4-tilings of benzenoid graphs

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Abstract

A benzenoid graph is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one. A benzenoid graph $G$ is elementary if every edge belongs to a 1-factor of $G$. A hexagon of an elementary benzenoid graph is peripheral if it has some edge lying on the boundary of the graph. A peripheral hexagon $h$ of an elementary benzenoid graph $G$ is reducible if the removal of the internal vertices and edges of the common path of the peripheries of $h$ and $G$ results in an elementary benzenoid graph. The vertices of the inner dual $I(G)$ of a plane graph $G$ are the finite faces of $G$, two vertices being adjacent if and only if the corresponding faces share an edge in $G$. If $S$ is a set of edges of $I(G)$ which do not belong to the infinite face of $I(G)$ such that $I(G) \setminus S$ is the graph where every finite face is a 4-cycle, then $S$ is called a 4-tiling of $G$. We describe a procedure to compute a 4-tiling of an elementary benzenoid graph in linear time. This computation is the basis for an optimal algorithm to find the sequence of reducible hexagons that decompose a graph of this class.

1 Introduction and preliminaries

A benzenoid graph is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one. A benzenoid graph $G$ is catacondensed if any triple of hexagons of $G$ has empty intersection, otherwise it is pericondensed. It is well known that benzenoid graphs possess very natural chemical background. In particular, the skeleton of carbon atoms in a benzenoid hydrocarbon is a benzenoid graph. The interested reader is invited to consult the books [1, 3] dedicated to these class of graphs.

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A hexagon $h$ of a benzenoid graph $G$ is called a pendant hexagon if a common path of the peripheries of $h$ and $G$ is a path of length five.

A graph $G$ is called bipartite if it is connected and its vertex set can be divided in two disjoint sets $V_1$ and $V_2$ such that $V_1 \cup V_2 = V(G)$ and no two vertices from the same set are joined by an edge. Every benzenoid graph is clearly bipartite. A peak (valley) of a benzenoid graph is a vertex that is above (below) all its first neighbors. Throughout this paper all benzenoid graphs considered are drawn so that an edge-direction is vertical and the peaks are colored black (cf. Fig. 1).

A matching of a graph $G$ is a set of pairwise independent edges. A matching is a 1-factor, if it covers all the vertices of $G$.

A bipartite graph $G$ is called elementary if $G$ is connected and every edge belongs to a 1-factor of $G$. It is well known that catacondensed benzenoid graphs are elementary.

Let $M$ be a 1-factor of $G$. A cycle $C$ is $M$-alternating if the edges of $C$ appear alternately in and off the $M$. An $M$-alternating cycle $C$ of $G$ is said to be proper (improper) if every edge of $C$ belonging to $M$ goes from white (black) end-vertex to black (white) end-vertex by the clockwise orientation of $C$.

Let us call the boundary of the infinite face of $G$ the outer boundary or the outer cycle.

A matching of a graph $G$ is a set of pairwise independent edges. A matching is a 1-factor, if it covers all the vertices of $G$. It is well known that the number of vertices is linear in the number of edges and the number of hexagons of a benzenoid graph.

The symmetry difference of finite sets $A$ and $B$ is defined as $A \oplus B := (A \cup B) \setminus (A \cap B)$. If $h$ is a hexagon of a benzenoid graph $G$ and $M$ a 1-factor of $G$ then in the $M \oplus h$ operation, $h$ is always regarded as the set of edges bounding the hexagon.

A 1-factor $M$ is said to be peripheral if the outer cycle of $G$ is $M$-alternating. The next proposition shows that the minimal and the maximal 1-factor of $G$ are peripheral.

**Proposition 1.** [11] Let $G$ be an elementary benzenoid graph. Then the outer cycle of $G$ is improper $M_0$-alternating as well as proper $M_1$-alternating.

Note that the minimal (and the maximal) 1-factor of an elementary benzenoid graph can be computed in linear time using the concept of the rightmost (leftmost) perfect path system. See [4, 11] for the details.

Let $f$ denote a face of a plane bipartite graph $G$ and $P$ a common path of the peripheries of $f$ and $G$. Let then $G - f$ denote the resultant subgraph of $G$ by removing the
internal vertices and edges of \( P \).

A face \( f \) of a plane bipartite graph \( G \) is peripheral if the peripheries of \( G \) and \( f \) have a nonempty intersection. Let \( f \) be a peripheral face of \( G \). If \( G - f \) is elementary then we call \( f \) a reducible face of \( G \).

**Theorem 1.** [19] If \( G \) is a plane elementary bipartite graph with at least three finite faces, then \( G \) has at least two reducible faces.

In the next section we show that a 4-tiling of an elementary benzenoid graph \( G \) is induced by a peripheral 1-factor of \( G \). In particular, this is also true for the minimal and maximal 1-factor of \( G \). Moreover, this relation can be reversed: every 4-tiling of \( G \) induces a peripheral 1-factor of \( G \). In Section 3 we prove that the number of 4-tilings of an elementary benzenoid graph \( G \) equals the number of 1-factors of \( G - C \), where \( C \) is a boundary cycle of \( G \). Section 4 conclude the paper by presenting a simple linear algorithm to find a reducible face decomposition for an elementary benzenoid graph.

## 2 4-tilings and peripheral 1-factors

The vertices of the inner dual of a plane graph \( G \) are the finite faces of \( G \), two vertices being adjacent if and only if the corresponding faces share an edge in \( G \). The inner dual of a benzenoid graph, denoted \( I(G) \), is a subgraph of the regular triangular grid. Clearly, the inner dual of a catacondensed benzenoid graph is a tree with maximum vertex degree three.

An edge \( e \) of \( I(G) \) is peripheral, if it belongs to the infinite face of \( I(G) \) and internal, otherwise. If \( h \) is a hexagon of a benzenoid graph, then \( h \) will also denote the corresponding vertex of \( I(G) \).

Let \( I(G) \) be the inner dual of a benzenoid graph \( G \) and let \( S \) denote a subset of internal edges of \( E(I) \). Then \( S \) is a 4-tiling of \( G \) if \( I(G) \setminus S \) is the graph where every finite face is a 4-cycle (cf. Figure 1). If \( S \) is a 4-tiling of \( G \), then we set \( IS(G) := I(G) \setminus S \).

The following theorem shows that the concept of 4-tiling is intrinsically connected with elementary benzenoid graphs.

**Theorem 2.** [12] A benzenoid graph \( G \) is elementary if and only if \( G \) admits a 4-tiling.

The main theorem of this section indicates that a 4-tiling of an elementary benzenoid graph can be constructed by using its peripheral 1-factor.

Let \( M \) denote a peripheral 1-factor of an elementary benzenoid graph \( G \). Let us define the set of edges \( SM(G) \) as follows: an internal edge \( hi \, hj \) of \( I(G) \) belongs to \( SM(G) \) if and only if the common edge of the corresponding hexagons \( hi \) and \( hj \) belongs to \( M \).
Figure 1: A benzenoid graph with its a. inner dual b. 4-tiling.

**Theorem 3.** Let $M$ denote a peripheral 1-factor of an elementary benzenoid graph $G$. Then $S_M(G)$ is a 4-tiling of $G$.

**Proof.** Let $C$ denote the outer cycle of $G$. Suppose that $M$ is a peripheral 1-factor of an elementary benzenoid graph $G$, such that $C$ is improper $M$-alternating. We prove the theorem by showing that $S_M(G)$ in the subgraph of $I(G)$, induced by a hexagon $h \in G$ together with hexagons adjacent to (or "near") $h$, locally admits a 4-tiling.

Suppose first that $h$ possesses six adjacent hexagons. The situation is depicted if Fig. 2, where $h$ is filled with gray color and the hexagons adjacent to $H$ are labeled $1, \ldots, 6$. Note also that the vertices and the edges of $I(G) \setminus S_M(G)$ are drawn gray. The figure show all possible ways to cover the vertices of $h$ by $M$ up to the obvious symmetries.
From Fig. 2a clearly follows that $S_M(G)$ in the subgraph, induced by a hexagon $h$ together with its adjacent hexagons, locally admits a 4-tiling. Situation in Fig. 2b is little more involved. Note first that the hexagon $h'$ has to exist in $G$. To see this suppose to the contrary that $h'$ does not belong to $G$. But then the edge of hexagon 1 which is (in Fig. 2b) adjacent to $h'$ as well as the edge of hexagon 6 which is (in Fig. 2b) adjacent to $h'$ belong to the outer cycle of $G$. Since the edge in the intersection of hexagons 1 and 6 belongs to $M$, these two consecutive edges of the outer cycle do not belong to $M$ and proposition 1 yields a contradiction. Analogously we can see that $h''$ also belongs to $G$. It is easy to derive now that $S_M(G)$ in the subgraph, induced by a hexagon $h$ together with its adjacent hexagons as well as hexagons $h'$ and $h''$, locally admits a 4-tiling. Cases in Figs. 2c, 2d, and 2e can be proven analogously.

The situation with $h$ adjacent to five hexagons is depicted if Fig. 3. Note first that one of the edges of $h$ (in the figure labeled with $e$) as well as two adjacent edges of hexagons 1 and 2 (labeled $e'$ and $e''$) belong to the boundary of $G$. Therefore either $e$ or both of $e'$ and $e''$ belong to $M$. Fig. 3 show all possible cases with $h$ covered by $M$ up to the obvious symmetries. We can prove analogously as above that every configuration of $S_M(G)$ in the subgraph, induced by $h$ and hexagons adjacent to (or "near") $h$, locally admits a 4-tiling.

Figs. 4, 5 and 6 show configurations with four, three and two hexagons adjacent to $h$, respectively. Using the same arguments than above, we can in a similar manner show that every depicted configuration locally admits a 4-tiling. Note also that the claim trivially follows for the pendant hexagon.
We showed that $S_M(G)$ in the neighborhood of every hexagon of $G$ locally admits a 4-tiling. If $M$ is a peripheral 1-factor of an elementary benzenoid graph $G$, such that $C$ is proper $M$-alternating, the proof goes analogously. This argument concludes the proof.

**Corollary 1.** Let $M_0$ denote the minimal 1-factor of a benzenoid graph $G$. Then $G$ is elementary if and only if $S_{M_0}(G)$ is a 4-tiling of $G$. 
Figure 6: Two adjacent hexagons.

Proof. It follows from Theorem 2 and Proposition 1.

Since the minimal and the maximal 1-factors of an elementary graph $G$ can be computed in linear time, Theorems 3 give a means to construct a 4-tiling of $G$ within the same time bound. The details are depicted in Section 4.

Let $M$ denote a 1-factor of an elementary benzenoid graph $G$. If $S_M(G)$ is a 4-tiling of $G$, we say that $M$ induces the 4-tiling $S_M(G)$ of $G$.

Let $G$ be an elementary benzenoid graph and let $C$ denote the boundary cycle of $G$. Define then the set $M_0(C)$ ($M_1(C)$) as a matching of $C$ such that $C$ is proper (improper) $M_1(C)(M_0(C))$-alternating.

Let $S$ be a 4-tiling of $G$. If $hh'$ is an edge of $S$ connecting hexagons $h$ and $h'$ of $G$ and $e$ the common edge of $h$ and $h'$ in $G$, then we say that $e$ is crossed by $hh'$.

Let us define two subsets of $E(G)$ as follows.

$M_{S_0} := \{e; e \in E(G) \text{ and } e \text{ is crossed by an edge of } S\} \cup M_0(C)$

$M_{S_1} := \{e; e \in E(G) \text{ and } e \text{ is crossed by an edge of } S\} \cup M_1(C)$

Theorem 3 demonstrates that every peripheral 1-factor of an elementary benzenoid graph induces 4-tilings of $G$. The next proposition shows that this implication can be reversed, namely every 4-tiling also induces 1-factors.

**Proposition 2.** Let $G$ be an elementary benzenoid graph and $S$ a 4-tiling of $G$. Then $M_{S_0}$ ($M_{S_1}$) is a peripheral 1-factor of $G$.

Proof. Let $C$ denote the boundary cycle of $G$ and let $\partial C$ denote the set of edges of $G$ with one end vertex in $C$ and the other not in $C$. We show first that $M_{S_0}$ is a matching. Note that by the definition of the 4-tiling an edge of $\partial C$ cannot belong to $M_{S_0}$. Moreover, since $M_0(C)$ is a matching in $C$, the claim clearly holds for the boundary cycle of $G$. To show the assertion for the internal edges of $G$, note first that an edge of $G$ crossed by an edge of $S$ lies inside a four cycle of $I_S(G)$. This implies that all edges of $G$ which are crossed by edges of $S$ are have to be independent. Thus, this claim is settled.

In order to finish the prove, we have to show that every vertex of $G$ is covered by an edge of $M_{S_0}$. By definition of $M_{S_0}$, this holds for $C$. To establish the assertion for the internal vertices of $G$ note that every internal vertex $v$ is of degree three. Let $v$ be
a vertex in the intersection of hexagons \(h_1, h_2, h_3\) (see Fig. 7a). We have to show that there always exists an adjacent vertex \(u\) such that \(uv\) is crossed by an edge of \(S\). To see this suppose to the contrary that \(uv\) is not crossed by an edge of \(S\) for any \(u\) adjacent to \(v\). But this implies that the hexagons \(h_1, h_2, h_3\) induce a triangle in \(I(G) \setminus S\). This contradiction concludes the proof.

\[\square\]

3 4-tiling count

Let \(G\) be a benzenoid graph with a 1-factor. A subgraph of \(H\) of \(G\) is said to be *nice* if \(G - V(H)\) has a 1-factor.

![Figure 7: a. Internal vertex \(v\) with its hexagons. b. Coronene.](image)

Let \(H\) be any nice subgraph of an elementary bipartite graph \(G\). Join its end vertices by a path \(P_1\) of odd length (first ear). Then proceed inductively to build a sequence of bipartite graphs as follows: if \(G_{r-1} = H + P_1 + P_2 + \ldots + P_{r-1}\) has already been constructed, add the \(r\)th ear \(P_r\) (of odd length) by joining any two vertices of different colors in \(G_{r-1}\) such that \(P_r\) has no internal vertices in common with \(G_{r-1}\). The decomposition \(G_r = H + P_1 + P_2 + \ldots + P_r\) is called an (bipartite) ear decomposition of \(G_r\).

**Theorem 4.** \([9]\) A bipartite graph is elementary if and only if it has an (bipartite) ear decomposition.

It is well known that some properties of an elementary benzenoid graph \(G\) depends on whether \(G\) possesses a coronene (see Fig. 7b) as its nice subgraph or does not.

**Lemma 1.** Let \(H_C\) denote a coronene which is a nice subgraph of an elementary benzenoid graph \(G\) and let \(h_c\) denote the central hexagon of \(H_C\). Then \(G - h_c\) is elementary.

**Proof.** Since \(H_C\) is a nice subgraph in \(G\), \(G\) admits a bipartite ear decomposition \(G = H_C + P_1 + P_2 + \ldots + P_r\). Let \(C\) denote the outer cycle of \(H_C\). Obviously, the sequence of ears \(P_1 + P_2 + \ldots + P_r\) starting with \(C\) gives \(G - h_c\). More formally \(G - h_c = C + P_1 + P_2 + \ldots + P_r\). Since \(C\) is obviously a nice cycle in \(G - h_c\), it follows that \(C + P_1 + P_2 + \ldots + P_r\) is a bipartite ear decomposition of \(G - h_c\). Theorem 4 now yields the assertion. \[\square\]
Lemma 2. [15] Let $G$ be an elementary benzenoid graph. Then $G$ has no coronene as its nice subgraph if and only if for any pair of disjoint cycles that form a nice subgraph of $G$ their interiors are disjoint.

Let $G$ be a benzenoid graph. Then the vertex set of the resonance graph $R(G)$ of $G$ consists of the 1-factors of $G$, two 1-factors being adjacent whenever their symmetric difference forms the edge set of a hexagon of $G$. The concept of a resonance graph has been introduced in chemistry and later introduced in mathematics under the name Z-transformation graphs. An extensive survey on resonance graphs of plane bipartite graphs was presented by Zhang [14], see also [2, 6, 7, 12, 11].

The hypercube of order $n$ and denoted $Q_n$ is the graph $G = (V,E)$ where the vertex set $V(G)$ is the set of all binary strings $b_{n-1}, \ldots b_1, b_0$. Two vertices $x, y \in V(G)$ are adjacent in $Q_n$ if and only if $x$ and $y$ differ in precisely one place.

Let $G = (V,E)$ be a connected graph and $u, v \in V$. Then the distance $d_G(u,v)$ between $u$ and $v$ is the number of edges on a shortest $u,v$-path. A subgraph $H$ of a graph $G$ is isometric if for any vertices $u$ and $v$ of $H$ holds $d_H(u,v) = d_G(u,v)$.

Isometric subgraphs of hypercubes are called partial cubes.

Let $G$ denote a plane elementary graph. Let $F$ be the set of all finite faces and let $M$ be the set of all 1-factors of a graph $G$, respectively. For each $M \in M$, a function $\phi_M$ is defined on $F$ as follows: for any $f \in F$, $\phi_M(f)$ is the number of cycles in $M \oplus M$ with $f$ in their interiors. Particularly, $M_0$ is constantly zero, i.e. every value on the inner faces is 0.

It was shown in [17] that the resonance graph of a plane elementary bipartite graph is a partial cube. For each 1-factor $M$, the function $\phi_M$ on $F$ is naturally transformed to $\tilde{\phi}_M$ as follows: for each $f \in F$, $\tilde{\phi}_M(f)$ is a sequence of length $\phi_M(f)$ such that first $\phi_M(f)$ positions from the left side are all placed 1 and the others 0. If $G$ is a benzenoid graph, then $\tilde{\phi}$ is an isometric embedding of $R(G)$ into a hypercube.

Lemma 3. [17] Let $G$ denote an elementary benzenoid graph. For $M, M' \in M$, $M$ and $M'$ are adjacent in $R(G)$ if and only if $|\phi_M(h) - \phi_{M'}(h)| = 1$ for $h = h_0$, where $h_0$ is a hexagon bounded by the cycle $M \oplus M$ and 0 for the other hexagons of $G$.

Since 1-factors compile pairwise independent edges, all the cycles induced by $M \oplus M_0$ have to be disjoint. It follows that for every peripheral hexagon $h$, $\phi_M(h)$ is either 1 or 0. Note also that for every peripheral hexagon $h$, we have $\tilde{\phi}_M(h) = \phi_M(h)$.

The following lemma shows that the value of $\phi$ in a peripheral hexagon $h$ depends on the position of the peripheral edges of $h$ that belong to a 1-factor.

Lemma 4. [12] Let $e$ be an edge on the boundary of an elementary benzenoid graph $G$ and let $h$ be the hexagon of $G$ containing $e$. For a 1-factor $M'$ of $G$ let $e \in M'$ and let...
If $M$ is an arbitrary 1-factor of $G$, then $\phi_M(h) = i$ if and only if $M$ contains $e$.

**Proposition 3.** Let $G$ be an elementary benzenoid graph. Then $G$ admits exactly one 4-tiling if and only if $G$ has no coronene as its nice subgraph.

**Proof.** Suppose first that $G$ possesses a coronene as its nice subgraph. Let $H_C$ denote a coronene which is a nice subgraph in $G$ and let $h_c$ denote the central hexagon in $H_C$. From Lemma 1 it follows that $G - h_c$ is elementary. Let then $M'_0$ denote the minimal 1-factor of $G - h_c$ and let $M_c$ denote three edges of $h_c$, such that the edges of $M_c$ form improper $M_c$-alternating cycle in $h_c$. It is straightforward to see that $M_0 := M'_0 \cup M_c$ is a peripheral 1-factor of $G$. Moreover, $M_0 \oplus h_c$ is also a peripheral 1-factor of $G$. Since $M_0$ and $M_0 \oplus h_c$ induce two distinct 4-tilings in $G$ (see Fig. 8), this part of the proof is complete.

Figure 8: Two 1-factors in a coronene which is a nice subgraph.

Suppose now that $G$ possesses no coronene as its nice subgraph. Suppose also that $G$ admits two 4-tilings. By Theorem 3 the minimal 1-factor $M_0$ of $G$ induces the 4-tiling $S_{M_0}$. Let then $S$ denote the other 4-tiling of $G$ distinct from $S_{M_0}$. From Proposition 2 it also follows that $S$ induces the 1-factor $M_{S_0}$. Observe now 1-factors $M_{S_0}$ and $M_0$. From Lemma 1 and from the definition of $M_{S_0}$ it follows that the outer cycle of $G$ is improper $M_0$-alternating and also $M_{S_0}$-alternating. Let then $M_0 = M_1, M_2, \ldots, M_k = M_{S_0}$ denote a shortest path between $M_0$ and $M_{S_0}$ in $R(G)$. From Lemma 3 it follows that for every pair of 1-factors $M_i$ and $M_{i+1}$, $i = 1, \ldots, k - 1$, we get $M_i \oplus M_{i+1} = h_0$, where $h_0$ is a hexagon of $G$.

Since the edges on the outer cycle of $G$ that belong to $M_0$ also belong to $M_{S_0}$, from Lemma 4 it follows that for every peripheral hexagon $h$ we get $\phi_{M_0}(h) = \phi_{M_{S_0}}(h)$. Moreover, since $R(G)$ is a partial cube, the same is true for every 1-factor on a shortest path between $M_0$ and $M_{S_0}$ in $R(G)$ (eg. [5, p. 20]). More formally, we get $\phi_{M_0}(h) = \phi_{M_i}(h) = j$, $j = 0, 1$ and $i = 2, \ldots, k$.

From the arguments above than it follows that for every pair of 1-factors $M_i$ and $M_{i+1}$, $i = 1, \ldots, k - 1$, $M_i \oplus M_{i+1} = h$, where $h$ has to be an internal hexagon of $G$. The cycle
induced by $h$ is then clearly disjoint with the boundary cycle of $G$. But then from Lemma 2 it follows that $G$ has a coronene as its nice subgraph and we obtain a contradiction.

**Theorem 5.** Let $C$ be the outer cycle of an elementary benzenoid graph $G$. Then the number of 4-tilings of $G$ equals the number of 1-factors of $G - C$.

**Proof.** Let $n_f$ and $n_t$ denote the number of 1-factors of $G - C$ and the number of 4-tilings of $G$, respectively. If $G$ has no coronene as its nice subgraph then $n_t = n_f = 1$ as follows from Proposition 3 (see also the proof).

Suppose then $n_f > 1$ and let $M$ and $M'$, $M \neq M'$, denote a pair of 1-factors of $G - C$. Let $B$ denote a 1-factor of $C$ and let us set $M_c := M \cup B$ and $M'_c := M' \cup B$. Since $M_c$ and $M'_c$ are not equal, there exist at least one edge $e_{i,j}$ of $G - C$ in the intersection of hexagons $h_i$ and $h_j$, such that $e_{i,j} \in M_c$ and $e_{i,j} \notin M'_c$. Since from definition of $S_M(G)$ it follows that $S_{M_c}(G) \neq S_{M'_c}(G)$, this implies $n_t \geq n_f$.

Suppose now that $n_t > 1$ and let $S$ and $S'$, $S \neq S'$, denote a pair of 4-tilings of $G$. We can show analogously as above that the 1-factors induced by $S$ and $S'$ are not equal. It follows that $n_f \geq n_t$ and the proof is complete.

4 Decomposition of elementary benzenoid graphs

Let $G$ be an elementary benzenoid graph. The sequence of hexagons $h_1, h_2, h_3, \ldots, h_r$ is called *reducible* if $h_i$ is a reducible hexagon of $G_i$ such that $G_r = G$, $G_{i-1} = G_i - h_i$, $i = r, r - 1, \ldots, 2$ and $h_1 = G_1$.

The characterization above is the basis for an algorithm which finds the sequence of reducible hexagons that decompose an elementary benzenoid graph in $O(n^2)$ time [11]. Moreover, an algorithm which decomposes a less general graph (an elementary benzenoid graph with at most one pericondensed component) in linear time is presented in the same paper. We will show in this section that the best possible complexity can be obtained for all elementary benzenoid graphs.

Let $G$ be a benzenoid graph without a pendant hexagon and with a 4-tiling $S$. The walk in a clockwise direction along the vertices of $I_S(G)$ induces three types of turns. The turns and the corresponding hexagons are denoted $\pi_3$, $2\pi_3$, and $-\pi_3$ in a natural way. All turns are depicted in Figure 9.

Let $G$ be a benzenoid graph with a 4-tiling and let $C$ be the outer cycle of $G$. Let $h$ be a hexagon that corresponds to a vertex of $C$. Then the hexagon $h$ is called *removable* if

- $h$ is a $\pi_3$ turn and the corresponding vertex in $I(G) \setminus S$ is of degree two, or
- $h$ is a $-\pi_3$ turn and the corresponding vertex in $I(G) \setminus S$ is of degree three.
Figure 9: Turns.

From Theorem 2 it clearly follows that a removable hexagon of an elementary benzenoid graph $G$ is also reducible. Note also that a pendant hexagon of $G$ is also trivially reducible. The following lemma was stated in [12] in slightly different form.

**Lemma 5.** Let $G$ be an elementary benzenoid graph without a pendant hexagon. Then a 4-tiling of $G$ admits at least one removable hexagon.

This observation together with Theorem 3 is the basis for the next algorithm.

**Algorithm Optimal RFD**

**input** - an elementary benzenoid graph $G$.

**output** - a reducible sequence of hexagons $L_i$, $i = 1, \ldots, r$.

1. $i := 1$.


3. $M_0 :=$ the minimal 1-factor of $G$.

4. $S :=$ the 4-tiling induced by $M_0$.

5. $H := \{h; h$ is a pendant or removable hexagon of $G\}$.

6. repeat
   
   (a) $L_i :=$ a hexagon of $H$.
   
   (b) $H := H \setminus \{L_i\}$.
   
   (c) $I_G := I_G - L_i$.
   
   (d) update $H$.
   
   (e) $i := i + 1$.

7. until $I(G)$ is a single hexagon $h'$.

8. $L_i := h'$. 
Theorem 6. Algorithm Optimal RFD finds a reducible sequence of hexagons of an elementary benzenoid graph $G$ and can be implemented to run in $O(n)$ time.

Proof. The correctness of the algorithm follows from Theorem 3 and Lemma 5. Starting from $G = G_r$, the algorithm at each execution of the loop finds a reducible hexagon in $G = G_i$ and then removes this hexagon from $G_i$. The obtained graph $G_{i-1}$ is elementary, therefore we can repeat the procedure till the last hexagon.

Concerning the time complexity of the algorithm, note that a vertex of $G$ and $I(G)$ possesses at most three and six adjacent vertices, respectively. Thus, the complexities of basic operations: deleting an edge, deleting a vertex, deleting all edges incident with a vertex etc., are constant notwithstanding a representation of $G$ and $I(G)$.

For Steps 2, 4, 5 it follows from the discussion above that they can be implemented in linear time. For Step 3 we invoke the routine RPS presented in [4] which compute the so called rightmost perfect path system of $G$ in linear time. As shown in [11], this implies that the computation of the minimal 1-factor can be executed within the same time bound.

We are left to show that the body of the loop is executed in constant time. Since we choose an arbitrary hexagon of $H$, Step 6(a) can be implemented to run in constant time. For Step 6(d) observe that $H$ can only be augmented with hexagons adjacent to $L_i$. Since the number of hexagons adjacent to $L_i$ is constant, this yields that this step can be executed in constant time. The same argument can be applied for Step 6(c). Since the number of hexagons is linear in the number of vertices of $G$, it follows that the overall time complexity of the algorithm is $O(n)$. \qed

References


