' has degree 2. Hence, by the inductive assumption, G' is 1-cycle resonant. Consider a cycle C of G. If P_{s+1} has length ≥ 3, denote by $\widehat{M}$ the unique perfect matching of the path obtained from P_{s+1} by deleting its ends, otherwise, i.e., if P_{s+1} has length 1, denote by $\widehat{M}$ the empty set.

Case 1: C does not contain an edge of P_{s+1}.
In this case C is a cycle of G', hence, is alternating in G', i.e., there exists a perfect matching of G', M' say, such that C is M'-alternating. It is clear that $M' \cup \widehat{M}$ is a perfect matching of G such that C is $(M' \cup \widehat{M})$-alternating.

Case 2: C contains an edge of P_{s+1}.
Then C contains P_{s+1}. The union of the path P_{s+1} and an odd path of the boundary of G', P' say, is a cycle, the boundary of an inner face of G.

Case 2.1: C contains an edge of P'.
Since each inner vertex of G has degree two, it follows that C contains the whole path P'. Hence, $C = P_{s+1} \cup P'$. The outer face of G' is alternating in G'. Hence, there exists a perfect matching M' of G' such that P' is M'-alternating and the edge(s) of P' incident with the ends of P' is (are) in M'. Again, note that $M' \cup \widehat{M}$ is a perfect matching of G such that $C = P_{s+1} \cup P'$ is $(M' \cup \widehat{M})$-alternating.

Case 2.2: C does not contain an edge of P'.
Let P'' be the path obtained by removing the inner vertices of P_{s+1} (and the incident edges) from C. Thus, $C = P_{s+1} \cup P''$. It is clear that $P' \cup P''$ is a cycle in G', hence, is alternating in G'. Thus, there exists a perfect matching of G', M' say, such that the edge(s) of P'' incident with the ends of P'' is (are) in M'. It is clear that $M' \cup \widehat{M}$ is a perfect matching of G such that $C = P_{s+1} \cup P''$ is $(M' \cup \widehat{M})$-alternating.

This proves Theorem 2.1.

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