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Normal components, Kekulé patterns, and Clar patterns in plane bipartite graphs *

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As a general case of molecular graphs of polycyclic alternant hydrocarbons, we consider a plane bipartite graph G with a Kekulé pattern (perfect matching). An edge of G is called nonfixed if it belongs to some, but not all, perfect matchings of G. Several criteria in terms of resonant cells for determining whether G is elementary (i.e., without fixed edges) are reviewed. By applying perfect matching theory developed in plane bipartite graphs, in a unified and simpler way we study the decomposition of plane bipartite graphs with fixed edges into normal components, which is shown useful for resonance theory, in particular, cell and sextet polynomials. Further correspondence between the Kekulé patterns and Clar (resonant) patterns are revealed.

KEY WORDS: benzenoid, Kekulé structure, Clar pattern, plane bipartite graph, normal component

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1. Introduction

Some important graph-theoretical approaches, such as Herndon's work [1] and Randić conjugated circuit model [2], were established during the last two decades for general resonance theory of polycyclic aromatic hydrocarbons (benzenoid systems). The sextet polynomial for counting sextet patterns of benzenoid or coronoid systems was found by Hosoya and Yamaguchi [3]. In fact the sextet polynomial reflects the combinatorial background of Clar's concept of the aromatic sextet [4,5], and was used for the calculation of the resonance energy of benzenoid hydrocarbons [6,7]. Gutman [9] and John [8] extended the sextet polynomial to define the so-called cell polynomial of polycyclic unsaturated *alternant* hydrocarbons for counting Clar (or resonant) patterns.

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A certain correspondence between the Clar patterns and Kelulé patterns was established [5,9–11].

A fixed bond (edge) of polycyclic unsaturated alternant hydrocarbons cannot be contained in any conjugated circuits and thus has no contribution to π-resonance energies of the corresponding molecules. The decomposition of such molecular graphs with fixed bonds into normal components enables one to simplify greatly the computations of some graph-theoretical models as mentioned above.

As a mathematical framework of polycyclic unsaturated alternant hydrocarbons, in this paper we consider a plane bipartite graph with perfect matchings, which embraces benzenoid and coronoid systems [7,12,13].

A plane graph G is an (intersection-free) embedding in the Euclidian plane. A subgraph H of G is a plane graph that can be viewed as the restriction of the embedding of G on H. The boundary of the infinite face is simply referred to as the boundary of G, denoted ∂G. A vertex not belonging to the boundary of G is said to be *interior vertex* of G. An *outerplane graph* is a 2-connected plane graph without interior vertices. A finite face of G is called a *cell* if its boundary is a cycle. For convenience, a cell may be referred to its boundary.

A *Kekulé pattern* (or 1-factor, perfect matching [14] and Kekulé structure [13]) of G is a set of pairwise disjoint edges of G that cover all of its vertices. For a 1-factor M of G, a cycle C of G is called *M-alternating* (or *conjugated*) if the edges of C alternate on and off the M. Such a cycle C is said to to be *resonant*. A set S of pairwise disjoint cells of G is called *Clar* (or *resonant*) *pattern* if G has a 1-factor M such that all cells in S are simultaneously M-alternating.

An edge of G is called a *fixed single edge* if it belongs to no 1-factor; *fixed double edge* if it belongs to all 1-factors. A bipartite graph with 1-factor is called *normal* (or *elementary*) if it is connected and has no fixed single edges. The components of the subgraph of G formed by all nonfixed edges are normal and thus called *normal components* of G. Fast algorithms were designed [15–17] to determine all normal components and fixed edges of bipartite graphs.

It is known that an elementary bipartite graph with more than two vertices is 2-connected. Several equivalent results for a bipartite graph to be elementary were described in [14]. In case of plane bipartite graphs [18] (including benzenoid systems [19] and coronoid systems [20]), some special fundamental structural properties were given. In section 2 we shall list such characterizations in term of resonant faces.

Much works [13,21–25] were done on benzenoid systems with fixed edges, which were viewed as "essentially disconnected". In fact it has been rigorously proved by Hansen and Zheng [23] that an essentially disconnected benzenoid system has at least two normal components, and every normal component is a normal benzenoid system.

For plane bipartite graphs with fixed edges, the situation is somewhat complicated. For example, the coronoid system G shown in figure 1 has three normal components G_1, G_2 and G_3; both G_1 and G_2 are normal benzenoid systems, where every interior

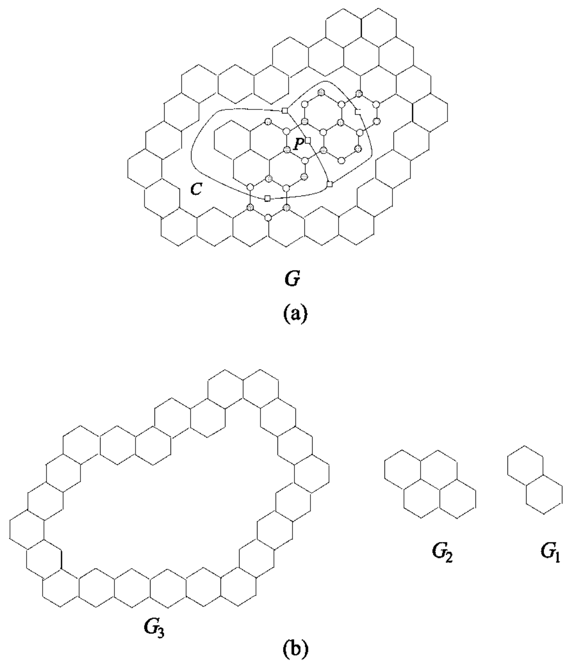

Figure 1. (a) A coronoid system G with fixed single edges. (b) Normal components of G.

face is a face of G, such normal components are called *normal blocks*; while G_3 is a coronoid system with a "hole" that is not face of the original graph G, that means that G_3 is not a normal block.

Even though, it is shown in section 3 that a plane bipartite graph G with fixed edges and the minimum degree not less than 2 has at least two normal components and at least *one* normal block. As an immediate consequence, we have that for any 1-factor M of G, an M-alternating cell exists. In section 4 some extremal cases are characterized. For example, it is proved that every normal component of G is normal block if and only if G is weakly elementary.

Finally we will give some applications of the results obtained above to resonance theory. It is shown that the sextet polynomial of a benzenoid or coronoid system can be expressed as the product of those sextet polynomial of its normal components; such an result holds for the cell polynomial of a plane bipartite graph G if and only if G is weakly elementary. A surjection from the Kekué patterns to the Clar patterns of G is established; it is shown that such a surjection is an one-to-one correspondence if and only if G is is weakly elementary and for any pair of resonant cycles their interior regions are disjoint.

Throughout this paper, the vertices of a bipartite graph G are colored white and black such that adjacent vertices receive distinct colors; denote $V(G)$ and $E(G)$ the vertex-set and edge-set of G, respectively; $\delta(G)$ the minimum degree of G and $\mathcal{G}$ the family of connected plane bipartite graphs with 1-factor.

2. Resonance faces of elementary plane bipartite graphs

A bipartite graph is *elementary* if the union of its 1-factors forms a connected subgraph. Various equivalent results on elementary bipartite graphs can be found in [14]. For example, a connected bipartite graph is elementary if and only if every edge belongs to a 1-factor; if and only if the deletion of any pair of distinct colored vertices results in a graph having a 1-factor. For a plane bipartite graph G, a face f of G is called *resonant* if G has a 1-factor M such that the boundary of f is an M-alternating cycle. In case of plane bipartite graphs, the following special characterization in terms of resonant faces was given.

Theorem 2.1 [18]. Let G be a plane bipartite graph with 1-factors. Then G is elementary if and only if every face of G is resonant.

If all interior vertices of G are of the same degree, a simpler criterion is given as follows.

Theorem 2.2 [18]. Let G be a connected and bipartite plane graph. Suppose all the interior vertices of G are of the same degree. Then G is elementary if and only if the exterior face of G is resonant.

Three distinct types of such graphs are exemplified in figure 2. A *benzenoid system* is 2-connected plane bipartite graph in which every interior region is bounded by a unit regular hexagon. A *coronoid system* is a benzenoid system with *holes* (i.e., nonhexagonal interior faces), but every edge is contained in a hexagon. Since all interior vertices of a benzenoid system are of degree three, so theorem 2.2 implies the following

Corollary 2.3 [19]. Let H be a benzenoid system with 1-factors. Then H is normal if and only if the exterior face of H is resonant.

For coronoid system, the following criterion was obtained by Zhang and Zheng.

Theorem 2.4 [20]. Let C be a coronoid system with 1-factors. Then C is normal if and only if every nonhexagonal face is resonant.

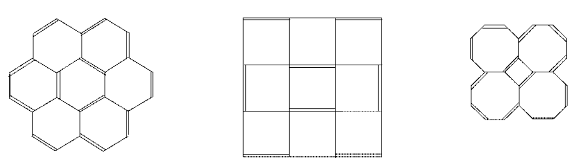

Figure 2. Some types of plane bipartite graphs that its interior vertices are of the same degree.

3. Normal components

Fast algorithms were designed [15–17] to determine all normal components and fixed single edges of bipartite graphs. One is outlined as follows. First, we orient all edges of any given 1-factor M from white towards black end-vertices. Then we orient all the other edges of G from black towards white end-vertices. Finally, by depth first search we determine the strongly connected components of the resulting digraph in linear times. These strongly connected components correspond to normal components of G.

It is useful to introduce a (*geometric*) *dual* graph G^* [26] of a plane graph G in characterizing a plane bipartite graph with fixed single edges: G^* has a vertex f^* for every face f of G, where f^* is placed inside f; corresponding to an edge e of G which is adjacent to two faces X and Y of G, there is an edge e^* of G^* joining the vertices X^* and Y^* of G^* and e^* crosses only the edge e of G. For $E \subseteq E(G)$, put $E^* := \{e^* \mid e \in E\}$. Note that the dual graph G^* is a connected plane graph and may contain self-loops and multiple edges.

A set S of edges of a connected graph G is called a *cutset* if $G - S$ is not connected and $G - S'$ remains connected for any proper subset S' of S.

Lemma 3.1 [26]. Edges in a plane graph G form a cutset in G if and only if the corresponding dual edges form a cycle in G^*.

Definition 3.1. Let G be a connected plane bipartite graph. A cutset C of G is called *elementary edge cut* (*e-cutset*) of G if all edges of C are incident with white vertices of one component of $G - C$. This component is called the *white* bank of C, denoted by $G_{\mathrm{w}}(C)$. The other component is called the *black* bank of C, denoted by $G_{\mathrm{b}}(C)$. The corresponding cycle C^* of G^* is called an *elementary closed cut line* (simply *e-cutline*) of G (see figure 1).

Note that the concept *e-cutline* here can be viewed as a generalization of cut (broken) segments appeared previously in benzenoid and coronoid systems [12,19,27,28]. Let H be a subgraph of G. Denote $w(H)$ and $b(H)$ the numbers of white and black vertices, respectively. Let $G \in \mathcal{G}$. The following theorem gives a criterion to determine whether G has a fixed single edge.

Theorem 3.2 [18]. Let $G \in \mathcal{G}$. Then G is not elementary if and only if G has an e-cutset C such that $b(G_{\mathrm{b}}(C)) = w(G_{\mathrm{w}}(C))$, i.e., all edges of C are fixed single.

Recall that a normal component of G is called a *normal block* if every interior face of it is a cell of the original graph G. Although any normal component of G is not necessarily a normal block as shown in introduction, we have the following

Theorem 3.3. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. Then G has at least one normal block.

Proof. If G is elementary, the result is trivial. Suppose that G has a fixed single edge. Then by theorem 3.2, there exists an e-cutline C^* corresponding to e-cutset C such that all the edges of C are fixed single. Suppose that C^* is minimal in the sense that there is no other e-cutset $\overline{C}$ consisting of fixed single edges such that the component of $G - \overline{C}$ lying in the interior of $\overline{C}^*$ is a proper subgraph of the component of $G - C$ lying in the interior of C^*. Without loss of generality, assume that the component of $G - C$ lying in the interior of C^* is the white bank, i.e., $G_{\mathrm{w}}(C)$. Since $G \in \mathcal{G}$ and the restriction of every 1-factor of G on $G_{\mathrm{w}}(C)$ is also a 1-factor of $G_{\mathrm{w}}(C)$, so $G_{\mathrm{w}}(C) \in \mathcal{G}$. It is easily seen that every black vertex in $G_{\mathrm{w}}(C)$ is of the same degree ($\geqslant 2$) as in G. So $G_{\mathrm{w}}(C)$ has at least 4 vertices.

It suffices to prove that $G_{\mathrm{w}}(C)$ is elementary: if $G_{\mathrm{w}}(C)$ is elementary and has more than two vertices, its edges are nonfixed. Moreover, all edges of C are fixed single implies that $G_{\mathrm{w}}(C)$ is a normal component of G. Since every cell of $G_{\mathrm{w}}(C)$ is that of G, $G_{\mathrm{w}}(C)$ is a normal block of G.

Suppose that $G_{\mathrm{w}}(C)$ has a fixed single edge. Then by theorem 3.2 $G_{\mathrm{w}}(C)$ has also an e-cutset $\overline{C}$ whose edges are all fixed single. From the dual graph G^*, delete the vertices lying in the exterior of C^* and contract the cycle C^* into a vertex c^* to result in the dual graph of $G_{\mathrm{w}}(C)$. If the corresponding e-cutline $\overline{C}^*$ of $G_{\mathrm{w}}(C)$ does not pass through c^*, then $\overline{C}$ is identical with an e-cutset of G and the component of $G - \overline{C}$ lying in the interior of $\overline{C}^*$ is a proper subgraph of $G_{\mathrm{w}}(C)$, which contradicts the minimality of C^*. Thus $\overline{C}^*$ passes through c^*. When c^* is recovered to the cycle C^* of G^*, $\overline{C}^*$ either remains a cycle or becomes a path of G^*, denoted by P^*. For the former case, a contradiction would occur as before. We consider the latter case, in $C^* \cup P^*$ there exists a cycle C'^* that is an e-cutline of G (see figure 1), the interior of which contains the white bank. Obviously all edges of the corresponding e-cutset C' are fixed single. However, the component of $G - C'$ lying in the interior of C'^* is a proper subgraph of $G_{\mathrm{w}}(C)$, which also contradicts the minimality of C^*. □

Definition 3.2. Suppose $G \in \mathcal{G}$ has fixed single edges. A normal component G_i of G is said to be *extreme* if (i) G_i is a (white or black) bank of an e-cutset of G, and (ii) G_i has exactly one face which is not a face of G.

Corollary 3.4. Suppose $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. If G has a fixed single edge, then G has at least two extreme normal components.

Proof. The proof of theorem 3.3 implies that G has a normal component that is a bank of an e-cutline C^* and contained in the interior of it, which must be extreme; the existence of another extreme normal component can be verified when considering always the exterior region of C^*. □

Corollary 3.5. Suppose $G \in \mathcal{G}$. If all vertices with degree one of G are of the same color and lie on the boundary of G, then G has at least one normal block.

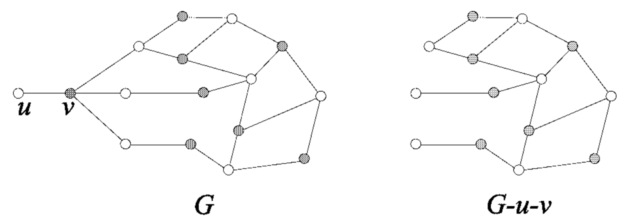

Figure 3.

Proof. Without loss of generality, assume that all vertices with degree one of G are of white color. Let u be a white vertex incident with a unique edge uv. Then uv is a pending, and thus fixed double edge. The other edges incident with v are fixed single edges. Deleting the vertices u and v together with incident edges, the resulting graph G' has the following properties (see figure 3):

(i) Every interior face of G' remains a face of G;

(ii) G' has black vertices, and every black vertex remains the same degree ($\geqslant 2$) as in G; and

(iii) If G' has a vertex with degree 1, then it is of white and lies on the boundary of G'.

Repeating the above procedure, by the finiteness of G we finally obtain a subgraph, denoted by G'', satisfying that every interior face is a face of G and the minimum degree $\geqslant 2$. By theorem 3.3, G'' and thus G has a normal block. □

Lemma 3.6 [18]. Let G be a plane elementary bipartite graph with more than two vertices. Then for every 1-factor M of G, it has an M-alternating cell.

Corollary 3.7. Let $G \in \mathcal{G}$. If all vertices with degree one of G are of the same color and lie on the boundary of G, or if $\delta(G) \geqslant 2$, then for every 1-factor M of G, there exists an M-alternating cell.

Proof. By theorem 3.3 and corollary 3.5, G has a normal block G_1. For every 1-factor M of G, the restriction $M|_{G_1}$ is also 1-factor of G_1. Then by lemma 3.6, G_1 and thus G has an M-alternating cell. □

4. Some extremal cases

From theorem 3.3, we know that a plane bipartite graph with a fixed single edge and the minimum degree $\geqslant 2$ has at least one normal block. In this section we shall discuss when a plane bipartite graph has exactly one normal block and all normal components are normal blocks, respectively. In addition, we estimate the number of normal blocks when a single cycle is a normal block.

4.1. Exactly one normal block

Definition 4.1. Let $G \in \mathcal{G}$. Let G_1 and G_2 be two disjoint subgraphs of G and f a finite face of G_2. Then G can be represented as $G := G_1 \leqslant_f G_2$, if

(i) G_1 lies in the interior of face f of G_2;

(ii) Let $G' := G - V(G_1 \cup G_2)$. Then G' lies in the interior of f and the exterior of G_1 and G' has a unique 1-factor; and

(iii) Let $E_0 = E(G)\backslash E(G_1 \cup G_2)$. Then E_0 lies in the interior of f and the exterior of G_1 and only the vertices with the same color of G_1 (respectively G_2) are incident with edges of E_0.

"$\leqslant_f$" is, in fact, an operation between two plane bipartite graphs. For an example, see figure 4. Furthermore, we can define the operations $\leqslant_f$ among many graphs in turn, for example, $G_1 \leqslant_{f_1} G_2 \leqslant_{f_2} G_3 = (G_1 \leqslant_{f_1} G_2) \leqslant_{f_2} G_3$. Note that the operation "$\leqslant_f$" satisfies the associate law but not the commutative law. For convenience, the subscript f may be omitted if no confusion may arise.

Theorem 4.1. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. Then G has exactly one normal block if and only if G can be represented as $G := G_1 \leqslant G_2 \leqslant \cdots \leqslant G_k$ $(k \geqslant 1)$, where the G_i's are the normal components of G.

Proof. Let $G_1, G_2, \ldots, G_k$ $(k \geqslant 1)$ denote the normal components of G. If G can be represented as $G := G_1 \leqslant G_2 \leqslant \cdots \leqslant G_k$, by definition 4.1 it is obvious that G has a unique normal block G_1.

We shall prove the necessity by the induction on the number k of normal components of G. If $k = 1$, then by corollary 3.4 G itself is elementary and the result is trivial. In what follows, suppose that $k \geqslant 2$. By the proof of theorem 3.3, G has an e-cutline C^* such that the component of $G - C$ lying in the interior of C^* is a normal block, denoted by G_1. The component of $G - C$ lying in the exterior of C^* is denoted by G'. We assert that C^* does not pass through the vertex of G^* corresponding to the exterior of G. Otherwise every interior face of G' is a cell of G, and by corollary 3.4 G' also contains a normal block of G, a contradiction. Thus G' has exactly one interior face f_1' which is

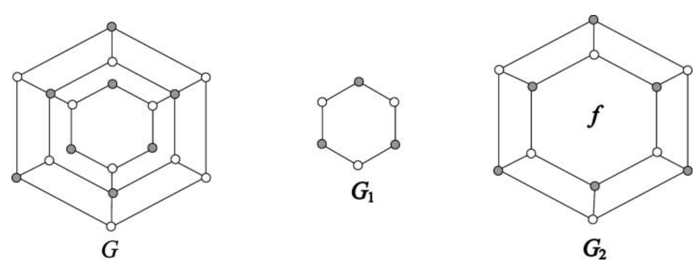

Figure 4. Illustration of $G := G_1 \leqslant_f G_2$.

not a cell of G. If G' has vertices of degree 1, they must be of the same color and lie in the boundary of f_1'. By the proof of corollary 3.5, repeatedly deleting those vertices with degree 1 and their adjacent vertices together with their incident edges in turn, the resulting graph G'' has the following properties: (i) G'' is connected and the minimum degree $\geqslant 2$, (ii) G'' has exactly one finite face f_1 which is not face of G, and (iii) G'' has $k-1$ normal components. Thus $G = G_1 \leqslant_{f_1} G''$. On the other hand, G'' has exactly one block G_2, which must contain the face f_1 of G'. By the induction hypothesis we have that $G'' := G_2 \leqslant \cdots \leqslant G_k$, where the G_i's are the normal components of G''. Thus $G := G_1 \leqslant G_2 \leqslant \cdots \leqslant G_k$. The proof is complete. □

Corollary 4.2. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. If G has exactly one normal block, then the exterior face of G is resonant.

Proof. By theorem 4.1, the exterior face of G is also that of the normal component G_k. By theorem 2.1 the exterior face of G_k, and thus of G is resonant. □

As an immediate consequence, we have

Corollary 4.3. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. If G has a fixed single edge lying in the boundary of G, then G has at least two normal blocks.

4.2. All normal blocks

Definition 4.2. Let $G \in \mathcal{G}$. An edge of G is called *allowed* if it belongs to a 1-factor. G is called *weakly elementary* [18], if for any resonant cycle C of G, the edges that are incident with the vertices of C and lie in the interior of C are allowed.

Lemma 4.4 [18]. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. Then G is weakly elementary if and only if for every resonant cycle C, the subgraph of G formed by C together with the interior is elementary.

Theorem 4.5. Let $G \in \mathcal{G}$. Then every normal component of G is a normal block if and only if G is weakly elementary.

Proof. Suppose that every normal component of G is a normal block. Let C be any resonant cycle of G. Then C must be contained in a normal component G_i of G. Since G_i is also normal block, the edges lying in the interior of C are allowed. Then G is weakly elementary.

Conversely, suppose that G is weakly elementary. Let $G_1, \ldots, G_k$ $(k \geqslant 1)$ be the normal components of G. Since each G_i $(1 \leqslant i \leqslant k)$ is a plane elementary bipartite graph, the boundary ∂G_i of G_i is a resonant cycle. Let $I[\partial G_i]$ denote the subgraph of G formed by ∂G_i and the interior. By lemma 4.4 $I[\partial G_i]$ is elementary. Thus $I[\partial G_i] = G_i$, i.e., G_i is a normal block of G. □

Corollary 4.6. Let $G \in \mathcal{G}$ be weakly elementary and $\delta(G) \geqslant 2$. If G has a fixed single edge, then G has at least two normal blocks.

Obviously elementary plane bipartite graphs are weakly elementary. Other types of known weakly elementary bipartite graphs are hexagonal systems, square systems and other systems exclusively formed by regular squares and octagons as cells (see figure 2), etc., which have the important properties that the interior vertices have the same degree and if the boundary is a resonant cycle, then they are elementary. Theorem 4.5 and corollary 4.6 can be viewed as extension of the corresponding results in hexagonal systems. Furthermore, we are interested in seeking for novel types of weakly elementary plane bipartite graphs.

4.3. Small normal blocks

Theorem 4.7. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. Assume that G has more than one cycle and all vertices of degree 2 lie on the boundary of G. If G has a cycle as normal block, then G has at least two normal blocks.

Proof. Let a cycle C of G be a normal block. Suppose that G has exactly one normal block, which must be C. Since G has more than one cycle, G has fixed single edges and thus at least two normal components. By theorem 4.1 we know that the vertices of C are interior vertices of G and thus of degree $\geqslant 3$; on the other hand, only the same colored vertices (say white) are incident with edges not belonging to C, the black vertices of C are thus of degree 2, a contradiction. □

Theorem 4.8. Let $G \in \mathcal{G}$ be 2-connected and weakly elementary. Assume that G has more than one cycle and all vertices of degree 2 lie on the boundary of G. If G has m ($m \geqslant 1$) distinct cycles as normal blocks, then G has $m + 2$ normal blocks.

Proof. It is obvious that G contains fixed single edges and every normal component is normal block (theorem 4.5). By corollary 3.4, G has two extremely normal blocks G_1 and G_2 such that only the same colored vertices of G_1 (respectively G_2) are incident with edges not belonging to G_1 (respectively G_2). We assert that neither G_1 nor G_2 is a cycle. Suppose that G_1 is a cycle. Since G is 2-connected, G has a path P only end-vertices u and v of which lie on C. Then u and v are of the same color (say white). Furthermore, P and a path P' of C from u to v form a cycle. The interior of the cycle lies in the exterior of C. So P' has a black vertex x of degree 2, which must be an interior vertex of G, a contradiction. The assertion is verified. Thus G has at least $m + 2$ normal blocks. □

Remark. In [23] Hansen and Zheng showed that, if benzenoid systems with fixed edges has a single hexagon as its normal component, then it has at least three normal components. Such a result is now extended to weakly elementary bipartite graphs in a simpler way. A type of benzenoid systems with exactly $m+2$ normal components are illustrated

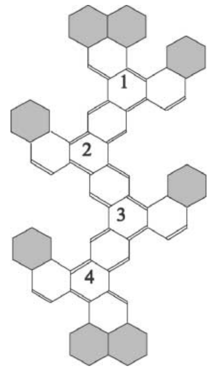

Figure 5. A hexagonal system with 6 normal components (shadowy parts).

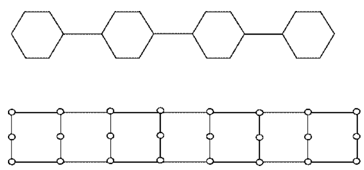

Figure 6. Two weakly elementary bipartite graphs in which every normal block is a cycle.

in figure 5, where m is the number of single hexagons as normal components. In addition, if the conditions of theorem 4.8 are violated, the result does not necessarily hold. For example, all normal components (blocks) of two weakly elementary plane bipartite graphs shown in figure 6 are cycles.

5. Clar patterns and cell polynomial

For $G \in \mathcal{G}$, let S be a set of pairwise disjoint cells of G and denote by $G - S$ the plane graph obtained from G by removing all vertices of cells in S together with their incident edges. Then S is called a *Clar* (or *resonant*) pattern of G if $G - S$ either has a 1-factor or is empty. It is obvious that S is a Clar pattern of G if and only if G has a 1-factor M such that every cell in S is M-alternating. Furthermore, a Clar pattern S of G is called *sextet pattern* if every cell in S is a hexagon (or 6-membered ring). Let $c(G)$ and $k(G)$ denote the number of Clar patterns and sextet patterns of G, respectively. A *pair of resonant cycles* C_1 and C_2 means that C_1 and C_2 are disjoint and $G - C_1 - C_2$ has a 1-factor or empty.

5.1. Cell polynomial

We now describe an definition of cell polynomial of G due to Gutman [9] and John [8]. If the cells of G are labelled by $C_1, C_2, \ldots,$ every cell C_i is assigned a weight $w_i := w(C_i)$. Then the weight of a Clar pattern S is defined as $W(S) := \prod_{C \in S} w(C)$;

in particular, the weight of an empty Clar pattern is 1. The cell polynomial of G can be defined as follows:

$$f_G = f_G(w_1, w_2, \ldots) = \sum_S W(S),$$

where the summation goes over all Clar pattern S of G.

In [8] an algorithm for computing the cell polynomial of an outerplane bipartite graph was designed. We first give a reduction method for computing the cell polynomial of a plane bipartite graph G with fixed edges by decomposing G into its normal components. Let $G_1, \ldots, G_k$ denote the normal components of G_i. Denote by F_i the set of some cells of G_i that are not cells of G; such cells are called "forbidden". The restricted cell polynomial of G_i with respect to forbidden cells is defined as

$$f^*_{G_i} = f^*_{G_i}(w_1, w_2, \ldots) = \sum_S W(S),$$

where the summation goes over all Clar pattern S of G_i containing no forbidden cells of G_i. Of course, if $F_i = \emptyset$ (i.e., G_i is a normal block), $f^*_{G_i} = f_{G_i}$.

Theorem 5.1. Let $G_1, \ldots, G_k$ be the normal components of $G \in \mathcal{G}$. Then

$$f_G = \prod_{i=1}^{k} f^*_{G_i}.$$

Proof. Let S be any Clar pattern of G. Since any cell in S contains no fixed edges, it must be a cell of exactly one normal components of G. Thus the restriction of S on G_i is also a Clar pattern of G_i that contains no forbidden cells of G_i; that means that any Clar pattern of G are composed of Clar patterns of G_i, for $i = 1, \ldots, k$, containing no forbidden cells of G_i and vice versa. □

The cell polynomial sometimes can be taken in various "coarsened" ways. For example, let us compute the cell polynomial of the graph G shown in figure 4, which has two normal components G_1 and G_2. If a cell C is assigned a weight $w_{|C|}$, $f_{G_1} = 1 + w_6$ and $f^*_{G_2} = 1 + 6w_4 + 9w_4^2 + 2w_4^3$. The cell polynomial reads as $f_G(w_4, w_6) = (1 + w_6)(1 + 6w_4 + 9w_4^2 + 2w_4^3)$, which implies that G has exactly $f_G(1, 1) = 36$ Clar patterns.

Theorem 5.2. Let $G_1, \ldots, G_k$ be the normal components of $G \in \mathcal{G}$. Then

$$f_G = \prod_{i=1}^{k} f_{G_i}$$

if and only if G is weakly elementary.

Proof. By theorem 5.1 $f_G = \prod_{i=1}^{k} f_{G_i}^*$. In general $f_{G_i}^*$ is only a part of f_{G_i}. Thus $f_G = \prod_{i=1}^{k} f_{G_i}$ holds if and only if $f_{G_i}^* = f_{G_i}$ for all i. Furthermore, if and only if every cell of G_i is also a cell of G. Otherwise, suppose that a cell C of some G_i is not a cell of G. By theorem 2.1 $\{C\}$ is a Clar pattern of G_i, but contains a forbidden cell. It implies that $f_{G_i}^* \neq f_{G_i}$, a contradiction. □

Corollary 5.3. Let $G \in \mathcal{G}$ and $\delta(G) \geqslant 2$. If the cell polynomial of G is irreducible on the polynomial ring $\mathbb{Z}[w_1, w_2, \ldots]$, then G has exactly one normal block, and the other normal components are cycles (if it has other).

Proof. By theorem 3.3, denote $G_1, \ldots, G_k$ $(k \geqslant 1)$ the normal components of G, where G_1 is a normal block. Then $f_{G_1}^* = f_{G_1} \neq 1$. By theorem 5.1 we have $f_G = \prod_{i=1}^{k} f_{G_i}^*$, which implies that $f_{G_i}^* = 1$, for all $2 \leqslant i \leqslant k$, and none of the G_i are normal block. Furthermore, by theorems 2.1 and 4.1 it easily follows that the G_i for all $i \geqslant 2$ are cycles. □

Definition 5.1 [29]. Let M be a 1-factor of $G \in \mathcal{G}$. An M-alternating cycle C of G is called *proper* if every edge of C belonging to M goes from white end-vertex to black end-vertex by the clockwise orientation of C; otherwise C is *improper*.

Lemma 5.4 [29]. For any $G \in \mathcal{G}$ there exists a unique 1-factor M without proper M-alternating cycles. Such 1-factor is called the *root* 1-*factor*.

Theorem 5.5. Let $G \in \mathcal{G}$. Then $c(G) = f_G(1, 1, \ldots) \leqslant k(G)$, and the equality holds if and only if G is weakly elementary and for any pair of resonant cycles their interior regions are disjoint.

Proof. We establish a mapping ϕ from the Kekulé patterns to the Clar patterns of G as follows. For any 1-factor M of G, define $\phi(M)$ as the set of all proper M-alternating cells of G. It is obvious that $\phi(M)$ is a Clar pattern of G. Furthermore, it will be shown that ϕ is a surjection. For any Clar pattern S of G, by lemma 5.4 we take the root 1-factor M_0 of $G - S$ (i.e., without proper M_0-alternating cycles), and a 1-factor M_1 of the subgraph formed by all cells in S such that all cells in S are proper M_1-alternating. It follows that $M_0 \cup M_1$ is a 1-factor of G and $\phi(M_0 \cup M_1) = S$. So $c(G) = f_G(1, 1, \ldots) \leqslant k(G)$.

The equality holds if and only if ϕ is a one-to-one correspondence between the 1-factors and the Clar patterns of G. Suppose that G is weakly elementary and for any pair of resonant cycles their interior regions are disjoint. Let M_1 and M_2 be two 1-factors of G such that $\phi(M_1) = \phi(M_2) = S_0$. It will be shown that $M_1 = M_2$. Let M_1' and M_2' be the restrictions of M_1 and M_2 on $G - S_0$, respectively. If $M_1 \neq M_2$, then $M_1' \neq M_2'$. Then the symmetric difference $M_1' \oplus M_2' := (M_1 \cup M_2) \setminus (M_1 \cap M_2)$ contains an alternating cycle C in M_1' and M_2'. Without loss of generality we may say that C is proper M_1'-alternating. Let $G[C]$ denote the subgraph of G

formed by C together with the interior. Then $G[C]$ is a subgraph of $G - S_0$, and it is elementary by theorem 4.4. However, $G[C]$ has a proper M_1'-alternating cell of G, which would belong to S_0, a contradiction.

Conversely, if G has a pair of resonant cycles C_1 and C_2 such that C_1 lies in the interior of C_2; that means that G has a 1-factor M such that both C_1 and C_2 are M-alternating. By corollary 3.5 $G[C_1]$ has an M-alternating cell C of G. So C and C_2 are a pair of resonant cycles. Let $G_0 := G - C$. We choose a 1-factor M_1 of G such that C is proper M_1-alternating and $M_1|_{G_0}$ is the root 1-factor of G_0. It is obvious that $\phi(M_1) = \{C\}$. On the other hand, since C_2 is a resonant cycle of G_0, it must be contained in a normal component of G_0. We choose a cell C_2' of this normal component so that its interior contains the cell C of the original graph. By lemma 5.4 we can construct another 1-factor M_2 of G such that both C and C_2' are proper M_2-alternating and $M_2|_{G_0 - C_2'}$ is the root 1-factor of $G_0 - C_2'$. Then $M_1 \neq M_2$. But it follows that $\phi(M_2) = \{C\}$; otherwise, if other proper M_2-alternating cell C' of G other than C would occur, C' is disjoint with C, must lie in the interior of C_2' and intersect C_2', which contradicts that C_2' is a cell of a normal component of G_0.

On the other hand, if G is not weakly elementary, G has a resonant cycle C_2 such that $G[C_2]$ contains a fixed single edge of G. Then C_2 must be contained in a normal component G_1 of G, which is not a normal block; that is, G_1 has a cell C that is not a cell of G. We choose two 1-factors M_1 and M_2 of G so that M_1 is the root 1-factor of G, C is proper M_2-alternating cycle and $M_2|_{G-C}$ is the root 1-factor of $G - C$. Similarly, it follows that $\phi(M_1) = \phi(M_2) = \emptyset$, a contradiction. $\square$

Corollary 5.6 [10]. Let $G \in \mathcal{G}$. Then $c(G) = f_G(1, 1, \ldots) \leqslant k(G)$; the equality holds if G is an outerplane bipartite graph.

5.2. Sextet polynomial

In this subsection we discuss the sextet polynomial of benzenoid or coronoid systems G, which is defined as [3,5]

$$B_G(x) = \sum_S x^{|S|} = \sum_{i=1}^{m} \sigma(G, i)x^i,$$

where the first summation goes over all sextet patterns of G, $\sigma(G, i)$ denotes the number of sextet patterns with exactly i hexagons and m is the maximum size of sextet patterns.

The sextet polynomial of a benzenoid system can be reduced from its cell polynomial by assigning all hexagons the same weight x; further the sextet polynomial of a coronoid systems can reduced from its restricted cell polynomial when all “holes” are viewed as forbidden faces.

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

Theorem 5.7. Let G be a benzenoid or coronoid system and $G_1, \ldots, G_k$ its normal components. Then

$$B_G(x) = \prod_{i=1}^{k} B_{G_i}(x).$$

Proof. It follows from a fact that a set S of pairwise disjoint hexagons in G is a sextet pattern of G if and only if the restriction of S on every normal component G_i is also a sextet pattern of G_i. □

Lemma 5.8 [19]. Let G be a benzenoid system. Then $c(G) = B_G(1) \leqslant k(G)$, and the equality holds if and only if G contains no coronene (the first one on the left-hand side in figure 2) as its nice subgraph.

Theorem 5.9. Let G be a coronoid system. Then $B_G(1) \leqslant k(G)$, and the equality holds if and only if every normal component of G is benzenoid system that contains no coronene as its nice subgraph.

Proof. By theorem 5.5 we have that $B_G(1) \leqslant c(G) = f_G(1, 1, \ldots) \leqslant k(G)$. Let $G_1, \ldots, G_k$ denote the normal components of G. Combining by theorem 5.7 and a fact $k(G) = \prod k(G_i)$, we have that $B_G(1) = k(G)$ if and only if $B_{G_i}(1) = c(G_i) = k(G_i)$ for all $1 \leqslant i \leqslant k$. It implies that G_i are benzenoid systems, i.e., G_i contains no holes (nonhexagon interior faces). Otherwise, such a hole itself can form a Clar pattern, other than sextet pattern, a contradiction. The second result follows by lemma 5.8. □

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