An optimal perfect matching with respect to the Clar problem in 2-connected plane bipartite graphs

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Abstract
We provide an optimality criteria for a perfect matching with respect to the Clar problem in 2-connected plane bipartite graphs.

1 Introduction
The class of graphs considered here are the 2-connected plane bipartite graphs with perfect matchings. We use $G \equiv G(V, E, F)$ to denote an arbitrary graph in this class, where $V$ is the set of vertices, $E$ is the set of edges and $F$ is the set of inner faces. It will be assumed that the vertices of $G$ are bi-colored, black and white say, such that the end vertices of each edge have different colors. A special type of 2-connected plane bipartite graphs are the so-called hexagonal systems. A hexagonal system is a 2-connected plane graph in which every inner face is a regular hexagon of side length one. Hexagonal systems with perfect matchings, i.e., Kekuléan benzenoid systems, are interesting graphs in chemical graph theory [1, 2] since they represent
the chemical compounds known as benzenoid hydrocarbons. Throughout this paper, the examples provided are drawn from these graphs.

An interesting optimization problem in 2-connected plane bipartite graphs with perfect matchings is the so-called Clar problem, a definition [3] of which follows. Let $P$ be a set of inner faces of $G$. We call $P$ a resonant set of $G$ (or a generalized Clar formula of $G$) if the faces in $P$ are pair-wise disjoint and there exists a perfect matching of $G$ that contains a perfect matching of each face in $P$. Let us recall here that every perfect matching of $G$ contains a perfect matching of an inner face of $G$ [4, 5]. The maximum of the cardinalities of all the resonant sets is called the Clar number [6]. It was Clar [7] who noticed the significance of this number in the chemistry of benzenoid hydrocarbons. A maximum cardinality resonant set (or a Clar formula) is a resonant set whose cardinality is the Clar number. By solving the Clar problem, we mean obtaining a maximum cardinality resonant set.

The Clar problem can be solved in polynomial time using linear programming algorithms [8, 9, 10, 5]. However, no polynomial-time combinatorial algorithm is available for the Clar problem. The purpose of this paper is to contribute to the development of such an algorithm within the framework described in [11]. Here, it should be noted that polynomial-time combinatorial algorithms for the Clar problem in two special classes of hexagonal systems with perfect matchings do exist [5, 12, 13]. In the remainder of this section, the framework suggested in [11] to solve the Clar problem is reviewed and the contribution of this paper is further specified, but more definitions are needed.

Let $M$ a perfect matching of $G$ and $P$ be a set of inner faces of $G$. We call $P$ an $M$-resonant set of $G$ if the faces in $P$ are pair-wise disjoint and the perfect matching $M$ contains a perfect matching of each face in $P$. It is noted that a set of inner faces of $G$ is resonant if and only if it is $M$-resonant for some perfect matching $M$ [11]. A maximum cardinality $M$-resonant set is an $M$-resonant set whose cardinality is the maximum of the cardinalities of all the $M$-resonant sets. It is noted that a maximum cardinality $M$-resonant set for some perfect matching $M$ is not necessarily a maximum cardinality resonant set [11]. A perfect matching $M$ is optimal with respect to the Clar problem if the maximum of the cardinalities of all the $M$-resonant sets is the Clar number.

The Clar problem can be solved in two stages [11]. We obtain a perfect matching $M$ that is optimal with respect to the Clar problem and then obtain a maximum cardinality $M$-resonant set. It was shown [11] that a maximum cardinality $M$-resonant set can be obtained in polynomial time by a combinatorial algorithm. This paper provides optimality criteria for a perfect matching with respect to the
Clar problem. In order to present this optimality criteria, we need to introduce an optimization problem on 2-connected plane bipartite graphs with perfect matching that is closely related to the Clar problem. It is the minimum weight cut cover problem. This will be the subject of section 2 and the optimality criteria will be given in section 3. For graph theory terminology, the reader is referred to [14].

![Figure 1: Closed cut lines.](image)

2 The minimum weight cut cover problem

Let \( G^* \) be a plane dual of \( G \). Let \( C \) be a cycle of \( G^* \) and \( E_C \) be the set of edges of \( G \) intersected by \( C \). It can be easily seen that \( G - E_C \) has exactly two components. The cycle \( C \) is called a closed cut line of \( G \) if all the edges of \( E_C \) are incident with black vertices of one of the components of \( G - E_C \) and white vertices of the other one [6, 15]. Fig. 1 shows examples of closed cut lines of benzo[a]pyrene.

A closed cut line of \( G \) intersects a face of \( G \) if the vertex of \( G^* \) corresponding to the face is one of the vertices of the closed cut line. A cut cover [6] of \( G \) is a set of closed cut lines of \( G \) such that each inner face of \( G \) is intersected by a closed cut line in the set; it is perfect if each inner face is intersected by exactly one closed cut line. Fig. 2 shows both a perfect cut cover and a cut cover that is not perfect.

For every closed cut line \( C \) of \( G \), the number of matched edges of \( G \) intersected by \( C \) is independent of the perfect matching [6, 5, 9] and is called the weight of
The weight of a cut cover is the sum of the weights of its closed cut lines. A minimum weight cut cover is a cut cover whose weight is the minimum of the weights of all the cut covers.

Hansen and Zheng [6] showed that for a hexagonal system with perfect matchings, the maximum cardinality of a resonant set is at most the minimum weight of a cut cover and conjectured that equality holds. Abeledo and Atkinson [5, 9] proved the conjecture for 2-connected plane bipartite graphs with perfect matchings; that is,

**Theorem 2.1** ([5, 9]). Let $G$ be a 2-connected plane bipartite graph with perfect matchings. The maximum of the cardinalities of all the resonant sets of $G$ is equal to the minimum of the weights of all the cut covers of $G$.

![Figure 2: Cut covers.](image)

3 The optimality criteria

**Remark 3.1** ([5]). If a closed cut line of $G$, $C$ say, intersects a face of $G$, then $E_C$ contains exactly two edges of the boundary of that face. Moreover, if the boundary of that face is $M$-alternating, where $M$ is a perfect matching of $G$, then exactly one of these two edges is matched.

**Remark 3.2.** Given a perfect matching of $G$ and a cut cover $C$ of $G$, the contribution of a matched edge $e$ to the weight of $C$ is the number of closed cut lines in $C$ that intersect $e$. The sum of the contributions of all the matched edges is the weight of the cut cover $C$.

**Lemma 3.3.** Let $G$ be a 2-connected plane bipartite graph with perfect matchings. Let $C$ be a minimum weight cut cover of $G$. Let $M$ be a perfect matching of $G$
that is optimal with respect to the Clar problem. For every maximum cardinality $M$-resonant set $P$ of $G$, every matched edge not in the boundary of a face in $P$ is not intersected by a closed cut line in $C$.

Proof. Let $P$ be a maximum cardinality $M$-resonant set of $G$. Assume that a matched edge not in the boundary of a face in $P$ is intersected by a closed cut line in $C$. It follows from Remarks 3.1 and 3.2 that the weight of $C$ exceeds the cardinality of $P$. Since $M$ is optimal with respect to the Clar problem, $P$ is a maximum cardinality resonant set of $G$. Hence, the weight of a minimum weight cut cover of $G$ exceeds the cardinality of a maximum cardinality resonant set of $G$, a contradiction to Theorem 2.1.

\[\square\]

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{An application of Theorem 3.4.}
\end{figure}

**Theorem 3.4.** Let $G$ be a 2-connected plane bipartite graph with perfect matchings. Let $C$ be a minimum weight cut cover of $G$ that is perfect. Let $M$ be a perfect matching of $G$. The following statements are equivalent.

i. The perfect matching $M$ is optimal with respect to the Clar problem.

ii. For every maximum cardinality $M$-resonant set $P$ of $G$, every matched edge not in the boundary of a face in $P$ is not intersected by a closed cut line in $C$. 

iii. There exists a maximum cardinality $M$-resonant set $P$ of $G$ such that every matched edge not in the boundary of a face in $P$ is not intersected by a closed cut line in $C$.

Proof. (i) implies (ii): This follows from Lemma 3.3. (ii) implies (iii): This is obvious. (iii) implies (i): Let $P$ be a maximum $M$-resonant set of $G$ such that every matched edge not in the boundary of a face in $P$ is not intersected by a closed cut line in $C$. Since $C$ is a perfect cut cover, it follows from Remarks 3.1 and 3.2 that the weight of $C$ is equal to the cardinality of $P$. By Theorem 2.1, this implies that $P$ is a maximum cardinality resonant set. Hence, the perfect matching $M$ is optimal with respect to the Clar problem. \hfill \Box

Here it is further clarified how to use Theorem 3.4 to determine whether a given perfect matching is optimal with respect to the Clar problem. It should be emphasized that a minimum weight cut cover that is perfect, $C$ say, should be available to apply Theorem 3.4. Given a perfect matching $M$, a maximum cardinality $M$-resonant set, $P$ say, is constructed. If every matched edge not in the boundary of a face in $P$ is not intersected by a closed cut line in $C$ then the perfect matching is optimal with respect to the Clar problem, otherwise it is not. Figure 3 illustrates an application of Theorem 3.4.

![Phenanthrene: Clar number=2](image)

Figure 4: When Theorem 3.4 fails.

Remark 3.5. Theorem 3.4 fails if the condition that the minimum weight cut cover should be perfect is relaxed. Figure 4 shows a minimum weight cut cover that is not perfect, $C$ say, a perfect matching, $M$ say, and a maximum cardinality $M$-resonant set, $P$ say. It is clear that every matched edges not in the boundary of a hexagon in $P$ is not intersected by a closed cut line in $C$, yet the perfect matching $M$ is not optimal with respect to the Clar problem.
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References


