

## Z-transformation graphs of perfect matchings of plane bipartite graphs: a survey\*

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Dedicated to Professor Fuji Zhang on the occasion of his 70th birthday

### Abstract

From a mathematical point of view, in 1988 F. Zhang, X. Guo and R. Chen introduced “Z-transformation graph” (Randić named after “resonance graph” in chemical literature) of perfect matchings of hexagonal systems: from a perfect matching to another is joined by an edge provided they only differ in a hexagon. Afterwards, this concept was extended naturally to general plane bipartite graphs. Its nature can be explained in many ways from chemical resonance to mathematical cycle space and distributive lattice. We now survey rich theoretical results on this field made by several groups in main directions: chemical application, basic properties, connectivity, forcing edge, lattice structure, distance and median graphs, coding, as well as some miscellaneous problems.

## 1 Introduction

A *hexagonal system* is a connected plane bipartite graph without cut vertices and each interior face of which is surrounded by a regular hexagon of side length one. The carbon-skeleton of a benzenoid hydrocarbon is a hexagonal system  $H$  with a Kekulé structure, a set of pairwise disjoint edges that cover all vertices of  $H$ , which coincides with perfect matching or 1-factor in graph theory. Various graph-theoretical researches on benzenoid hydrocarbons are referred to books [7, 8, 17, 18].

In 1988 Zhang, Guo and Chen [54, 55] introduced a kind of transformation graphs, named after *Z-transformation graph* on the set of perfect matchings of hexagonal systems:

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from a perfect matching to another is joined by an edge provided they only differ in a hexagon (equivalently, the symmetric difference of these two perfect matchings is just the hexagon), and revealed many basic properties and an application [60]. In mathematics, it originates from perfect matching polyhedron [41]: two vertices are adjacent if and only if their corresponding perfect matchings form a unique alternating cycle. Thus  $Z$ -transformation graph of a hexagonal system is a spanning subgraph of its perfect matching graph [38]. In chemistry, this idea originates from Herndon's resonance theory [24] put forward in 1973:  $RE = 2(\chi_1\gamma_1 + \chi_2\gamma_2)/K$ , where  $\gamma_1$  and  $\gamma_2$  are constants, and  $\chi_1$  and  $\chi_2$  stand for the numbers of pairs of Kekulé structures which are transformed one into the other by cyclically permuting 3 and 5 double bonds respectively. An example is illustrated in Gutman and Cyvin [18]. In fact  $\chi_1$  corresponds the number of edges of  $Z$ -transformation graph. Then,  $Z$ -transformation graph has been introduced by Gründler [15, 16], and Randić [42, 43, 44] in 1997 under the name "resonance graph"; El-Basil [9, 10] carried on such transformations on partial hexagons (eg. end-hexagons of cata-benzenoids) to produce lattice graph or hypercubes. In 1997 Randić [43] showed that the leading eigenvalue ( $\lambda$ ) of the resonance graphs correlates with the resonance energy of benzenoids:  $RE = 0.78342\lambda + 0.60682$  with the coefficient of the correlation 0.9828, the standard err of the estimate 0.072, and the Fisher ratio 686. This represents a quite satisfactory correlation.

In 2003 J.C. Fournier [12] re-introduced  $Z$ -transformation graph under name "perfect matching graph" in investigating domino tiling spaces of Saldanha and Casarin [46]. Domino tilings and lozenge tilings of polygonal region in the plane are other sources of perfect matchings. A polyomino is a polygonal region consisting of regular squares. A *domino tiling* is a polyomino tiled or paved fully by dominoes ( $1 \times 2$  or  $2 \times 1$  rectangles). A domino tiling of a polyomino corresponds to a perfect matching of its inner dual. For example, the domino tiling in Fig. 1 corresponds to a perfect matching of  $3 \times 3$  chessboard.



Fig. 1. Domino tiling and matching.

We can use *lozenge* as a *brick* of tiling. A *lozenge* is a rhombus of side length 1 having angles of  $60^\circ$  and  $120^\circ$ . A *lozenge tiling* is a triangulated region, composed of triangles with all side lengths 1, is tiled fully by lozenges. A lozenge tiling of a triangulated region corresponds to a perfect matching of its inner dual. For example, the lozenge tiling in Fig. 2 (left) corresponds to a perfect matching of coronene (Fig. 2 (right)).

To date many theoretical researches on  $Z$ -transformation graphs have been made by several groups in the following main directions: (i) cata-benzenoids and outplane

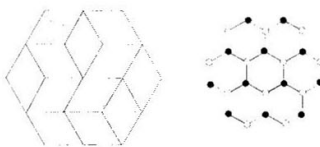


Fig. 2. A lozenge tiling and matching

bipartite graphs, (ii) basic properties and extension to general plane bipartite graphs, (iii) connectivity, (iv) orientation of Z-transformation graphs and lattice structure, (v) distance, median properties and coding, as well as some miscellaneous problems (Hamilton path, Fibonacci cubes and Clar number). In this article we summary such research progresses on Z-transformation graphs with some open problems.

## 2 Plane bipartite graphs and resonance faces

Thorough this article we restrict our consideration on finite and simple plane bipartite graphs with at least one perfect matching. Hexagonal systems, polyomino systems and boron-nitrogen fullerenes [13, 6] are classical examples of plane bipartite graphs.

By a plane graph  $G$  we mean an embedding of a planar graph in the plane. This embedding partitions the plane into an open set, every connected component of which is a region, called a face of  $G$ ; the infinite one is the *outer face* and the other ones are said to be *inner faces*. A subgraph  $H$  of a given plane graph  $G$  is a plane graph, which can be always regarded as a planar embedding restricted on  $G$ .

A *bipartite* graph means a graph for which the vertices are colored by white or black so that two adjacent vertices receive different colors. For a bipartite graph, such a 2-coloring (white-black) is always specified.

A plane graph is called an *outerplane* graph if all vertices lie on the boundary of the exterior face. Some examples of outerplane bipartite graphs are illustrated in Fig. 3. Catacondensed benzenoids [30, 32, 34, 42] are hexagonal systems that are a subclass of outerplane bipartite graphs.

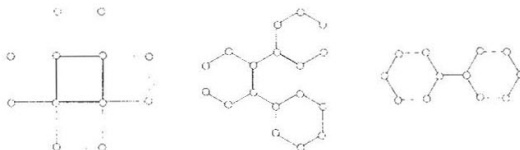


Fig. 3. Three examples of outerplane bipartite graphs.

Let  $G$  be a plane bipartite graph and  $M$  a perfect matching of  $G$ . A cycle  $C$  (resp. path  $P$ ) is  $M$ -alternating if the edges of  $C$  (resp.  $P$ ) appear alternately in  $M$  and  $E(G) \setminus M$ . The symmetric difference of two finite sets  $A$  and  $B$  is defined as  $A \oplus B := (A \cup B) \setminus (A \cap B)$ . This operation can be defined among many finite sets in a natural way and obey associative and commutative laws. Let  $M$  and  $M'$  be distinct perfect matchings. The symmetric difference  $M \oplus M'$  consists of mutually disjoint  $M$  and  $M'$ -alternating cycles of  $G$ . If  $C$  is an  $M$ -alternating cycle, then  $M \oplus C$  is also a perfect matching of  $G$ , where  $C$  may be regarded as its edge-set.

A bipartite graph  $G$  is called *elementary* or *normal* if  $G$  is connected and every edge belongs to a 1-factor of  $G$ . Elementary bipartite graphs have many important equivalent properties, see Lovasz and Plummer [38]. The complete graph  $K_2$  on two vertices is a trivial elementary bipartite graph. A non-trivial plane elementary bipartite graph is 2-connected and every face is bounded by a cycle.

A subgraph  $H$  of a bipartite graph  $G$  is *nice* if  $G - V(H)$  has a perfect matching. It is obvious that a cycle  $C$  of  $G$  is nice (or *resonant*) if and only if  $G$  has a perfect matching  $M$  such that  $C$  is  $M$ -alternating. A *generalized hexagonal system* means a connected subgraph of a hexagonal system. The following elegant characterizations for normal (generalized) hexagonal systems were obtained by Zhang, Chen and Zheng.

**Theorem 2.1.** [51] *Let  $H$  be a hexagonal system with perfect matchings. Then  $H$  is normal if and only if the boundary of  $H$  is a nice cycle.*

**Theorem 2.2.** [61] *Let  $G$  be a generalized hexagonal system with perfect matchings. Then  $G$  is normal if and only if the boundary of each non-hexagonal face is a nice cycle.*

A face of a plane bipartite graph is *resonant* if its boundary is a nice cycle. Some natural generalization on plane elementary bipartite graph can be described in terms of resonant faces as follows.

**Theorem 2.3.** [70] *Let  $G$  be a plane bipartite graph with perfect matchings. Then  $G$  is elementary if and only if each face is resonant.*

**Theorem 2.4.** [71] *Let  $G$  be a plane bipartite graph the interior vertices of which are of the same degree. Then  $G$  is elementary if and only if the exterior face of  $G$  is resonant.*

From the theorem we can know that 2-connected outerplane bipartite graph is elementary because it has no interior vertices and its boundary is a nice cycle.

For non-elementary plane bipartite graphs  $G$ , elementary components of  $G$  mean components of the subgraph obtained from  $G$  by the removal of all forbidden edges (or fixed single edges [58], those edges not contained in any perfect matchings). Further,  $G$  is called *weakly elementary* [70, 36, 47] if every interior face of every elementary component of  $G$  remains an interior face of the original  $G$ . It is known that hexagonal system, polyomino, etc., are this kind of graphs. However, an example of non-weakly graphs is illustrated in Fig. 4(a).



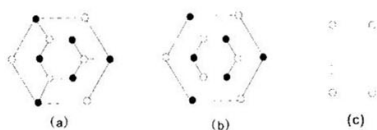


Fig. 4. (a) A non-weakly elementary plane bipartite graph  $G$ , (b) two elementary components, and (c)  $Z$ -transformation graph  $Z(G)$ .

**Lemma 2.5.** [70] *Let  $G$  be a plane bipartite graph with a perfect matching. Then  $G$  is weakly elementary if and only if for each nice cycle  $C$ , the subgraph of  $G$  formed by  $C$  together with the interior is elementary.*

### 3 Basic properties of $Z$ -transformation graphs

Given a plane bipartite graph  $G$  with a perfect matching  $M$ . If the boundary of an inner face is an  $M$ -alternating cycle  $C$ , a  $Z$ -transformation (*twist*, or *flip*) is an interchange between the  $M$ -matching and non-matching edges on  $C$ ; that is, it carries-once on the symmetric difference  $M \oplus E(C)$  to give another perfect matching. For example, Fig. 5 gives  $Z$ -transformations of perfect matchings of chessboard and coronene along a square and a hexagon respectively.

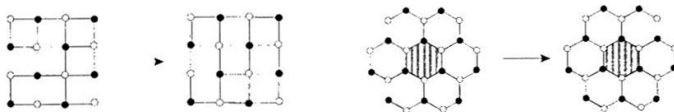


Fig. 5. Illustration for  $Z$ -transformation or twist for a square and hexagon.

**Definition 3.1.**  $Z$ -transformation graph, denoted by  $Z(G)$  (or *resonance graph*), of perfect matchings of  $G$  is a graph: the vertices are perfect matchings of  $G$ , and a pair of vertices  $M_1$  and  $M_2$  are joined by an edge provided they can be obtained from each other by a  $Z$ -transformation along an inner facial boundary.

For example, the  $Z$ -transformation graph of the cube graph  $Q_3$  is illustrated in Fig. 6(b); and the  $Z$ -transformation graph of the graph in Fig. 4(a) is the disjoint union of two copies of  $K_2$  (cf. Fig. 4(c)). Randić [43] ever drew  $Z$ -transformation graphs of quite many cata-condensed benzenoids.

The following basic properties of  $Z$ -transformation graph were first obtained by Zhang et al. [54] for hexagonal systems, then extended to general plane bipartite graphs.

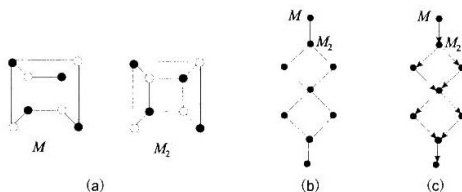


Fig. 6. (a) Perfect matchings  $M$  and  $M_2$ , (b) Z-transformation graph  $Z(Q_3)$ , and (c) Z-transformation digraph  $\bar{Z}(Q_3)$ .

**Theorem 3.1.** [54, 70] Let  $G$  be a plane bipartite graph with a perfect matching. Then  $Z(G)$  is a bipartite graph.

**Theorem 3.2.** Let  $G$  be a plane elementary bipartite graph. Then

- (i) [54, 70]  $Z(G)$  is connected,
- (ii) [54, 70]  $Z(G)$  has at most two vertices of degree one, and
- (iii) [68] the block-graph of  $Z(G)$  is a path.

**Theorem 3.3.** [54] Let  $H$  be a hexagonal systems with perfect matchings. Then either  $Z(H)$  is a path or  $Z(H)$  has girth 4 and  $Z(H) - V_m$  is 2-connected, where  $V_m$  denotes the set of monovalency vertices of  $Z(H)$ .

Zhang et al. [54] completely determined hexagonal systems whose Z-transformation graphs contain one monovalency vertex by establishing a coordinate system  $O-ABC$ , which divides the plane into three areas  $AOB$ ,  $BOC$  and  $COA$ ; three equivalent propositions are obtained (for example, the boundaries in three areas are all monotone); further hexagonal systems whose Z-transformation graphs contain precisely two monovalency vertices are just hexagonal benzenoids  $O(m, n, k)$  [57].

The concept of Z-transformation graph can be used to solve the forcing edge problem of hexagonal systems proposed by Harary et al. [23]. An edge of a graph  $G$  is called a *forcing edge* if it belongs to exactly one perfect matching of  $G$ . F. Zhang and X. Li [56] provided an algorithm to recognize the hexagonal systems with forcing edges. Further the same authors [57] showed that a hexagonal system  $H$  with perfect matchings has a forcing edge if and only if  $Z(H)$  has a vertex  $M$  of degree one and the unique resonant hexagon with respect to  $M$  is a boundary hexagon. A similar characterization was obtained by Hansen and Zheng [20] independently. Enumeration [57, 53] for hexagonal systems with forcing edges and Kekulé structure count [59] were discussed.

Che and Chen [3] recently introduce a novel concept ‘forcing hexagon’: a hexagon  $h$  of a hexagonal system  $H$  is called a *forcing hexagon* if  $H - h$  has exactly one perfect matching, and show that



Fig. 7. (a) A crossed polyomino  $T$ , (b)  $Z(T)$ .

**Theorem 3.4.** [3] *A hexagonal system has a forcing hexagon if and only if it has a forcing edge.*

A general consideration on forcing edges of plane bipartite graphs was made in terms of reducible face construction and ear decomposition [38]. The details are referred to [70].

## 4 Connectivity of Z-transformation graphs

The connectivity of a graph  $G$  is the least integer  $\kappa$  such that it is less than the number of vertices of  $G$  and it remains connected by deletion of fewer than  $\kappa$  vertices. For hexagonal systems and polyomino graphs, the connectivity of their Z-transformation graphs was determined completely; see the following theorems.

**Theorem 4.1.** [55] *For a hexagonal system  $H$ , the connectivity of  $Z(H)$  equals its minimum degree.*

**Theorem 4.2.** [62] *For a polyomino graph  $P$ , the connectivity of  $Z(P)$  equals its minimum degree except  $Z(T)$  and  $Z(T) \times K_2$  (see Fig. 7).*

Wang [50] showed that the Z-transformation graph of plane bipartite cubic graphs are connected. In general, a simple characterization for connected Z-transformation graphs was obtained by Fournier [12] and Zhang et al. [72] independently.

**Theorem 4.3.** [12, 72] *Let  $G$  be a plane bipartite graph with a perfect matching. Then  $Z(G)$  is connected if and only if  $G$  is weakly elementary.*

Fournier also gave a criterion of determining whether two perfect matchings of  $G$  belong to the same component of  $Z(G)$ . Along this line, further descriptions can be found in next section and ref. [63].

We now define the restricted Z-transformation graphs. Let  $G$  be a plane bipartite graph with perfect matchings. Let  $F(G)$  and  $F_0(G)$  denote the sets of all faces and interior faces of  $G$  respectively.

**Definition 4.1.** For  $F \subseteq F(G)$ , the Z-transformation graph of  $G$  with respect to  $F$ , denoted by  $Z_F(G)$ , is defined as a graph in which the vertices are the perfect matchings

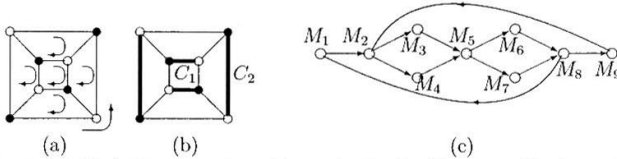


Fig. 8. (a) Clockwise orientation of faces of cube  $Q_3$ , (b) proper  $M_9$ -alternating face  $C_2$  and improper  $M_9$ -alternating face  $C_1$ , and (c)  $Z_t(Q_3)$ .

of  $G$  and two vertices  $M_1$  and  $M_2$  are joined by an edge provided they can be obtained from each other by a  $Z$ -transformation along a face of  $G$  belonging to  $F$ .

In particular, if  $F = F_0(G)$ , the restricted  $Z$ -transformation graph  $Z_F(G)$  with respect to  $F$  is the usual  $Z$ -Transformation graph  $Z(G)$  previously defined; if  $F = F(G)$ ,  $Z_F(G)$ , however, is the *total*  $Z$ -transformation graph of  $G$ , denoted by  $Z_t(G)$  [69].

**Theorem 4.4.** [72] *Let  $G$  be a plane elementary bipartite graph and let  $F \subseteq F(G)$ . If  $G$  has at least two faces not belonging to  $F$ , then the restricted  $Z$ -transformation graph  $Z_F(G)$  is not connected.*

From Lemma 2.5,  $G$  is said to be *second-weakly elementary* if for every nice cycle  $C$  of  $G$ , the subgraph of  $G$  formed by  $C$  together with either the interior or the exterior is elementary. For the total  $Z$ -transformation graph, we have the following results.

**Theorem 4.5.** [72] *Let  $G$  be a plane bipartite graph with a perfect matching. Then  $Z_t(G)$  is connected if and only if  $G$  is second-weakly elementary.*

**Theorem 4.6.** [72] *Let  $G$  be a 2-connected plane bipartite graph with perfect matchings. Then either  $Z_t(G)$  or each component of  $Z_t(G)$  is 2-connected.*

**Corollary 4.7.** *For plane elementary bipartite graph  $G$  with more than one cycle,  $Z_t(G)$  is 2-connected.*

Since every plane bipartite cubic graph is elementary, the corollary can be used to deduce 2-connection of matching transformed graphs due to Bau and Henning [1].

Let  $G$  be a plane bipartite graph with a perfect matching  $M$ . An  $M$ -alternating cycle  $C$  (resp. face  $f$ ) of  $G$  is called *proper* [67] if each edge of  $C$  (resp. of the boundary of  $f$ ) belonging to  $M$  goes from the white end-vertex to the black end-vertex along the clockwise orientation of  $C$  (resp.  $f$ ) to be suppressed, where the clockwise of face  $f$  means an orientation of its boundary such that the face  $f$  always lies on the right side when one goes along the direction; Otherwise  $C$  (resp.  $f$ ) is called *improper*. For example, see Fig. 8(a) and (b).

**Definition 4.2.** For  $F \subseteq F(G)$ , the Z-transformation digraph  $\bar{Z}_F(G)$  with respect to  $F$  is an orientation of  $Z_F(G)$ : an edge  $M_1M_2$  of  $Z_F(G)$  becomes an arc from  $M_1$  to  $M_2$  if and only if  $M_1 \oplus M_2$  forms a proper  $M_1$ - and improper  $M_2$ -alternating cycle.

**Theorem 4.8.** [72] *Let  $G$  be a plane bipartite graph with at least two perfect matchings. Then  $\bar{Z}_t(G)$  is strongly connected if and only if  $G$  is elementary.*

## 5 Lattice structure

The concepts for posets and lattices are referred to Birkhoff [2], Grätzer [14] or Stanley [48].

Let  $G$  be a plane bipartite graph with a perfect matching and  $\mathcal{M}(G)$  the set of all perfect matchings of  $G$ . For  $M \in \mathcal{M}(G)$ , an  $M$ -alternating cycle  $C$  of  $G$  is proper  $M$ -alternating if and only if it is improper  $M \oplus C$ -alternating.

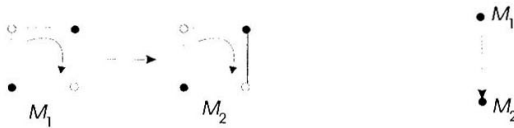


Fig. 9. Directed Z-transformation from  $M_1$  to  $M_2$ .

Recall directed Z-transformation graphs from Definition 4.2: An *orientation* of Z-transformation graph  $Z(G)$ , denoted by  $\bar{Z}(G)$ , is defined as follows: an edge  $M_1M_2$  is oriented from  $M_1$  to  $M_2$  if and only if  $M_1 \oplus M_2$  is proper  $M_1$ -alternating (and thus improper  $M_2$ -alternating). For example, see Figs. 6(c) and 9.

The Cartesian product of digraphs  $D_1$  and  $D_2$  is a digraph on  $V(D_1) \times V(D_2)$  such that there exists an arc from  $(u, v)$  to  $(u', v')$  if and only if either  $u = u'$  and  $(v, v')$  is an arc of  $D_2$  or  $(u, u')$  is an arc of  $D_1$  and  $v = v'$ .

**Lemma 5.1.** [63] *Let  $G_1, \dots, G_k$  denote the elementary components of  $G$ . Let  $F_i$  denote the set of inner faces of  $G_i$  belonging to  $F_0(G)$ . Then*

$$\bar{Z}(G) \cong \bar{Z}_{F_1}(G_1) \times \dots \times \bar{Z}_{F_k}(G_k).$$

**Lemma 5.2.** [68, 63]  *$\bar{Z}(G)$  has no directed cycles.*

**Definition 5.1.** A binary relation  $\preceq$  on  $\mathcal{M}(G)$  is defined as:  $M_1 \preceq M_2$ ,  $M_1, M_2 \in \mathcal{M}(G)$ , if and only if  $\bar{Z}(G)$  has a directed path from  $M_2$  to  $M_1$ .

**Lemma 5.3.** [37, 63]  *$(\mathcal{M}(G), \preceq)$  is a poset and its Hasse diagram corresponds the Z-transformation digraph.*



**Theorem 5.6.** [63] Let  $G$  be a plane elementary bipartite graph with  $n$  inner faces. Then

$$d(Z(G)) = h(\mathcal{M}(G)) \leq \lceil \frac{n(n+2)}{4} \rceil.$$

This upper bound enables one to design an efficient algorithm  $O(n^2)$  for generating the root perfect matching.

If some specific inner face  $f_0$ , in addition to the outer face, is *forbidden* in Z-transformation or twist, by Theorem 4.4 we can see that the restricted Z-transformation digraph or the corresponding poset is not connected. In fact, by Theorem 2.3, there exist 1-factors  $M$  and  $M_2$  such that  $M \oplus M_2$  is just the boundary of  $f_0$ . Then  $M$  and  $M_2$  belong to different components of the restricted Z-transformation graph. For example, see Fig. 12. For  $F \subseteq F_0(G)$ , let  $\mathcal{M}_F(G)$  be the poset implied by  $\tilde{Z}_F(G)$  as Definition 5.1

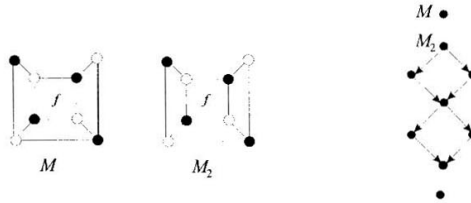


Fig. 12. The restricted Z-transformation digraph,  $f$  is forbidden.

**Theorem 5.7.** Let  $G$  be a plane elementary bipartite graph and  $F \subseteq F_0(G)$ . Then  $\mathcal{M}_F(G)$  is direct sum of distributive lattices.

It is well known that direct sum and product among posets obey distributive laws [48, page 102] and the Cartesian product of distributive lattices is also a distributive lattice [2, page 22]. Further, by Lemma 5.1 we have the following general result.

**Theorem 5.8.** [63] Let  $G$  be a plane bipartite graph with a perfect matching. Then  $\mathcal{M}(G)$  is direct sum of distributive lattices (see Fig. 4(c));  $\mathcal{M}(G)$  itself is distributive lattice if and only if  $G$  is weakly elementary.

It can be easily shown from the above method that the theorem still holds for a plane bipartite graph  $G$  that may have no perfect matchings, by extending naturally Z-transformation digraph on the set of maximum matchings of  $G$  [66].

A distributive lattice is called *irreducible* if it cannot be expressed as the Cartesian product of non-trivial distributive lattices.

**Theorem 5.9.** [64] Let  $G$  be a plane elementary bipartite graph. Then distributive lattice  $\mathcal{M}(G)$  is irreducible.

A distributive lattice on the set of orientations of a graph with a given flow difference was established by Propp [40] and Pretzel [39]. In particular, similar lattice structures on the  $f$ -factors of plane bipartite graphs and the flows, Eulerian orientations, spanning trees and Schnyder woods from planar graphs were found [40, 11, 28]. Rooted tree structures on the set of perfect matchings of plane bipartite graphs were given in [5, 67].

## 6 Distance formulae and Median graph

Given a connected graph  $H$  with vertices  $u$  and  $v$ , the *interval*  $I_H(u, v)$  (or simply  $I(u, v)$ ) between  $u$  and  $v$  consists of all vertices on shortest paths between  $u$  and  $v$ . A *median* of vertices  $u, v$  and  $w$  is a vertex that lies in  $I(u, v) \cap I(u, w) \cap I(v, w)$ . A graph is called a *median graph* if every triple of its vertices has a unique median (cf. [27]). Every median graph is a partial cube, i.e. it can be isometrically embedded in a hypercube. Various characterizations and recognitions for median graphs can be found in Imrich and Klavžar [27]. Accordingly, Klavžar, Žigert and Brinkmann [33] showed (2002) the following result.

**Theorem 6.1.** [33] *The Z-transformation graphs of catacondensed benzenoids are median graphs*

By the established distributive lattice on the set of perfect matchings and the developed techniques (cf. Theorem 5.4, or [37]), Lam, Shiu and Zhang showed that the above result holds generally for plane weakly-elementary bipartite graphs (i.e. we only require that the resonance graph is connected).

**Theorem 6.2.** [36] *The Z-transformation graph of a plane weakly-elementary bipartite graph  $G$  is a median graph.*

To prove the theorem three explicit formulae of distance  $d_{Z(G)}(M, M')$ , the length of a shortest path between a pair of vertices  $M$  and  $M'$  in Z-transformation graph  $Z(G)$ , were deduced.

**Theorem 6.3** (Distance Formula 1). [36]  $d_{Z(G)}(M, M') = \sum_{f \in \mathcal{F}} |\phi_M(f) - \phi_{M'}(f)|$ .

The above distance formula shows that the embedding  $\phi : \mathcal{M}(G) \rightarrow (\mathbb{Z}^+)^{\mathcal{F}}$  is also distance-preserving.

**Corollary 6.4** (Distance Formula 2). [36]  $d_{Z(G)}(M, M') = d_{Z(G)}(M \vee M', M \wedge M')$ .

**Corollary 6.5** (Distance Formula 3). [36]  $d_{Z(G)}(M, M') = \sum_{f \in \mathcal{F}} |\psi_{MM'}(f)|$ .

**Lemma 6.6.** [36] *For any  $M_1, M_2 \in \mathcal{M}(G)$ ,  $I_{Z(G)}(M_1, M_2) = I_{\mathcal{M}(G)}(M_1 \vee M_2, M_1 \wedge M_2)$ .*

The above distance formulas imply Lemma 6.6. This shows every triple  $M_1, M_2$  and  $M_3$  in  $\mathcal{M}(G)$  has a unique median:

$$(M_1 \wedge M_2) \vee (M_2 \wedge M_3) \vee (M_1 \wedge M_3) = (M_1 \vee M_2) \wedge (M_2 \vee M_3) \wedge (M_1 \vee M_3),$$



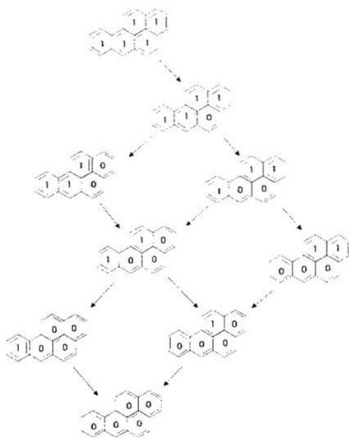


Fig. 13. Illustration for generation of  $\mathcal{M}$  and labelling of the perfect matchings.

which can imply Theorem 6.2.

Conversely, it is natural to ask what median graphs are Z-transformation graphs. Vesel [49] characterized Z-transformation graphs of catacondensed benzenoids and provided an recognition algorithm  $O(mn)$ , where  $m$  and  $n$  denote the numbers of edges and vertices of a given median graph respectively.

## 7 Labellings for perfect matchings

Based on Lemma 5.3 and Theorem 5.4, Ref. [36] gives a generation procedure of lattice  $\mathcal{M}(G)$ . The main principle is the well-known Jordan-Dedekind theorem in finite Distributive lattice: all maximal chains between a pair of elements have the same length. That is, all directed paths between any pair of vertices  $\vec{Z}(G)$  are of the same length whenever they exist. From Lemma 5.5, we immediately arrive in the following result.

**Lemma 7.1.** *For  $M, M' \in \mathcal{M}(G)$ ,  $M$  covers  $M'$  if and only if  $\phi_M(f) - \phi_{M'}(f) = 1$  for  $f = f_0$ , where  $f_0$  is an inner face bounded by the cycle  $M \oplus M'$ , and 0 for the other faces in  $\mathcal{F}$ .*

Recall that mapping  $\phi : M \mapsto \phi_M$  defines an embedding of the poset  $\mathcal{M}(G)$  into  $(\mathbb{Z}^+)^{\mathcal{F}}$  and  $\phi(\mathcal{M}(G))$  is a sublattice of  $(\mathbb{Z}^+)^{\mathcal{F}}$ . The vector or function  $\phi_M$  on  $\mathcal{F}$  can be regarded as a labelling of length  $|\mathcal{F}|$ , the number of inner faces of  $G$ , for a perfect matching  $M$ . Lemma 7.1 also enables one to give the embedding  $\phi$  of  $\mathcal{M}(G)$  into  $(\mathbb{Z}^+)^{\mathcal{F}}$ .

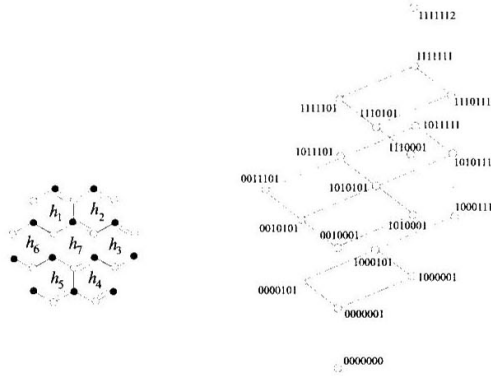


Fig. 14. The coronene and the distributive lattice on the 1-factors with labelling.

We now describe an outline. First construct the root 1-factor  $M_0$  and let  $\phi_{M_0} \equiv 0$ . The inductive procedure is as follows: suppose that a 1-factor  $M$  and its labelling  $\phi_M$  have been already given. Check each improper  $M$ -alternating face  $f_0$ :  $M \oplus f_0$  is another 1-factor covering  $M$ ; while  $\phi_{M \oplus f_0}(f_0) = \phi_M(f_0) + 1$  and the others remain unchanged. Note in the  $M \oplus f_0$  operation,  $f_0$  is always regarded as the set of edges bounding the face. For example, see Figs. 13 and 14.

The following result determines when  $\phi$  is a binary coding for perfect matchings of hexagonal systems.

**Theorem 7.2.** [36] *Let  $G$  be a hexagonal system. Then  $\phi$  is an embedding of  $\mathcal{M}(G)$  into  $\{0, 1\}^{\mathcal{F}}$  (i.e. Boolean algebra  $B_{1^{\mathcal{F}}}$ ) if and only if  $G$  has no coronene as its nice subgraph.*

For a catacondensed benzenoid  $G$  with  $d$  hexagons, there are  $2^d$  different ways by which the resonance graph can be isometrically embedded into a  $d$ -hypercube; for example, Refs. [29, 30] gave different binary codings. But  $\phi$  is both order-preserving and distance-preserving embedding. Ref. [36] designed a simple algorithm to generate such a binary coding by modifying Klavžar et al.'s method [30].

If  $d \geq 2$ ,  $G$  has a hexagon that share exactly one edge with the remainder of  $G$  when removing the hexagon. This hexagon corresponds to a mono-valency vertex of its inner dual graph (tree). Hence  $G$  has a sequence of hexagons  $h_1, h_2, \dots, h_d$ , so that each  $h_j$  shares one edge (say  $e_j$ ) with exactly one hexagon (say  $h_{a(j)}$ ) of  $h_1, \dots, h_{j-1}$ . We call it a *normal* sequence of hexagons of  $G$ .

For a given hexagon, the three thick edges in Fig. 15 are said to be in *proper positions*, the other thin edges in *improper positions*. So the common edge of two adjacent hexagons is in a proper position of one hexagon and in an improper position of the other one.

Based on this Hamiltonian path, Klavžar et al. [29] designed an algorithm for generating all perfect matchings. An extension to outerplane bipartite graphs was described as follows.

**Theorem 8.2.** [73] *The Z-transformation graph of an outerplane bipartite graph with a perfect matching has a Hamilton path.*

## 8.2 Fibonacci cubes

The Fibonacci cube,  $\Gamma_n$  introduced in [25, 26] as a model for interconnection networks, is a graph: the vertices are the binary strings  $b_1b_2 \cdots b_n$  containing no two consecutive ones, and two vertices are adjacent if they differ in precisely one bit. So it is an induced subgraph of  $n$ -hypercube. Klavžar and Žigert [31] showed that Fibonacci cubes are the Z-transformation graphs of zigzag hexagonal chains, called *Fibonaccenes*.

A non-branched catacondensed hexagonal system is called a *Fibonaccene* (or zigzag chain) if two vertices of degree 2 lying in each non-terminal hexagon are adjacent. Chemical graph theory of Fibonaccenes was surveyed by Gutman and Klavzar [19].

**Theorem 8.3.** [31] *Let  $G$  be a Fibonaccene with  $n$  hexagons. Then  $Z(G)$  is isomorphic to the Fibonacci cube  $\Gamma_n$ .*

Vesel further characterized Fibonacci cubes by applying  $\Theta$ -class and obtained the following result.

**Theorem 8.4.** [49] *Fibonacci cubes can be recognized in  $O(mn)$  times.*

## 8.3 Clar number

A set  $S$  of disjoint inner faces of  $G$  is called a *resonant pattern* if  $G$  has a perfect matching  $M$  such that the boundaries of all faces in  $S$  are  $M$ -alternating cycles. The maximum number of faces in resonant patterns of  $G$  is called the *resonant number* of  $G$ , denoted by  $res(G)$ . The resonant number of a hexagonal system is the so-called *Clar number* [21, 22].

**Theorem 8.5.** [34, 65] *Let  $G$  be a plane elementary bipartite graph. Then the dimension of a largest hypercube of  $Z(G)$  equals the resonant number of  $G$ .*

For a catacondensed benzenoid  $G$ , Klavžar and Žigert [32] found a min-max result: the smallest number of elementary cuts that cover  $G$  equals the dimension of a largest induced hypercube of the resonance graph of  $G$ . According to this method, Klavžar et al. [34] gave a simple computation to the Clar number of a catacondensed benzenoid. Zhang et al. [65] extended their results to 2-connected outerplane bipartite graph by applying Dilworth's min-max theorem on *poset* and by generalizing "elementary cut". Salem et al. [45] established a relation between the hypercubes in Z-transformation graph  $Z(G)$  and the resonant patterns of  $G$ .

**Theorem 8.6.** [45] *Let  $H$  be a hexagonal system with perfect matchings. Then there exists a surjective map  $f$  from the set of hypercubes of  $Z(H)$  to the set of all resonant patterns of  $H$  such that for each  $k$ -hypercube  $Q$ ,  $f(Q)$  is a resonant pattern of  $k$  hexagons.*

## 8.4 Open problems

- (1) Characterize Z-transformation graphs of plane bipartite graphs?
- (2) For a given elementary bipartite graph  $G$  that is planar, what relations have the total Z-transformation graphs of different planar embeddings of  $G$ ?
- (3) For a plane elementary bipartite graph  $G$ , determine the connectivity of Z-transformation graph  $Z(G)$ .
- (4) For a plane elementary bipartite graph  $G$ , the length of each directed cycle of the total Z-transformation digraph  $\tilde{Z}_t(G)$  is divisible by the number  $f$  of faces of  $G$ . Can the lengths of all directed cycles of  $\tilde{Z}_t(G)$  compose of consecutive times of  $f$  (for example,  $f, 2f, 3f, \dots$ )?
- (5) For a plane elementary bipartite graph  $G$ , determine the smallest integer  $m$  such that  $\mathcal{M}(G)$  can be embedded into  $(\mathbb{Z}^+)^m$ , the Cartesian product of  $m$  copies of  $\mathbb{Z}^+ = \{0, 1, 2, \dots\}$  with the usual order. We may conjecture that the such smallest integer  $m$  is equal to the resonant number of  $G$ . For coronene, Fig. 14 shows that the conjecture holds since its resonant number equals 3.
- (6) For a general hexagonal system  $G$ , how to design an algorithm as Algorithm 7.3 to generate  $\phi_M$ , labelling of length  $|\mathcal{F}|$  for all 1-factors  $M$ , avoiding the generation of lattice  $\mathcal{M}(G)$ ?

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