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Forcing on Perfect Matchings – A Survey

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Abstract

The notions of a forcing edge and the forcing number of a perfect matching first appeared in a 1991 paper [15] by Harary, Klein and Živković. The root of these concepts can be traced to the works ([24] and [36]) by Randić and Klein in 1985-1987, where the forcing number was introduced under the name of "innate degree of freedom" of a Kekulé structure, which plays an important role in the resonance theory in chemistry. Over the past two decades, more and more mathematicians were attracted to the study on forcing sets (including forcing edges and forcing faces, etc.) and the forcing numbers of perfect matchings of a graph. The scope of graphs in consideration has been extended from polyhexes to various bipartite graphs and non-bipartite graphs. Some varied topics such as global forcing matchings and anti-forcing matchings also emerged recently. Here we will present a brief survey on the known results, as well as some open problems and conjectures in this growing field.

1 Introduction

1.1 Origin and Importance

The idea of "forcing" has long been used in many research fields, such as colorings, orientations, geodetics and dominating sets in graph theory, as well as Latin squares, block designs and Steiner systems in combinatorics (see [14] and the references therein). Recently, the "forcing" on perfect matchings has been attracting more researchers' attention. In this survey we focus on the study of forcing sets (including forcing edges and forcing faces) and forcing numbers of perfect matchings of a graph.

The notions of a forcing edge and the forcing number of a perfect matching first appeared in a 1991 paper [15] by Harary, Klein and Živković. The root of these concepts can be traced to the works ([24] and [36]) by Klein and Randić in 1985–1987, where they introduced the innate degree of freedom (the forcing number) of a Kekulé structure (perfect matching) which plays an important role in the resonance theory in chemistry. For a Kekulé structure M of a benzenoid hydrocarbon, the edges in M are called *double bonds*; *single bonds* otherwise. An edge is called a *forcing bond* (or, *forcing edge*) if it is contained in exactly one Kekulé structure. A forcing bond between two carbon atoms r and s in a given benzenoid hydrocarbon has the smallest positive *Pauling bond order* $P_{rs} = \frac{K_{rs}}{K}$, where K_{rs} is the number of Kekulé structures such that there is a double bond between r and s, and K is the total number of Kekulé structures of the benzenoid hydrocarbon. The Pauling bond order was successfully correlated with experimentally determined bond lengths of various benzenoid hydrocarbons. Kekulé structures with a larger innate degree of freedom play more important role in resonance theory. For details of the related study in chemistry, the reader is referred to the recent paper [34] by Randić (2003). For various mathematical concepts in chemistry we refer to the book [19] by Gutman and Polansky (1986).

Over the past two decades, more and more mathematicians were attracted to the study on forcing sets (including forcing edges and forcing faces, etc.) and forcing numbers of perfect matchings of a graph. The scope of graphs in consideration has been extended from hexagonal systems (also called polyhexes, or benzenoid systems) to plane bipartite graphs, bipartite graphs, as well as non-bipartite graphs. Some varied topics such as global forcing matchings and anti-forcing matchings also emerged in the past few years. Here we will present a brief survey on the known results, as well as some open problems and conjectures in this growing field.

1.2 Preliminaries

All graphs considered in this survey are connected simple graphs with at least one perfect matching.

Definition 1.1 A *perfect matching* (or 1-*factor*) M of a graph G is a set of disjoint edges that covers all vertices of G.

Perfect matchings of a molecule graph G are also called *Kekulé structures* of G in chemistry, which play a key role in the molecule resonance energy and aromaticity of organic molecules.

Definition 1.2 A *forcing set* S of a perfect matching M of a graph G is a subset of M contained in no other perfect matchings of G.

Note that the empty set is a forcing set of a perfect matching M of G if and only if M is the unique perfect matching of G.

A set S of independent edges of a graph G is a forcing set if and only if $G - V(S)$ has a unique perfect matching or is empty, where $V(S)$ denotes the set of end vertices of edges in S.

Definition 1.3 The *forcing number* (or, *innate degree of freedom*) of a perfect matching M of a graph G is defined as

$$f(G, M) = \min \{|S|\colon S \text{ is a forcing set of } M\}.$$

Definition 1.4 The *forcing number* (or, minimum forcing number) of a graph G is defined as

$$f(G) = \min\{f(G, M)\colon M \text{ is a perfect matching of } G\}.$$

Definition 1.5 The *maximum forcing number* of a graph G is defined as

$$F(G) = \max\{f(G, M)\colon M \text{ is a perfect matching of } G\}.$$

Note that $f(G)$ and $F(G)$ are defined only for graphs with at least one perfect matching. Clearly, $0 \leq f(G) \leq F(G) \leq \frac{|V(G)|}{2} - 1$, $f(G) = 0$ if and only if $F(G) = 0$ if and only if G has a unique perfect matching.

Definition 1.6 The *spectrum of forcing numbers* of a graph G is defined as

$$Spec(G) = \{f(G, M) : M \text{ is a perfect matching of } G\}$$

Afshani et al (2004) [1] showed that any finite set of positive integers can be realized by the spectrum of a plane bipartite graph.

Theorem 1.7 [1] For any finite set A of positive integers, there is a plane bipartite graph G such that $Spec(G) = A$.

Definition 1.8 A *forcing edge* of a graph G is an edge contained in exactly one perfect matching of G. (It constitutes a forcing set with cardinality 1.)

Note that a graph G has a forcing edge if and only if $f(G) = 0$ or 1. If G has at least two perfect matchings, then G has a forcing edge if and only if $f(G) = 1$.

By definitions, we immediately have the following proposition.

Proposition 1.9 Let G be a graph with a perfect matching. Then

(i) $Spec(G) = \{0\}$ if and only if G has a unique perfect matching if and only if $0 \in Spec(G)$ if and only if $f(G) = 0$.

(ii) $Spec(G) = \{1\}$ if and only if G has more than one perfect matching and every perfect matching M contains a forcing edge of G.

Proposition 1.10 Let G be a graph with a perfect matching. Then $Spec(G) = \{0\}$ or $\{1\}$ if and only if after deleting all forcing edges of G the resultant graph has no perfect matchings.

Proof. The necessity can be proved by contradiction. Assume that the resultant graph after the deletion of forcing edges has a perfect matching M. It is clear that M is also a perfect matching of G which contains no forcing edges. So $f(G, M) > 1$. This contradicts the condition that $Spec(G) = \{0\}$ or $\{1\}$.

The sufficiency can also be shown by contradiction. Assume that $Spec(G) \neq \{0\}$ or $\{1\}$. Then G must have a perfect matching M such that $f(G, M) > 1$, that is, M does not contain any forcing edge of G, and so M is a perfect matching of the resultant graph after the deletion of forcing edges of G. This contradicts the assumption that the resultant graph has no perfect matchings. So the sufficiency is proved. This completes the proof. □

The largest possible forcing number $f(G)$ for a graph G is $f(G) = \frac{1}{2}|V(G)| - 1$. Assume that $|V(G)| = 2n$. It is clear that $f(G) = n-1$ if and only if $Spec(G) = \{n-1\}$. For example, $f(K_{2n}) = f(K_{n,n}) = n - 1$.

Proposition 1.11 For any integer $n > 1$,

(i) there exists a (bipartite) graph G that has n perfect matchings and $f(G) = 1$.

(ii) there exists a (bipartite) graph G with $f(G) = 1$ such that $f(G, M) = n$ for some perfect matching M of G.

Proof. (i) A linear hexagonal chain H with $n-1$ hexagons has n perfect matchings and forcing number $f(H) = 1$. See the graph at the top of Fig. 1 (i) for an example with $n = 6$.

(ii) An example for $n = 4$ is depicted in Fig. 1 (ii). The desired graph is the G_n constructed in [1] by replacing alternate edges in C_{2n} by a cycle of size 4 whose one edge is identical to the replaced edge in C_{2n}. □

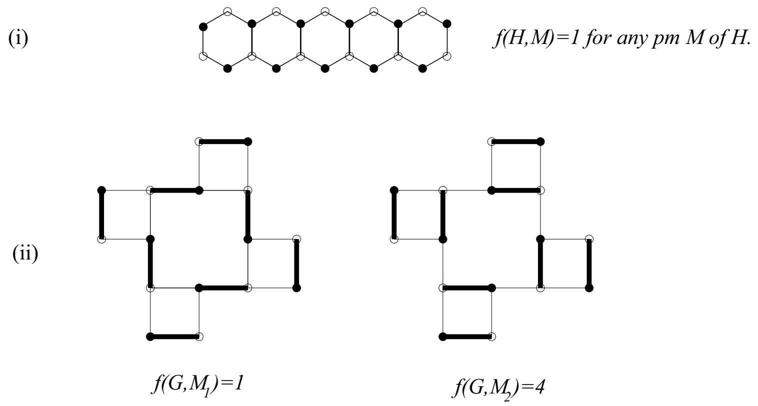

Figure 1. Examples of forcing numbers of graphs.

The problems of finding the smallest forcing number and finding a smallest forcing set of graphs are both NP-complete by the following two theorems by Afshani et al (2004) [1] and Adams et al (2004) [2].

Theorem 1.12 [1] Finding the smallest forcing number is NP-complete for bipartite graphs with maximum degree 4.

Theorem 1.13 [2] Finding the smallest forcing set of a perfect matching is NP-complete for bipartite graphs with maximum degree 3.

Remark. For plane bipartite graphs G, however, Pachter and Kim (1998) [29] made the remark that forcing sets of perfect matchings of G can be found in polynomial time using the $O(n^3)$ algorithm by Gabow [16] for finding feedback sets of a plane digraph.

2 Important Tools and General Results

2.1 Three Classical Results

In this section, we state three classical results which are fundamental in the study of forcing on perfect matchings of a graph: Kotzig's theorem (1959) on the unique perfect matching of a general graph, Lovász and Plummer's theorem (1986) on the unique perfect matching of a bipartite graph, and the minimax theorem on the disjoint directed cycles in a planar directed graph by Lucchesi and Younger (1978), an extended version of which was given by Barahona et al. in 1994.

Theorem 2.1 [23] (Kotzig) If a connected graph G has a unique perfect matching M, then G has a bridge in M.

Kotzig's theorem immediately implies that any 2-connected graph G with a perfect matching has at least two perfect matchings. If G is a connected graph with a perfect matching M and $S \subset M$ ($S \neq M$) is a forcing set of M, then $G - V(S)$ must have a bridge which belongs to M. Hence, any k-connected graph G with a perfect matching has the forcing number $f(G) \geq \lfloor \frac{k}{2} \rfloor$.

Let $G = (B, W)$ be a bipartite graph with two partite sets B and W. If G has a unique perfect matching, then vertices of G can be labeled $B = \{b_1, b_2, \cdots, b_m\}$ and $W = \{w_1, w_2, \cdots, w_m\}$ such that for every edge $b_i w_j$, $i \geq j$ (see page 139 in [26] by Lovász and Plummer). It follows immediately that b_1 and w_m must be degree-1 vertices (or, pendent vertices) in G. Therefore, the following theorem comes immediately.

Theorem 2.2 [26] (Lovász and Plummer) A bipartite graph with a unique perfect matching must contain at least one pendent vertex in each partite set.

By Theorem 2.2, for any bipartite graph G with a perfect matching, if G does not have a pendent vertex in each partite set, then G has at least two perfect matchings. It is well known that any regular bipartite graph has a perfect matching. So any connected regular bipartite graph with more than two vertices has at least two perfect matchings. If a bipartite graph G is k-extendable (i.e., any k-matching is contained in a perfect matching of G) and for any k-matching S, $G - V(S)$ does not have a pendent vertex in each partite set, then $f(G) > k$.

Finally, we introduce Lucchesi and Younger's minimax theorem (1978) on the disjoint directed cycles in a planar directed graph. A *feedback arc set* (or briefly, *feedback set*) in a directed graph D is a set of arcs of D that contains at least one arc of each directed cycle in D.

Theorem 2.3 [28] (Lucchesi and Younger) For a finite planar directed graph, a minimum feedback set has the cardinality equal to that of a maximum disjoint collection of directed cycles.

An extension of this theorem was given by Barahona et al. in 1994.

Theorem 2.4 [3] (Barahona et al.) For any directed graph without $K_{3,3}$ minor, the cardinality of a minimum feedback set is equal to the maximum number of arc disjoint cycles.

A directed graph is said to have the *cycle-packing property* if the minimum cardinality of a feedback set equals the maximum number of arc disjoint directed cycles. A graph G is said to have the *cycle-packing property* if every orientation of G results in a directed graph that has the cycle-packing property. So Theorems 2.3 and 2.4 can be restated as the following.

Theorem* Any graph without $K_{3,3}$ minor (for example, any planar graph) has the cycle-packing property.

2.2 Three Key Concepts

In this section, we will introduce three key concepts which are useful in the study on forcing perfect matchings of a graph: alternating cycles (or, conjugated circuits in chemistry), trailing vertices, and Z-transformation graphs (or, resonance graphs in chemistry). We will also state main results on forcing perfect matchings related to these three concepts.

Definition 2.5 [26] Let M be a perfect matching of a graph G. An M*-alternating cycle* of G is a cycle of G whose edges are alternately in M and $E(G) \setminus M$.

An M-alternating cycle is simply called an *alternating cycle* if there is no need to specify the perfect matching M.

Close relationship between a forcing set and alternating cycles of a perfect matching in a graph has been realized and studied by many researchers. By definition, we can see that M is the unique perfect matching of G if and only if G has no M-alternating cycles. Patcher and Kim (1998) presented the following equivalent form employing the forcing number.

Lemma 2.6 [29] Let G be a graph with a perfect matching M. Then $f(G, M) > 0$ if and only if G has an M-alternating cycle.

A necessary and sufficient condition for a forcing set S of a perfect matching M comes immediately.

Proposition 2.7 Let G be a graph with a perfect matching M. Then a subset $S \subset M$ is a forcing set of M if and only if $G - V(S)$ contains no M-alternating cycles.

The special case of this result for hexagonal systems was given by F. Zhang and H. Zhang [52] in 1995. Necessity of Proposition 2.7 was observed by Riddle [32] in 2002, and a special case of Proposition 2.7 on bipartite graphs was given by Kleinerman [22] in 2006.

For any graph G with a perfect matching M, it is easy to see that the forcing number $f(G, M)$ is bounded below by the maximum number of disjoint M-alternating cycles. The minimax theorem of Lucchesi and Younger (1978) motivated Pachter and Kim (1998) to consider a class of bipartite graphs G with the *cycle-packing property*. They showed that for any perfect matching in such a graph G, the forcing number $f(G, M)$ can be obtained by counting the maximum number of disjoint M-alternating cycles in G.

Theorem 2.8 [29] Let G be a bipartite graph with the cycle-packing property. Then for any perfect matching M of G,

(i) $f(G, M) = C(G, M)$, the maximum number of disjoint M-alternating cycles in G.
(ii) $f(G, M) \leq \left\lfloor \frac{p}{q} \right\rfloor$, where $p = |V(G)|$ and $q =$ the girth of G.

Due to the minimax Theorem 2.3 by Lucchesi and Younger (1978) and its extended version Theorem 2.4 by Barahona et al. (1994), Theorem 2.8 can be applied to all bipartite graphs without $K_{3,3}$ minor (for example, all plane bipartite graphs).

Theorem 2.9 [29] [32] Let G be a bipartite graph without $K_{3,3}$ minor. Then for any perfect matching M of G,

(i) $f(G, M) = C(G, M)$, the maximum number of disjoint M-alternating cycles in G,

(ii) $f(G, M) \leq \left\lfloor \frac{p}{q} \right\rfloor$, where $p = |V(G)|$ and $q =$ the girth of G.

Remark 2.10 (i) Riddle (2002) stated Theorem 2.9 in [32]; but it was not explicitly stated by Pachter and Kim (1998) in [29]. That may be the main reason why this important result has not been widely known. (For example, on page 510 in [33] byRandić (2002) or on page 3472 in [34] byRandić (2003), where the special case of this result for G being a hexagonal system was listed as a conjecture.)

(ii) Theorem 2.9 (i) generalizes a result by Hansen and Zheng (1994) that the innate degree of freedom of a Kekulé structure in a cata-condensed benzenoid hydrocarbon is equal to the maximum number of disjoint hexagons containing three double bonds [21].

Theorem 2.8 shows that the forcing number of a bipartite graph with cycle-packing property (for example, a plane bipartite graph) can be obtained by counting the maximum number of disjoint alternating cycles. But it does not hold for many nonplanar bipartite graphs. To find a lower bound for the forcing numbers of bipartite graphs without cycle-packing property such as torus and hypercubes, Riddle (2002) introduced the trailing vertex method for a bipartite graph $G = (B, W)$ in [32], which gives a lower bound on the forcing number of a bipartite graph by the minimum number of trailing vertices in one partite set B over all possible ordering of B. It reduces a problem on all perfect matchings of a bipartite graph G to a single problem on the vertices in one partite set of G.

Definition 2.11 [32] Let $G = (B, W)$ be a bipartite graph with a perfect matching. Assign an ordering to all vertices in B. A vertex $b \in B$ is called a *trailing vertex* if it is not the largest one in the neighborhood $N(w)$ for any vertex $w \in W$; a *leading vertex* otherwise.

Theorem 2.12 [32] The forcing number of a bipartite graph $G = (B, W)$ is bounded below by the minimum number of trailing vertices in B over all possible orderings of B.

Riddle (2002) also gave a weaker lower bound on the forcing number of a bipartite graph $G = (B, W)$ using the smallest possible *maximum excess* over all orderings of

B, which is easier to compute in some cases such as when G is a torus. Assign an ordering $b_1 < b_2 < \cdots < b_n$ on all vertices of B and denote $\overline{B}_k = \{b_{k+1}, b_{k+2}, \cdots, b_n\}$ for $0 \leq k \leq n-1$. The *excess* of $\overline{B}_k$ is defined as $\epsilon(\overline{B}_k) = |N(\overline{B}_k)| - |\overline{B}_k|$. The *maximum excess* for an ordering of B is defined as

$$\max_{0\leq k\leq n-1} \epsilon(\overline{B}_k) = \max_{0\leq k\leq n-1} \{|N(\overline{B}_k)| - |\overline{B}_k|\}.$$

By the definition, it is easily to see that for an ordering $b_1 < b_2 < \cdots < b_n$ on B, a vertex b_i is a leading vertex if and only if $\epsilon(\overline{B}_{i-1}) \geq \epsilon(\overline{B}_i)$, and b_i is a trailing vertex if and only if $\epsilon(\overline{B}_{i-1}) = \epsilon(\overline{B}_i) - 1$.

Theorem 2.13 [32] The forcing number of a bipartite graph $G = (B, W)$ is bounded below by the smallest possible maximum excess for all orderings of B.

Kleinerman (2006) [22] determined the conditions under which the lower bound given in Theorem 2.12 by Riddle is sharp in terms of edge-packing; he also provided an infinite family of graphs for which the lower bound is arbitrarily weak. An *edge-packing* of a bipartite graph $G = (B, W)$ is a disconnected collection E of edges in G along with an injective weight function $w : E \to \{1, 2, ..., |E|\}$ on these edges extended to a weight function on their endpoints as well, by inheriting the edge-weight, and in which no vertices in W are adjacent to vertices in B of greater weight. The set of edges constituting an edge-packing P will be denoted $E(P)$. A *maximal edge-packing* P_{max} of a graph G is an edge-packing of G such that $|E(P_{max})| \geq |E(P)|$ for all edge-packings P of G. Kleinerman (2006) [22] showed that for a bipartite graph $G = (B, W)$, given an ordering on the vertices of B, there is an edge-packing P for which $|E(P)|$ is equal to the number of leading vertices in that ordering. Conversely, given an edge-packing P, there is an ordering on the vertices of B for which the number of leading vertices in that ordering equals $|E(P)|$.

Theorem 2.14 [22] The lower bound on the forcing number given in Theorem 2.12 is sharp exactly when some maximal edge-packing P_{max} of the graph G in question has $E(P_{max})$ extendable to a perfect matching M of G.

Kleinerman (2006) [22] also provided a family of graphs for which the minimum number of trailing vertices in a partite set B is 1 over all possible orderings of B, but the

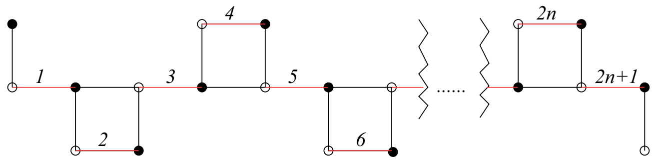

Figure 2. An example of a bipartite graph with forcing number n, where the numbered red edges represent an edge-packing.

forcing number diverges, see Fig. 2 provided in [22]. This shows that the lower bound given in Theorem 2.12 can be arbitrarily weak.

Wang, Ye and Zhang (2008) [47] improved the lower bound given in Theorem 2.12 by using the minimum number of trailing vertices in B over all *canonical orderings* of B for a bipartite graph $G = (B, W)$. An ordering $b_1 < b_2 < \cdots < b_n$ on all vertices of B is said to be *canonical* (or, *standard*) if its smallest leading vertex is larger than the largest trailing vertex; *non-canonical* (or, *non-standard*) otherwise. Wang et al [47] showed that for a canonical ordering of B, the maximum excess is equal to the number of trailing vertices. If S is a minimum forcing set of a perfect matching of $G = (B, W)$, then there exists a canonical ordering of B such that $V(S) \cap B$ is the set of trailing vertices and $B \setminus V(S)$ is the set of leading vertices.

Theorem 2.15 [47] The forcing number of a bipartite graph $G = (B, W)$ is bounded below by the minimum number of trailing vertices in B over all canonical orderings of B.

Wang (2009) [46] improved the trailing vertex method by Riddle, and gave a necessary condition for a given natural number k being in the spectrum of forcing numbers of a bipartite graph. He also provided a necessary and sufficient condition for the minimum forcing number of a bipartite graph being equal to the minimum number of trailing vertices of all standard orderings of a color set.

Let $G = (B, W)$ be a bipartite graph. For an ordering $b_1 < b_2 < \cdots < b_n$ on all vertices of B, the excess of $\overline{B}_i = \{b_{i+1}, b_{i+2}, \cdots, b_n\}$ is defined as $\epsilon(\overline{B}_i) = |N(\overline{B}_i)| - |\overline{B}_i|$. The excess of b_i is defined to be $\epsilon(b_i) = \epsilon(\bar{B}_{i-1}) - \epsilon(\bar{B}_i)$. The vertex b_i is called an m-excess vertex if $\epsilon(b_i) = m$. For an ordering of B, a vertex $b_i \in B$ is a trailing vertex if and only if b_i is a (-1)-excess vertex, and $b_i \in B$ is a leading vertex if and only if b_i is a nonnegative excess vertex. Wang showed that in a bipartite graph $G = (B, W)$ with a perfect matching, for any given non-standard ordering of B, there exists a standard ordering such that the two orderings have the same number of trailing vertices.

For a standard ordering of B with k trailing vertices, denote the set of all positive-excess vertices by B_+, the set of 0-excess vertices by B_0, and the set of trailing vertices by B_-. Then $B = B_+ \cup B_0 \cup B_-$. Define

$$N^*(b_i) \equiv N(b_i) \setminus N(\bar{B}_i) = N(\bar{B}_{i-1}) \setminus N(\bar{B}_i),$$

Theorem 2.16 [46] Let $G = (B, W)$ be a bipartite graph with a perfect matching. If $k \in Spec(G)$, then there exists a standard ordering with k trailing vertices such that the induced subgraph $G[(B_+ \cup B_- \cup (\cup_{b_i \in B_+} N^*(b_i))]$ has a perfect matching.

Theorem 2.17 [46] Let $G = (B, W)$ be a bipartite graph with a perfect matching and δ_G be the smallest number of tailing vertices among all standard orderings of B. Then $f(G) = \delta_G$ if and only if there exists a standard ordering with the number of trailing vertices δ_G such that the induced subgraph $G[(B_+ \cup B_- \cup (\cup_{b_i \in B_+} N^*(b_i))]$ has a perfect matching.

The concept of Z-transformation graph of a hexagonal system was introduced by mathematicians Zhang, Guo and Chen [49] in 1988. The same concept was also introduced and studied independently by the chemist Gründler [17, 18] in (1982, 1983) under the name *resonance graph*. The concept Z-transformation graphs was further extended to plane bipartite graphs by F. Zhang and H. Zhang [54] in 2000. It plays an important role on the study of forcing edges and forcing faces in plane bipartite graphs including hexagonal systems, see [8], [9], [50], [54].

Definition 2.18 [54] Let G be a plane bipartite graph with a perfect matching. The *Z-transformation graph* of G, denoted by $Z(G)$, is the graph whose vertices are the perfect matchings of G where two vertices M_1 and M_2 are adjacent if and only if their symmetric difference $M_1 \oplus M_2$ is the periphery of some finite face of G.

Zhang, Guo and Chen (1988) proved that if a hexagonal system H has at least one perfect matching, then $Z(H)$ is a connected bipartite graph. Furthermore, $Z(H)$ is either a path or a graph with girth 4; and $Z(H) - V_m$ is 2-connected, where V_m is the set of pendent vertices in $Z(H)$, see Fig. 3. They also gave structural characterizations for those hexagonal systems whose Z-transformation graphs have a pendent vertex.

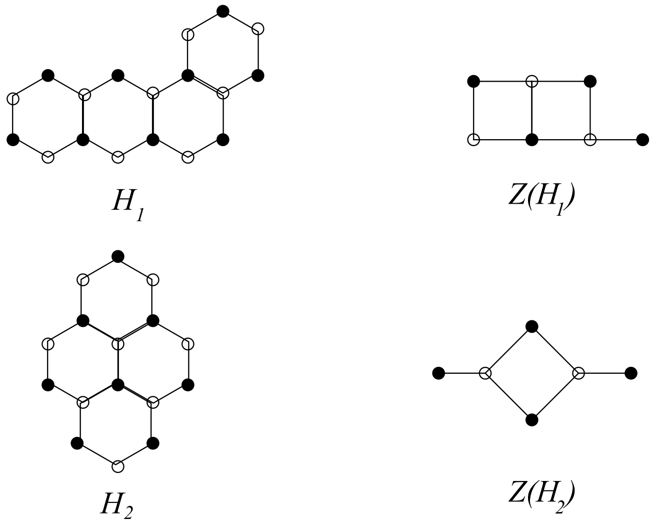

Figure 3. Examples of Z-transformation graphs.

Theorem 2.19 [49] Let H be a hexagonal system. Then $Z(H)$ has a pendent vertex M if and only if one of the following is true:

(i) H has a perfect matching M which is 3-dividable w.r.t. an $O - ABC$ coordinate system;

(ii) The periphery of the inner dual of H is monotone w.r.t. an $O - ABC$ coordinate system.

Zhang and Li (1995) showed that $Z(H)$ has at most 2 pendent vertices and gave structural characterizations for those hexagonal systems H whose $Z(H)$ has exactly two pendent vertices. They also provided a generating function for enumerating hexagonal systems with forcing edges. H. Zhang and F. Zhang (2000) showed that $Z(H)$ is a path if and only if H is a linear hexagonal chain, which was proved by Che and Chen (2006) in a different way. To study various molecule structures, H. Zhang and F. Zhang (2000) extended the concept of Z-transformation graph for a hexagonal system to that for a plane bipartite graph in [54]. The following lemma in [54] presents some properties of the Z-transformation graph of a plane bipartite graph, which are especially useful in the study of forcing edges and forcing faces (including forcing hexagons) in plane bipartite graphs.

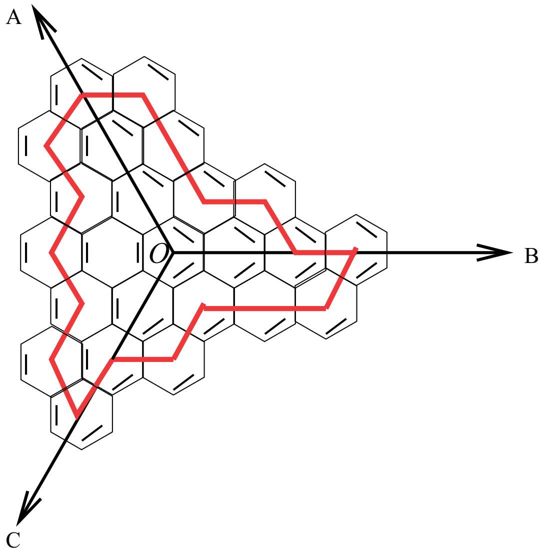

Figure 4. A perfect matching M of H is 3-dividable w.r.t. $O - ABC$; periphery of the inner dual of H is monotone w.r.t. $O - ABC$.

Lemma 2.20 [54] Let G be a plane elementary bipartite graph. Then

(i) $Z(G)$ is a connected bipartite graph,

(ii) $Z(G)$ has at most two vertices of degree one, and

(iii) if $Z(G)$ has a vertex of degree ≥ 3, then the girth of $Z(G)$ is 4; otherwise, $Z(G)$ is a path.

For more results on Z-transformation graphs, the reader is referred to the recent survey [48] by H. Zhang (2006). In the rest of the paper, we will organize the known results on perfect matching forcing in two categories: bipartite graphs (including plane bipartite graphs and nonplanar bipartite graphs) and non-bipartite graphs. We also will give a brief survey on some emerging varied topics such as global forcing matchings and anti-forcing matchings. We conclude the paper with open questions and conjectures.

3 Bipartite graphs

3.1 Hexagonal Systems

Forcing edges and forcing numbers of a hexagonal system have been investigated intensively because they are closely related to the study of molecule resonance structure in chemistry. The forcing number of a perfect matching M was also called the innate degree of freedom of the Kekulé structure M byRandić and Klein (1985) in [36].

A *hexagonal system* (also called *polyhex*, or *benzenoid system*) is a 2-connected plane bipartite graph such that each interior face is a unit hexagon. We only consider those *simple hexagonal systems* which are 2-connected subgraphs of a regular hexagonal lattice. A vertex of a hexagonal system belongs to at most three hexagons. A vertex is called an *interior vertex* if it is shared by three hexagons. A hexagonal system is called *cata-condensed* if it has no interior vertices; *peri-condensed* if it has at least one interior vertex. The inner dual H^* of a hexagonal system H is the graph each vertex of which corresponds to the center of a hexagon of H and two vertices are adjacent in H^* if the two corresponding hexagons have a common edge in H. A cata-condensed hexagonal system is called a *hexagonal chain* if its inner dual is a path, and *linear hexagonal chain* if its inner dual is a straight path.

Harary, Klein and Živković (1991) [15] characterized when each edge of a hexagonal system is a forcing edge. Characterizations for a hexagonal system with forcing edges were given by Zhang and Li (1995) [50] using the concept of Z-transformation of hexagonal systems. They completely determined the existence and location of the forcing edges of a cata-condensed benzenoid system. Zhang and Li (1996) [51] gave a linear algorithm to determine if an indicted edge of a benzenoid system is a forcing edge. Furthermore, by Polya's theorem, they enumerated all cata-condensed benzenoid systems with forcing edges: the number of non-isomorphic cata-condensed benzenoid system with forcing bonds and with h hexagons is the nearest integer to $\frac{1}{12}(h+2)^2$, which is asymptotically equivalent to $\frac{h^2}{12}$. A new method on enumeration of Kekulé structures of hexagonal systems with forcing edges was obtained elegantly by F. Zhang and H. Zhang (1995) [52]. In 1997, Li [25] introduced the concept of a *forcing single edge* of a hexagonal system H, which is an edge of H belonging to all but one perfect matching of H. He determined all the hexagonal systems with a forcing single edge, and gave a generating function for the number of such systems. Pachter and Kim [29](1998) gave an upper bound for the forcing numbers of a hexagonal system as a corollary of Theorem 2.9. Kleinerman [22] (2006) used a constructive method to obtain the same upper bound for the forcing numbers of a hexagonal system (as well as an upper bound for the forcing numbers of subgraphs of a square grid).

Theorem 3.1 [15] The single-hexagon is the only polyhex in which every edge is a forcing edge.

Theorem 3.2 [50] A hexagonal system H has a forcing edge if and only if $Z(H)$ has a pendent vertex M and the unique M-alternating hexagon contains at least one edge on the periphery of H.

Theorem 3.3 [50] Let H be a hexagonal system whose $Z(H)$ has exactly one pendent vertex. Then H has at most 3 forcing edges. The three possible forcing edges are the three disjoint edges of a hexagon h if they lie on the periphery of H, where h is a periphery hexagon such that there exists a coordinate system $O-ABC$ w.r.t. h and H is monotone w.r.t. $O-ABC$.

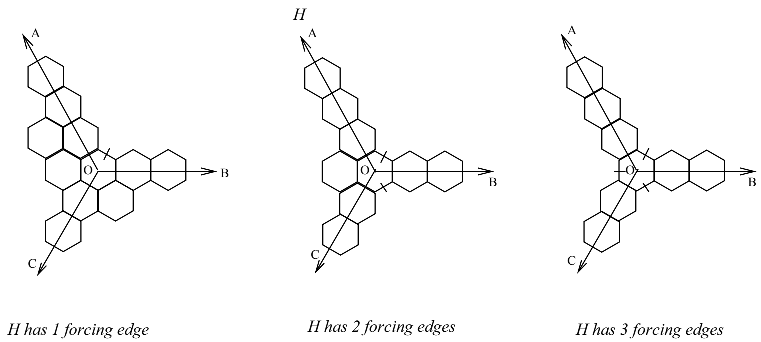

Figure 5. Forcing edges in H (marked by short bars) when $Z(H)$ has exactly one pendent vertex.

Theorem 3.4 [50] Let H be a hexagonal system whose $Z(H)$ has exactly two pendent vertices. Let H^* be the inner dual of H. Then one of the following three cases must occur:

(i) The perimeter of H^* is a big hexagon and H has no forcing edges.

(ii) The perimeter of H^* is a parallelogram with an angle equal to 120° and H has exactly 4 forcing edges, which belong to two hexagons centered at the corners of 120° angles of H^*.

(iii) H^* is a straight path with $n(\geq 1)$ vertices and H has $n + 5$ forcing edges.

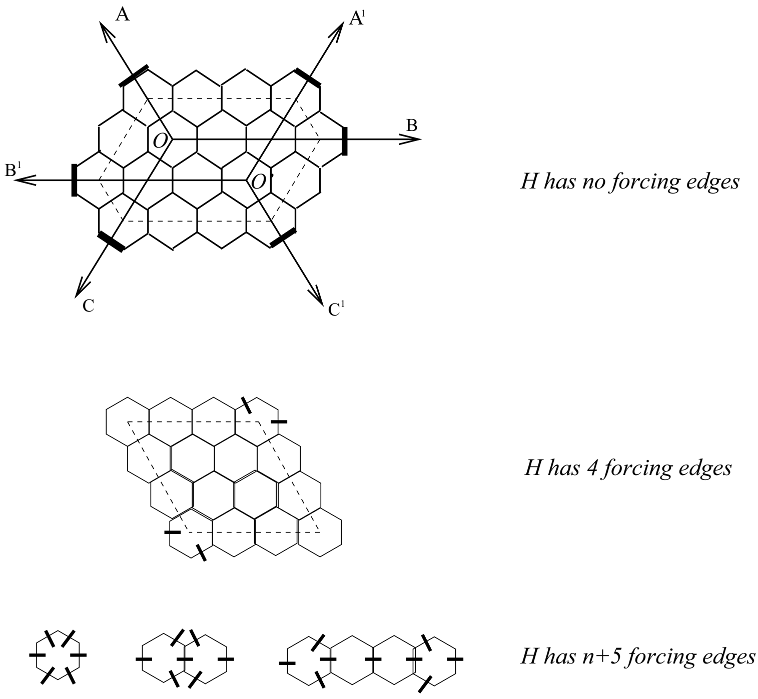

Figure 6. Forcing edges in H (marked by short bars) when $Z(H)$ has two pendent vertices.

Since $Z(H)$ has at most two pendent vertices, by Theorems 3.2, 3.3 and 3.4, we can have the following result immediately.

Corollary 3.5 The number of forcing edges in a hexagonal system is a nonnegative integer not equal to 5.

Zhang and Li (1996) [51] gave a linear algorithm to determine whether an edge e with one end incident to the boundary of a hexagonal system H is a forcing bond or not.

Algorithm 3.6 [51] Let e be an edge of a hexagonal system H with one end incident to the boundary of H.

Step 1. Delete the indicated edge e together with its two end vertices u and v to obtain a graph $H_1 = H \setminus \{u, v\}$.

Step 2. If H_i has a pendant edge, then delete the edge together with its end verities to obtain a graph H_{i+1}. If H_{i+1} has a pendant edge, then $H_i := H_{i+1}$, and go to Step 2. Otherwise, go to Step 3.

Step 3. If $H_i = \emptyset$, then e is a forcing bond. Stop. Otherwise, H_i is a connected subgraph of H without pendent vertices, so H_i has at least two perfect matchings by Theorem 2.2. Hence, e is not a forcing bond. Stop.

Theorem 3.7 [51] Algorithm 3.6 correctly recognizes whether the indicated edge e in a hexagonal system H is a forcing bond or not with complexity $O(n)$, where n is the number of vertices of H.

F. Zhang and H. Zhang's enumeration method (1995) on the Kekulé Structures of hexagonal systems with forcing edges is based on the following theorem.

Theorem 3.8 [52] Let H be a hexagonal system with a forcing edge e. Then the number of Kekulé structures of H is one more than the number of M-alternating cycles passing through e, where M is the Kekulé structure containing e.

Motivated by the concepts of forcing edges and Clar structures in a hexagonal system, Che and Chen (2006) introduced the concept of forcing hexagons in a hexagonal system.

Definition 3.9 [8] A hexagon h of a hexagonal system H is a forcing hexagon if $H - V(h)$ has a unique perfect matching.

(Note that the definition includes the case when H is a single hexagon, since the empty graph $H - V(h)$ is assumed to have a unique perfect matching by convention.)

We showed in [8] that any hexagonal system with a forcing hexagon is normal, that is, each edge of the hexagonal system is contained in some perfect matching. We further proved that a linear hexagonal chain has all its hexagons forcing, and other hexagonal systems may have 0, 1 or 2 forcing hexagons. Structural characterizations for the hexagonal systems with a given number of forcing hexagons were presented. Using the tool of

Z-transformation graphs, we also proved the co-existence property of forcing hexagons and forcing edges in a hexagonal system.

Theorem 3.10 [8] Let H be a hexagonal system with a perfect matching.

(i) If H has a forcing hexagon then H has no forbidden edges, that is, H is normal;

(ii) All hexagons of H are forcing if and only if H is a linear hexagonal chain;

(iii) If H is not a linear hexagonal chain, then a hexagon h of H is forcing if and only if h is a periphery hexagon and there is a perfect matching M of H that corresponds to a pendent vertex of $Z(H)$ such that h is M-alternating.

Parallel to Theorems 3.3 and 3.4, we gave structural characterizations for a hexagonal system H with forcing hexagons in Lemmas 3.11 and 3.12, from which the co-existence property of forcing edges and forcing hexagons in a hexagonal system was derived in Corollary 3.13.

Lemma 3.11 [8] Let H be a hexagonal system whose $Z(H)$ has exactly one pendent vertex. Then H has at most one forcing hexagon h, which is a periphery hexagon such that there exists a coordinate system $O - ABC$ w.r.t. h and H is monotone w.r.t. $O - ABC$. Furthermore, H has at most three forcing edges, which belong to h and are disjoint edges on the periphery of H.

Lemma 3.12 [8] Let H be a hexagonal system whose $Z(H)$ has exactly two pendent vertices. Let H^* be the inner dual of H. Then one of the following three cases must occur.

(i) The periphery of H^* is a big hexagon and H has neither forcing hexagons nor forcing edges.

(ii) The perimeter of H^* is a parallelogram with an angle equal to $120°$, and H has two forcing hexagons and four forcing edges. Furthermore, each forcing hexagon is centered at the corner of $120°$ angel of H^*, contains exactly two forcing edges.

(iii) H^* is a straight path and each hexagon of H is forcing. Furthermore, if H consists of the unique hexagon h, then each edge of h is a forcing edge; otherwise, each of the two end hexagons of H contains four forcing edges, and any other hexagon has the two vertical edges as forcing edges.

Corollary 3.13 [8] A hexagon h of a hexagonal system H is a forcing hexagon of a perfect matching M if and only if it contains a forcing edge of the same perfect matching M.

It is known that a bond between two carbon atoms in a benzenoid hydrocarbon H is a forcing bond if and only if its Pauling bond order reaches the minimum of all positive Pauling bond orders between carbon atoms of H. It is natural to ask the following

Question 3.1 [8] Which particular chemical (and physical) properties of benzenoid hydrocarbons are determined by the (number of) forcing hexagons in their molecular structures?

This question was first posted at the end of our 2006 paper [8]. It was raised again in Chen's talk (based on this survey) during the 2010 International Conference on Mathematical Chemistry in Xiamen, China. Professor Balaban was then in the audience, and he kindly provided a list of papers including [5, 6, 7, 30], which he thought should be relevant. After reading these papers we think that force hexagons have significance in the π-electron distribution of benzenoid hydrocarbons. According to Balaban and Randić [7], the π-electrons in benzenoid hydrocarbons can be counted in two different ways: (i) as partitions of π-electrons of the benzenoid (according to the conventions [34] that all resonance structures contribute equally, that shared double bonds resonance structures contribute with one π-electron to each of the condensed hexagons (the hexagons with a common bond), and that both π-electrons of an unshared double bond belong to the corresponding hexagon) and (ii)as benzenoid signature, i.e., a sequence of six real numbers counting for all resonance structures the numbers of times a hexagon is assigned according to the above conventions s_i π-electrons where i takes integer values between 1 and 6. An inventory of the distribution of π-electrons in hexagons of benzenoids is computed by summing up the number of times each hexagon achieves a count of 0,1,2,3,4,5 or 6 π-electrons according to the above conventions. The π-electron partition of a benzenoid is obtained by taking the average of the numbers of π-electrons assigned to each hexagon of the benzenoid.

From the data listed in these references on the π-electron partitions of some benzenoid hydrocarbons, we observed that if a benzenoid H has forcing hexagon(s) as well as non-forcing hexagon(s) (that is, H is not a linear hexagonal chain) then its forcing hexagon has smaller average number of π-electrons in the π-electron partition of H. This observation seems to be consistent with the coexistence of forcing edges and forcing hexagons. Note that chemical reactions of organic compounds involve the making and breaking of bonds, and a single bond between two given atoms is weaker than a double bond (that is, a double bond has more resistance to breaking). We know that a forcing bond in a benzenoid H is a weaker bond since it has the smallest positive pauling bond order among all bonds in H. Then the coexistence of forcing edges and forcing hexagons may indicate that a forcing hexagon in a benzenoid is a weaker hexagon that is easier to be broken during chemical reactions. So, it is reasonable to state the following chemical meaning of forcing hexagons:

In a benzenoid, a forcing hexagon has smaller average number of π-electrons than non-forcing hexagons, and it is easier to be broken during chemical reactions.

The forcing numbers of hexagonal systems are not easy to determine in general. So, upper bounds for forcing numbers of H are desirable. One upper bound was first given by Pachter and Kim (1998) as a corollary of Theorem 2.9 since a hexagonal system is a plane bipartite graph. Kleinerman (2006) used a constructive argument to obtain the upper bound of forcing numbers of planar bipartite graphs that are subgraphs of certain regular bipartite grids such as hexagonal grids and rectangular grids.

Corollary 3.14 [22][29] For any perfect matching M of a hexagonal system H, the forcing number $f(H,M) \le \left\lfloor \frac{|V(H)|}{6} \right\rfloor$, or equivalently, $f(H,M) \le \frac{|M|}{3}$.

On the other hand, by Theorem 2.1 or Theorem 2.2, any hexagonal system with a perfect matching has at least two perfect matchings since it is a 2-connected graph. So, the forcing numbers of a hexagonal system are bounded below by 1. Therefore, for any perfect matching M of a hexagonal system H, $1 \le f(H,M) \le \left\lfloor \frac{|V(H)|}{6} \right\rfloor$.

At the end of this section, let's recall the following definition introduced by Randić and Klein [36] in 1985.

Definition 3.15 The average forcing number $\overline{f}(G)$ of a graph G is defined as

$$\overline{f}(G) = \sum_{i=1}^{k} \frac{f(G,M_i)}{k}, \quad \text{where } M_i \ (1 \le i \le k) \text{ are all the perfect matchings of } G$$

The average forcing numbers for some small polyhexes were listed in [36].

3.2 Plane Bipartite Graphs - Forcing Edges and Forcing Faces

In order to extend various studies on hexagonal systems, H. Zhang and F. Zhang (2000) [54] conducted an extensive study on plane elementary bipartite graphs, by which many important known results in hexagonal systems can be generalized. In particular, they extended the concept of forcing edges from hexagonal systems to connected plane bipartite graphs. Parallel to their work, Che and Chen (2008) [9] extended the concept of forcing hexagons of hexagonal systems to forcing faces of connected plane bipartite graphs. The concepts of Z-transformation graph and a reducible face decomposition (briefly, RFD) of a plane bipartite graph played an important role on studying plane bipartite graphs with forcing edges or forcing faces. It turned out that many nice properties on hexagonal systems with forcing edges or forcing hexagons can be extended to plane bipartite graphs. For example, if G is a plane bipartite graph with minimum vertex degree $\delta(G) > 1$ and it has a forcing edge or forcing face, then G has no forbidden edges, that is, G is elementary. On the other hand, some properties of forcing edges or forcing faces in a hexagonal system is no longer valid in plane bipartite graphs. For example, for any integers n and k with $n \geq 4$ and $n \geq k \geq 0$, there exists a plane elementary bipartite graph G such that exactly k of the n finite faces of G are forcing, while any hexagonal system which is not a linear hexagonal chain has at most two forcing hexagons. Also, the co-existence property of forcing edges and forcing faces in hexagonal systems does not hold in plane bipartite graphs with minimum vertex degree > 1: where the existence of forcing edges implies the existence of forcing faces, but not vice versa.

Definition 3.16 [9] A finite face s of a plane bipartite graph G is said to be a forcing face of G if the subgraph of G obtained by deleting all vertices of s together with their incident edges, denoted by $G - s$, has exactly one perfect matching.

The following two lemmas are special cases of Proposition 2.7 when the forcing set is a forcing edge or a forcing face in a plane bipartite graph.

Lemma 3.17 [54] Let M be a perfect matching of a plane bipartite graph G. An edge e in M is forcing if and only if e is on every M-alternating cycle.

Lemma 3.18 [9] Let G be a plane elementary bipartite graph. Then a finite face s of G is forcing if and only if there is a perfect matching M of G such that s is M-resonant and each M-alternating cycle of G has at least one edge in common with the periphery of s.

Bau and Henning [4] showed that for any perfect matching M of a connected cubic plane bipartite graph G, there are at least two disjoint M-resonant faces (one of which could be the infinite face) in G. Their proof for the above result is quite long, we gave a much short proof of the above result and provided the following corollary in [9].

Corollary 3.19 [9] Any cubic plane bipartite graph has no forcing faces.

The following two theorems tell that if a plane bipartite graph has a forcing edge or a forcing face, then it is elementary.

Theorem 3.20 [54] Let G be a connected plane bipartite graph with $\delta(G) > 1$. Then G has a forcing edge if and only if the following two conditions hold:

(i) G has no forbidden edge, that is, G is elementary, and

(ii) G has a perfect matching M such that G has exactly two M-resonant faces (exterior face allowed) and their boundaries have at least one common edge.

(A forbidden edge of G is an edge that does not belong to any perfect matching of G.)

Theorem 3.21 [9] Let G be a connected plane bipartite graph with $\delta(G) > 1$. If G has a forcing face, then G is elementary.

H. Zhang and F. Zhang (2000) showed that any plane bipartite graph with more than two vertices is elementary if and only if it has a reducible face decomposition. They also applied RFD to provide a structural characterization for a plane bipartite graph G whose $Z(G)$ is a path.

Definition 3.22 [54] A reducible face decomposition (RFD) of a plane bipartite graph G can be defined as following: Start from an edge e, and join its two end vertices by a path P_1 of odd length (called the "first ear") to form a finite face $G_1(= s_1)$ of G. Then proceed inductively to build a sequence of plane bipartite graphs as follows: if $G_i = e + P_1 + P_2 + \cdots + P_i$ has already been constructed, add the $(i + 1)$th ear P_{i+1} of odd length by joining any two vertices in different colors of G_i such that P_{i+1} lies in the exterior of G_i and P_{i+1} and a part of the periphery of G_i surround a finite face (s_{i+1}) of

G for all $1 < i < n-1$. The decomposition $G = G_n = e + P_1 + P_2 + \cdots + P_n$ is called reducible face decomposition of G, and denoted by $RFD(G_1, G_2, \cdots, G_n(= G))$, which is associated with a unique face sequence $s_1, s_2, \cdots, s_n$.

Theorem 3.23 [54] Let G be a plane elementary bipartite graph with more than two vertices. Then $Z(G)$ is a path if and only if G has an $RFD(G_1, G_2, ..., G_n(= G))$ associated with the face sequence $s_1, s_2, \cdots, s_n$ and the ear sequence $P_1, P_2, \cdots, P_n$ such that

(i) the P_i's start with black (resp. white) vertices and end with white (resp. black) vertices w.r.t. the clockwise orientation of the boundaries of the G_i's;

(ii) s_i and s_{i+1} have edges in common for all i; and

(iii) s_1 is a periphery face of $G_n(= G)$ or G_{n-1}.

Recall that each hexagon of a hexagonal system H is forcing if and only if $Z(H)$ is a path. But the sufficiency doe not hold in a plane bipartite graph by the following RFD structural characterization of a plane bipartite each finite face of which is forcing.

Theorem 3.24 [9] Let G be a plane elementary bipartite graph with more than two vertices. Then each finite face of G is forcing if and only if G has a RFD $(G_1, G_2, \cdots, G_n(= G))$ associated with the face sequence $s_1, s_2, \cdots, s_n$ and the ear sequence $P_1, P_2, \cdots, P_n$ satisfying

(i) the P_i's start with black (resp. white) vertices and end with white (resp. black) vertices w.r.t. the clockwise orientation of the boundaries of the G_i's;

(ii) s_i and s_{i+1} have edges in common for all i; and

(iii) s_1 is a periphery face of $G_n(= G)$.

By Theorems 3.23 and 3.24, if each finite face of a plane bipartite graph G is forcing, then $Z(G)$ is a path. But it is not true conversely.

Using the tool of $Z(G)$, characterizations of those plane elementary bipartite graphs with a forcing edge or a force face were given by H. Zhang and F. Zhang (2000), Che and Chen (2008) respectively.

Theorem 3.25 [54] Let G be a plane elementary bipartite graph with more than two vertices. Then G has a forcing edge if and only if one of the following statements holds:

(i) $Z(G)$ has a vertex M of degree one such that the unique M-resonant finite face is a periphery face of G. Moreover, the periphery of G must be an M-alternating cycle.

(ii) $Z(G)$ has a vertex M of degree two such that the two M-resonant finite faces of G have a path in common and the periphery of G is not an M-alternating cycle.

Theorem 3.26 [9] Let s be a finite face of a plane elementary bipartite graph G. Then s is a forcing face if and only if one of the following statements holds:

(i) $Z(G)$ has a vertex M of degree one such that s is the unique M-resonant finite face of G and s is a periphery face of G. Moreover, the periphery of G must be an M-alternating cycle.

(ii) $Z(G)$ has a vertex M of degree two such that s is one of the two M-resonant finite faces, and these two faces are adjacent. Furthermore, if the periphery of G is an M-alternating cycle, then s is periphery face of G.

(iii) $Z(G)$ has a vertex M of degree $n+1$ where $n \geq 2$ and s, s_i $(1 \leq i \leq n)$ are the M-resonant finite faces such that s is adjacent to each s_i for $1 \leq i \leq n$; s_i and s_j have disjoint boundaries whenever $1 \leq i \neq j \leq n$. Furthermore, if the periphery of G is an M-alternating cycle, then s is a periphery face of G.

By Theorems 3.25 and 3.26, we can see that for any plane elementary bipartite graph G, the existence forcing edges implies the existence of forcing faces in G, but not true conversely.

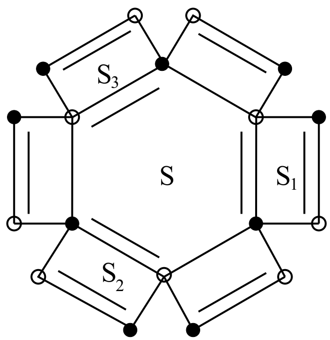

Figure 7. A plane bipartite graph with a forcing face s but no forcing edges.

Remark 3.27 Let G be a plane elementary bipartite graph with more than two vertices.

(i) If $e \in M$ is a forcing edge of a perfect matching M in G, then any M-resonant face of G containing e is a forcing face of M.

(ii) If s is a forcing face of a perfect matching M in G, it is possible that no edges in $s \cap M$ are forcing edges of M, but edges in $s \cap (M \oplus s)$ are forcing edges of $M \oplus s$. For example, see Fig. 1 (ii).

3.3 Plane Bipartite Graphs - Grids and Stop Signs

Sharp lower and upper bounds on forcing numbers of a $2n \times 2n$ square grid were first given by Pachter and Kim (1998) [29]. The bounds were also given by Lam and Pachter (2003) [27] as a special case of their main result on (n, k) stop signs.

Theorem 3.28 [29][27] Let M be a perfect matching of a square grid $P_{2n}\square P_{2n}$ where P_{2n} is a path with $2n$ vertices. Then the forcing number $f(P_{2n}\square P_{2n}, M)$ is bounded by

$$n \leq f(P_{2n}\square P_{2n}, M) \leq n^2,$$

and both bounds are sharp.

An (n, k) *stop sign* where $0 \leq k \leq n-1$ is the region obtained from the $2n \times 2n$ square grid by deleting the squares along the k diagonal closest to each of the four corners, see Fig. 8 provided in [27]. (n, k) stop signs generalize both square grids (when $k = 0$) and Aztec diamonds (when $k = n - 1$). Lam and Pachter (2003) [27] gave sharp lower and upper bounds on the forcing numbers of stop signs, and the bounds of Aztec diamonds and square grids follow as corollaries.

Theorem 3.29 [27] Let G be an (n, k)- stop sign and M be a perfect matching of G. Then the forcing number $f(G, M)$ is bounded by

$$n \leq f(G, M) \leq \left(n - \left\lceil \frac{k-1}{2} \right\rceil\right)\left(n - \left\lfloor \frac{k+1}{2} \right\rfloor\right)$$

and both bounds are sharp.

Corollary 3.30 [27] For any perfect matching M of an Aztec diamond G of order n, the forcing numer $f(G, M)$ is bounded by

$$n \leq f(G, M) \leq \begin{cases} \frac{n(n+2)}{4} & \text{for } n \text{ even} \\ \frac{(n+1)^2}{4} & \text{for } n \text{ odd} \end{cases}$$

and both bounds are sharp.

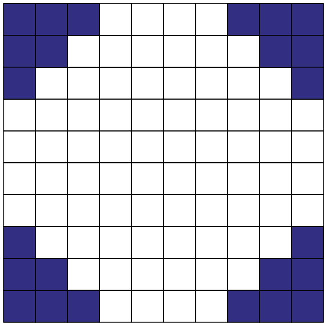

Figure 8. $(5,3)$ stop sign.

An induced subgraph G of a grid with vertex set $V(G)$ is called a *column continuous subgrid* if it has the following property: If (i_1, j), $(i_2, j) \in V(G)$ where $i_1 < i_2$, then for all integers i, such that $i_1 \leq i \leq i_2$, we have $(i, j) \in V(G)$. For example, both an (n, k) stop sign and a rectangle grid $P_m \Box P_n$ are column continuous. Afshani, Hatami and Mahmoodian (2004) gave the following result for the spectrum of a column continuous subgrid in [1].

Theorem 3.31 [1] There are no gaps in the spectrum of a column continuous subgrid.

Corollary 3.32 [1] Let G be an (n, k)-stop sign where $0 \leq k \leq n-1$. Then

$$Spec(G) = \left\{n, n+1, \cdots, \left(n - \left\lceil \frac{k-1}{2} \right\rceil\right)\left(n - \left\lfloor \frac{k+1}{2} \right\rfloor\right)\right\}$$

In particular,

(i) if $k = 0$, then G is a $2n \times 2n$ square grid $P_{2n} \Box P_{2n}$ and

$$Spec(P_{2n} \Box P_{2n}) = \{n, n+1, \cdots, n^2\},$$

(ii) if $k = n-1$, then G is an Aztec diamond of order n and

$$Spec(G) = \begin{cases} \left\{n, n+1, \cdots, \frac{n(n+2)}{4}\right\} & \text{for } n \text{ even} \\ \left\{n, n+1, \cdots, \frac{(n+1)^2}{4}\right\} & \text{for } n \text{ odd}\ . \end{cases}$$

Afshani et al (2004) [1] also gave the maximum forcing number of a rectangle grid $P_m \Box P_n$ and maximum forcing number of $P_m \Box C_{2n}$. They pointed out that finding the forcing number of $P_m \Box P_n$ does not seem to be easy and gave upper bounds on the forcing numbers of some special rectangular grids. Kleinerman (2006) [22] also gave the maximum forcing number of $P_{2m} \Box P_{2n}$ using a constructive method.

Theorem 3.33 [1] [22] Let $P_m \Box P_n$ be a rectangle grid. Then its maximum forcing number

$$F(P_m \Box P_n) = \left\lfloor \frac{m}{2} \right\rfloor \cdot \left\lfloor \frac{n}{2} \right\rfloor .$$

Theorem 3.34 [1] For every $k, n \geq 1$, the maximum forcing number for $P_m \Box C_{2n}$ is

$$F(P_m \Box C_{2n}) = \begin{cases} kn & \text{if } m = 2k \\ kn+1 & \text{if } m = 2k+1 . \end{cases}$$

Theorem 3.35 [1] The upper bounds on the forcing number of rectangle grid $P_{2k} \Box P_{(2k+1)l+r}$ and $P_{2k+1} \Box P_{(2k+2)l+2r}$ are:

(i) $f(P_{2k} \Box P_{(2k+1)l+r}) \leq kl + \lceil \frac{r-1}{2} \rceil$, where $0 \leq r \leq 2k$ and $l \geq 1$;

(ii) $f(P_{2k+1} \Box P_{(2k+2)l+2r}) \leq kl + r$, where $0 \leq 2r \leq 2k+1$ and $l \geq 1$.

3.4 Nonplanar Bipartite Graphs - Torus, Hypercubes, Toroidal Polyhexes

Afshani et al (2004) [1] gave an upper bound on the maximum forcing number of the special torus $C_{2n} \Box C_{2n}$: $F(C_{2n} \Box C_{2n}) \leq n^2 + \frac{n}{2}$. For torus $C_{2m} \Box C_{2n}$ $(m, n > 1)$, both the forcing number and the maximum forcing number are known.

Theorem 3.36 Let $C_{2m} \Box C_{2n}$ $(m, n > 1)$ be a torus. Then

(i) [32] (Riddle 2002) $\quad f(C_{2m} \Box C_{2n}) = 2\min\{m, n\}$,

(ii) [22] (Kleinerman 2006) $\quad F(C_{2m} \Box C_{2n}) = mn$.

For hypercubes Q_n, Pachter and Kim (1998) [29] conjectured that $f(Q_n) = 2^{n-2}$ for any positive integer n. The case when n is even was proved by Riddle (2002) [32]. It is still open for odd n.

Theorem 3.37 [32] (Riddle 2002) $f(Q_n) = 2^{n-2}$ for any even n.

The spectra of hypercubes were studied by Adams et al (2004) [2]. The vertices of a hypercube Q_n can be denoted by the set $\{0, 1, 2, \cdots, 2^n - 1\}$, where each vertex is viewed as a sequence of length n consisting of its binary representation with 0's and 1's. Two vertices are adjacent if and only if their sequence representations differ in exactly one component. For a given value k, $1 \leq k \leq n$, a set of edges of the form a_nb_n where a_n is any sequence having 0 in the kth component and b_n is obtained from a_n by changing the kth component to 1, is called a set of *parallel edges*, and the edges are said to be in the same direction.

Proposition 3.38 [2] Let M be a perfect matching of the hypercube Q_n consisting edges all in the same direction. Then $f(Q_n, M) = 2^{n-2}$.

Theorem 3.39 [2] Let Q_n be a hypercube where $n \geq 1$. Then

(i) $Spec(Q_n) = \{2^{n-2}\}$ for $n \leq 4$;

(ii) $Spec(Q_5) = \{8, 9\}$; and

(iii) $Spec(Q_n) \supseteq \{2^{n-2}, 2^{n-2}+1, \cdots, 2^{n-2}+2^{n-5}\}$ for $n \geq 5$.

A surprising result proved by Alon (see [32]) states that for sufficiently large n, there exists a perfect matching M of Q_n such that any one of its forcing sets almost contains all edges of M.

Theorem 3.40 (Alon 2002; in [32]) For sufficiently large n, there exists a perfect matching M of Q_n such that its forcing number $f(Q_n, M) > c2^{n-1}$ for any constant $c < 1$.

Alon's proof used the well known result that the number of perfect matchings equals the permanent of the biadjacency matrix and the proved (1979/80) Van der Waerden's permanent conjecture (1926) on the permanent of doubly stochastic matrix. In fact Alon's method can be applied to any k-regular bipartite graphs. Using Alon's method, Adams et al (2004) [2] obtained that for any k-regular bipartite graph G, as long as k is sufficiently large, there exists a perfect matching M of G such that any forcing set of M contains almost all the edges in M.

Theorem 3.41 [2] For any k-regular bipartite graph G with N vertices in each partite set,

$$F(G) \geq \left(1 - \frac{\log(2e)}{\log k}\right) N,$$

where e is the base of the natural logarithm.

A toroidal polyhex $H(p,q,t)$ with a torsion t (where integers $p \geq 1$, $q \geq 1$ and $0 \leq t \leq p-1$) is a cubic bipartite graph embedded on torus with every face being a hexagon. It can be obtained in the following way: Let P be a $p \times q$ parallelogram section cut from the hexagonal lattice such that every corner lies on the center of a hexagon, two lateral sides pass through q oblique edges, top and bottom sides pass through p vertical edges. identify the two lateral sides of P to form a cylinder, and then identify top and bottom sides with a torsion t hexagons. An example for $H(p,q,t)$ is depicted in Fig. 9 where $p = 8, q = 4$ and $t = 2$.

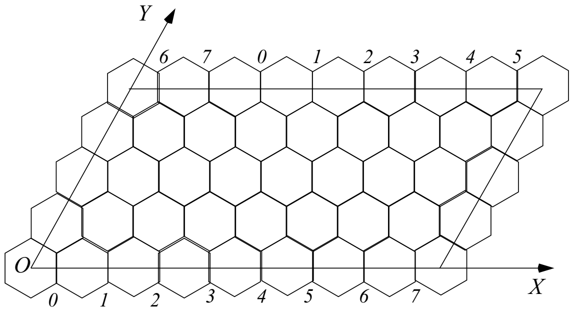

Figure 9. Toroidal polyhex $H(8,4,2)$.

Wang, Ye and Zhang (2008)[47] determined the forcing number of a toroidal polyhex, by improving Riddle's method for getting a lower bound of $f(G)$ for bipartite graphs G.

Theorem 3.42 [47] For any toroidal polyhex $H(p,q,t)$, its forcing number $f(H(p,q,t)) \geq \min\{p,q\}$, and equality holds for $p \leq q$ or $p > q$ and $t \in \{0, p-q, p-q+1, \cdots, p-1\}$. In general, $f(H(p,q,t))$ is equal to the side length of a maximum equilateral triangle on $H(p,q,t)$.

Based on the above result, they also presented a linear algorithm to compute the forcing number of $H(p,q,t)$.

4 Non-Bipartite Graphs

Most known results on forcing on perfect matchings of non-bipartite graphs are those of fullerene graphs. A fullerene graph is a 3-connected plane cubic graph with exactly 12 pentagonal faces and the other faces being hexagonal. For example, the dodecahedron is the fullerene C_{20} with 20 vertices, and the most important fullerene is buckminsterfullerene C_{60} obtained by leap-frog transformation of the fullerene C_{20}, see [20]. Fullerene graphs have been studied in chemistry as fullerene molecules which have extensive applications in physics, chemistry and material science. Zhang, Ye and Shiu (2010) showed that the forcing number of any fullerene graph was bounded below by 3, see [53]. Their proof uses Kotzig's classical theorem on unique perfect matching (1959) and two recent results on fullerene graphs G: the 2-extendability by H. Zhang and F. Zhang (2001) in [55], and the cyclically 5-edge-connectivity by Došlić (2003) in [10] and Qi and Zhang (2008) in [31].

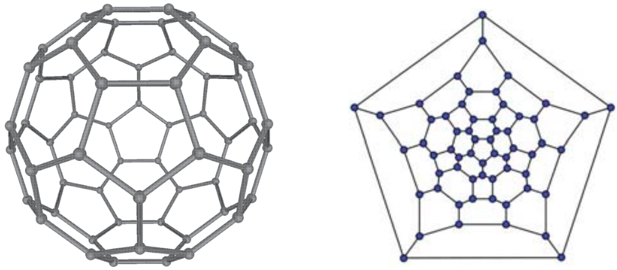

Figure 10. Buckminsterfullerene and its fullerene graph C_{60}.

Theorem 4.1 [53] For a fullerene graph G, $f(G, M) \geq 3$ for any perfect matching of G, and this lower bound can be achieved by infinitely many fullerene graphs.

Spectra of forcing numbers for some special fullerene graphs C_{20}, C_{60}, C_{70} and C_{72} have been established.

Theorem 4.2 Spectra of forcing numbers of C_{20}, C_{60}, C_{70}, and C_{72}:

(i) [53] Zhang, Ye and Shiu (2010)

$$Spec(C_{20}) = \{3\};$$

(ii) [42] Vukičević and Randić (2005)

$$Spec(C_{60}) = \{5, 6, 7, 8, 9, 10\};$$

(iii) [37] Randić and Vukičević (2006)

$$Spec(C_{70}) = \{5, 6, 7, 8, 9, 10, 11\};$$

(iv) [40] Vukičević, Gutman and Randić (2006)

$$Spec(C_{72}) = \{5, 6, 7, 8, 9, 10, 11, 12\}.$$

5 Other Related Work

5.1 Total (or Global) Forcing Number

Forcing sets and forcing numbers of perfect matchings of a graph are defined by the "local" approach, i.e., defined with respect to particular perfect matchings of a graph. Vukičević and Sedlar (2004) introduced "global" concepts on forcing perfect matchings in [43] without reference to a particular perfect matching, called the total forcing sets and the total forcing number of a graph.

A *total forcing set* of a graph G is a subset S of the edge set $E(G)$ that completely determines perfect matchings of G, which means that there are no two different perfect matchings of G coinciding on S. The *total forcing number* of a graph G is the smallest cardinality of a total forcing set of G.

Došlić (2007) gave equivalent formal definitions of the above concepts under the names of a global forcing set and the global forcing number of a graph in [11]. A *global forcing set* in a simple connected graph G with a perfect matching is a set of edges $S \subseteq E(G)$ such that the restriction of the characteristic function of perfect matchings of G on S is an injection. The number of edges in a global forcing set of the smallest cardinality is called the *global forcing number* of G, and denoted by $\gamma(G)$. The motivation for the study of global forcing sets comes from the large-scale computations involving manipulations of perfect matchings in fullerene graphs. By definition, a global forcing set can serve as binary codes for perfect matchings of a graph. If G is a graph with $K(G)$ perfect matchings, then $\gamma(G) \geq \lceil \log_2 K(G) \rceil$.

Vukičević and Sedlar (2004) studied the total forcing number of a square triangular grid T_n with n rows and n columns of vertices where n is even, see Fig. 11. They gave both a lower bound and an upper bound on the total forcing number $\gamma(T_n)$ and the limit of the ratio $\gamma(T_n)/|E(T_n)|$ as n tends to infinity.

Theorem 5.1 [43] Let T_n be a square triangular grid with n rows and n columns of vertices where n is even and $\gamma(T_n)$ be the total forcing number of T_n. Then

$$\frac{5}{4}n^2 - \frac{21}{2}n + \frac{41}{4} \leq \gamma(T_n) \leq \frac{5}{4}n^2 + n - 2,$$

and $\frac{\gamma(T_n)}{|E(T_n)|}$ tends to $\frac{5}{12}$ as n tends to infinity.

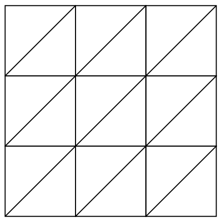

Figure 11. A square triangular grid T_4 with 4 rows and 4 columns of vertices.

Došlić (2007) [11] gave a characterization of global forcing sets and an upper bound on the global forcing number of a graph. He also proved several results concerning global forcing sets and numbers of benzenoid graphs. In particular, he proved that all cata-condensed benzenoids and catafused coronoids with n hexagons have the global forcing number equal to n, and that for peri-condensed benzenoids, the global forcing number is always strictly less than the number of hexagons.

Proposition 5.2 [11] Let G be a simple connected graph with a perfect matching. An edge set $S \subseteq E(G)$ is a global forcing set of G if and only if the graph induced by $E(G)\setminus S$ has at most one perfect matching.

A subgraph $H \subseteq G$ is *nice* if $G - H$ contains a perfect matching.

Proposition 5.3 [11] Let G be a simple connected graph with a perfect matching. Then $\gamma(G) \leq |E(G)| - |V(G)| + 1$. In particular, if G is a connected bipartite graph with a perfect matching, then $\gamma(G) = |E(G)| - |V(G)| + 1$ if and only if all even cycles in G are nice.

A *coronoid graph* is a graph obtained from a peri-condensed benzenoid by deleting some internal vertices and/or edges in such a way that no remaining vertices is of degree one, there is only one bounded nonhexagonal face, and this face is not adjacent to the unbounded face of the graph. A coronoid graph is *cataconfused* if it has no vertices shared between three hexagons.

Proposition 5.4 [11] (Došlić 2007) All cata-condensed benzenoids and catafused coronoids with n hexagons have the global forcing number equal to n, and that for peri-condensed benzenoids the global forcing number is always strictly smaller than the number of hexagons.

Vukičević and Došlić (2007) [39] showed how to compute the global forcing number of two classes of composite graphs: a link $G_1 \sim G_2$ and a splice $G_1 \cdot G_2$. A *link* of G_1 and G_2 anchored at the vertices $v \in V(G_1)$ and $w \in V(G_2)$ is a graph obtained by connecting vertices v and w by an edge, and denoted by $G_1 \sim G_2$. A *splice* of G_1 and G_2 is a graph obtained by selecting a vertex $v \in V(G_1)$ and identifying it with some vertex from $V(G_2)$, and denoted by $G_1 \cdot G_2$. They gave explicit formulas for global forcing numbers of grid graphs, complete bipartite graphs, complete graphs, and linear hexagonal chain.

Lemma 5.5 [39] Let G_1 and G_2 be simple connected graphs. Assume that $G_1 \sim G_2$ is their link anchored at the vertices $v \in V(G_1)$ and $w \in V(G_2)$, and $G_1 \cdot G_2$ is their splice at $v(w)$. Then their global forcing numbers are:

(i) $\gamma(G_1 \sim G_2) = \begin{cases} \gamma(G_1) + \gamma(G_2) & \text{if } |V(G_1)| \text{ is even} \\ \gamma(G_1 - v) + \gamma(G_2 - w) & \text{if } |V(G_2)| \text{ is odd}, \end{cases}$

(ii) $\gamma(G_1 \cdot G_2) = \gamma(G_1) + \gamma(G_2 - v)$, where $|V(G_1|$ is even.

Theorem 5.6 [39] Let $R_{i,j} = P_i \Box P_j$ be the Cartesian product of two paths P_i and P_j of i vertices and j vertices respectively. Then its global forcing number is

$$\gamma(R_{i,j}) = (i-1)(j-1) - \left\lfloor \frac{i-1}{2} \right\rfloor \left\lfloor \frac{j-1}{2} \right\rfloor .$$

Proposition 5.7 [39] The global forcing numbers of complete bipartite graph $K_{n,n}$, complete graph K_{2n}, and a linear hexagonal chain L_n with n hexagons are:

$$\begin{aligned} \gamma(K_{n,n}) &= (n-1)^2, \\ \gamma(K_{2n}) &= 2(n-1)^2, \\ \gamma(L_n) &= n. \end{aligned}$$

Vukičević and Došlić (2007) [39] also provided an explicit formula of vertex global forcing numbers of grid graphs. Let S be a subset of $V(R_{i,j})$ and $g : M(R_{i,j}) \rightarrow \{L, R, D, U\}^{ij}$ a function that to each perfect matching $M \in M(R_{i,j})$ assigns the directions of the edges that cover the vertices from $R_{i,j}$. A set $S \subseteq V(R_{i,j})$ such that $g|_S$ is an injection is called a *vertex global forcing set*, and the cardinality of smallest such set is called the *vertex global forcing number* of $R_{i,j}$, denoted by $\nu(R_{i,j})$.

Theorem 5.8 [39] Let $R_{i,j} = P_i \Box P_j$ be the Cartesian product of two paths P_i and P_j of i vertices and j vertices respectively. Then its vertex global forcing number is

$$\nu(R_{i,j}) = \left\lfloor \frac{i-1}{2} \right\rfloor \left\lfloor \frac{j-1}{2} \right\rfloor .$$

5.2 Anti-Forcing Number

Vukičević and Trinajstić (2007) introduced the concepts of anti-forcing number and anti-Kekulé number of a graph in [44]. Let $G = (V(G), E(G))$ be a graph G with a perfect matching. An *anti-forcing set* of G is a set $S \subseteq E(G)$ such that $G - S$ has a unique Kekulé structure. An anti-forcing set of the smallest cardinality is called a minimal anti-forcing set, and its cardinality is the *anti-forcing number* of G, denoted by $afn(G)$. An *anti-Kekulé set* of G is a set $S \subseteq E(G)$ such that $G - S$ is a connected graph and it has no Kekulé structures. An anti-Kekulé set of the smallest cardinality is called a minimal anti-Kekulé set, and its cardinality is the *anti-Kekulé number* of G and denoted by $akn(G)$. Vukičević and Trinajstić (2007) exemplified these concepts on damaged benzenoid parallelograms and obtained the anti-forcing number and anti-Kekulé number of a benzenoid parallelogram. A *benzenoid parallelogram* $B_{m,n}$ is a parallelogram-like shaped benzenoid that consists of $m \times n$ hexagons, arranged in m rows, each row consisting of n hexagons. The edges of $B_{m,n}$ can be divided into two classes E_1 and E_2, where edges in E_1 are drawn with normal lines and edges of E_2 with bold lines, see Fig. 12 provided in [44].

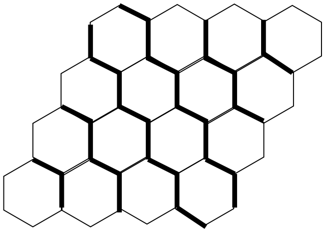

Figure 12. Benzenoid parallelogram $B_{4,4}$.

Theorem 5.9 [44] Let $B_{m,n}$ be a benzenoid parallelogram that consists of $m \times n$ hexagons, arranged in m rows, each row consisting of n hexagons. Then

(i) $afn(B_{m,n}) = 1$, for $m, n \geq 3$.

(ii) $akn(B_{m,n}) = 2$, for $m, n \geq 3$. Moreover, for every edge $e \in E_1$, there is a minimal anti-Kekulé set that contains e. There is no minimal anti-Kekulé set that contains any edge in E_2.

Vukičević and Trinajstić (2008) [45] showed that a cata-benzenoids has anti-Kekulé number either 2 or 3, and both classes are classified. A hexagon in a cata-condensed benzenoid is called a *branched hexagon* if it has three neighbors; Otherwise, it is called a *non-branched hexagon*. A cata-condensed benzenoid is a *more-branched cata-condensed benzenoid* if it has no two adjacent non-branched hexagons. Otherwise, it is a *less-branched cata-condensed benzenoid*.

Theorem 5.10 [45] Let B be a cata-condensed benzenoid. Then

(i) if B is less-branched, then its anti-Kekulé number $akn(B) = 2$;

(ii) if B is more-branched, then its anti-Kekulé number $akn(B) = 3$.

A *hexagonal chain* (or, *benzenoid chain*) with n hexagons (where $n > 2$) possesses two terminal hexagons and $n - 2$ non-terminal hexagons each of which has two neighbors. Assume that a hexagon h is adjacent to exactly two other hexagons h_1 and h_2. If the inner dual of of these three hexagons is a straight line, then h is called *linearly adhesive*; otherwise, *angularly adhesive*. Each branched and angularly connected hexagon in a cata-condensed hexagonal system is said to be a *kink*, in contrast to the terminal and linearly connected hexagons. A *linear chain* L_n with n hexagons is a hexagonal chain without kinks. A *fibonacene chain* F_n with n hexagons is a hexagonal chain without linearly adhesive hexagons. A *segment* is a maximal linear chain in a cata-condensed system, including the kinks and/or terminal hexagons at its end. A segment including a terminal hexagon is a *terminal segment*. The number of hexagons in a segment S is called its length and is denoted by $l(S)$.

For the anti-forcing number of a benzenoid chain B with k kinks (unbranched cata-condensed benzenoids) a formula $afn(B) = \lceil \frac{k}{2} \rceil$ was given by Vukičević and Trinajstić (2008)[45], see Theorem 5 on page 723 in [45]. We note that the formula is not correct. In the same paper they also gave a tight upper bound for the anti-forcing number of any cata-condensed benzenoid B with $n(> 1)$ hexagons: $afn(B) \leq \lfloor \frac{n}{2} \rfloor$, and showed that there is a cata-condensed benzenoid B_n with n hexagons such that $afn(B_n) = \lfloor \frac{n}{2} \rfloor$, see Theorem 6 on page 725 in [45]. In their proof, it was claimed that the zig-zag benzenoid B_n with n hexagons (see Fig. 10 on that same page) has $afn(B_n) = \lfloor \frac{n}{2} \rfloor$. We must point out that this is not correct either. To see the two anti-forcing numbers are wrong, we give the example in Fig. 13, where B is a benzenoid chain with $k = 7$ kinks and $n = 9$ hexagons. It is easy to check that $B - \{e_1, e_2, e_3\}$ has a unique perfect matching, and B has the anti-forcing number 3, which is less than both $\lceil \frac{k}{2} \rceil$ and $\lfloor \frac{n}{2} \rfloor$.

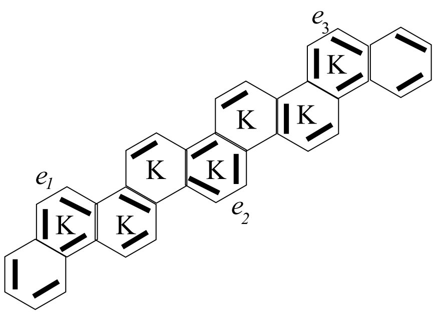

Figure 13. A counterexample to Theorem 5 on page 723 and to the tight upper bound of Theorem 6 on page 725 in [45].

Deng (2007) gave an algorithm for computing anti-forcing numbers of hexagonal chains and determined the bounds for the anti-forcing numbers of hexagonal chains [12].

Theorem 5.11 [12] Let G be a hexagonal chain with n hexagons. Then

(i) If the number of segments in G is s, then $afn(G) \leq \frac{s+1}{2}$;

(ii) If G is a fibonacene chain F_n, then $afn(F_n) = \lceil \frac{n}{3} \rceil$;

(iii) if G is neither a linear chain L_n nor a fibonacene chain F_n, then

$$1 = afn(L_n) < afn(G) < afn(F_n) = \left\lceil \frac{n}{3} \right\rceil .$$

Deng (2008) also determined the anti-forcing numbers of double hexagonal chains and characterized the extremal graphs in [13]. An *double hexagonal chain* consists of 2 condensed identical hexagonal chains. It can be constructed inductively from a naphthalene by a stepwise fusion of new naphthalene, and at each step, a type of fusion is selected from θ-type fusing, where $\theta \in \{\alpha, \beta\}$ explained in Figure 14 provided in [13].

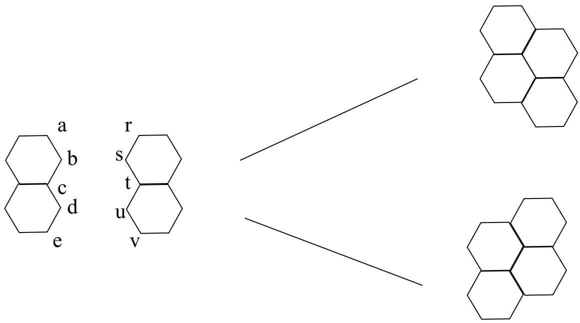

Figure 14. (1) α-type fusing: $b \equiv r$, $c \equiv s$, $d \equiv t$, $e \equiv u$,
(2) β-type fusing: $a \equiv s$, $b \equiv t$, $c \equiv u$, $d \equiv v$.

Let $B(\theta_1, \theta_2, \cdots, \theta_n)$ be the double hexagonal chain obtained from naphthalene B by θ_1-type, θ_2-type, $\cdots$, θ_n-type, fusing successively. Then $B(\theta_1, \theta_2, \cdots, \theta_n)$ has $n+1$ naphthalenes or $2(n+1)$ hexagons. If $\theta_i = \theta_{i+1}$ for each i, then $B(\theta_1, \theta_2, \cdots, \theta_n)$ is called the *double linear hexagonal chain* and denoted by DL_n; if $\theta_i \neq \theta_{i+1}$ for each i, then $B(\theta_1, \theta_2, \cdots, \theta_n)$ is called the double zig-zag hexagonal chain and denoted by DZ_n, see Figure 15 provided in [13].

Theorem 5.12 [13] Let $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ be a double hexagonal chain with $n+1$ naphthalenes and k segments. Then $afn(G) = k$.

Corollary 5.13 [13] Let $G = DZ_n$ be a double zig-zag hexagonal chain with $n+1$ segments. Then $afn(G) = \lfloor \frac{n}{2} \rfloor + 1$.

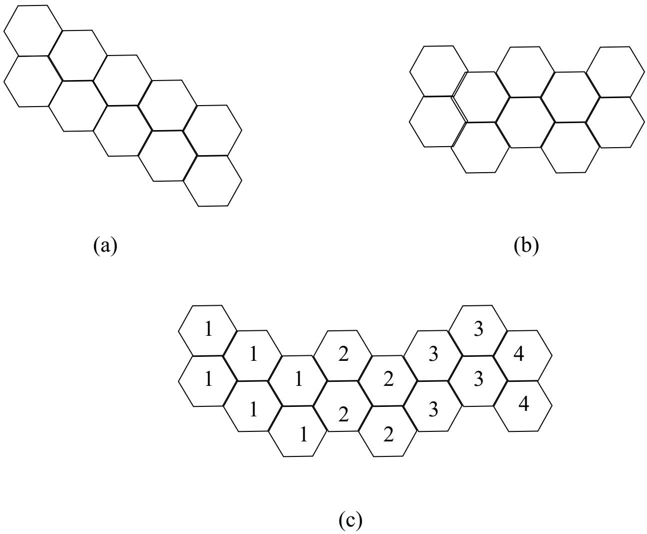

Figure 15. (a) Double linear hexagonal chain, $DL_4 = B(\alpha, \alpha, \alpha, \alpha)$;
(b) Double zig-zag hexagonal chain, $DZ_4 = B(\alpha, \beta, \alpha, \beta)$;
(c) Double hexagonal chain $B(\alpha, \alpha, \beta, \alpha, \beta, \beta, \alpha)$.

Corollary 5.14 [13] Let $G = B(\theta_1, \theta_2, \cdots, \theta_n)$ be any double hexagonal chain with $n+1$ naphthalenes. Then

$$1 = afn(DL_n) < afn(G) < afn(DZ_n) = \left\lfloor \frac{n}{2} \right\rfloor + 1 \ .$$

6 Open Questions and Conjectures

Question 6.1 Find $Spec(G)$ for specific graphs G.

- Find $Spec(P_m \Box P_n)$ for a general rectangular grid.
  - The spectrum is known for square grid $P_n \Box P_n$ (see Afshani, Hatami, Mahmoodian (2004) [1])
  - Afshani et al [1] found the maximum forcing matching number for $P_m \Box P_n$:
    $F(P_m \Box P_n) = \lfloor \frac{m}{2} \rfloor \lfloor \frac{n}{2} \rfloor$.
  - To find $Spec(P_m \Box P_n)$, we only need find $f(P_m \Box P_n)$, since it is kown that there is no gap in $Spec(P_m \Box P_n)$.

  - Afshani et al [1] pointed out that finding $f(P_m \Box P_n)$ does not seem to be so easy.

- Find $Spec(C_{2m} \Box C_{2n})$
  - Known: (Riddle 2002) $f(G) = 2min\{m, n\}$; (Kleinerman 2006) $F(G) = mn$.
  - It would be solved if we can show that there is no gap in $Spec(C_{2m} \Box C_{2n})$.

- Find $Spec(P_m \Box C_n)$.
  - Afshani, Hatami, Mahmoodian (2004) asked:
    (1) Find $f(P_m \Box C_n)$; (2) Find $F(P_{2m} \Box C_{2n+1})$.
  - They obtained: (1) $F(P_{2m} \Box C_{2n}) = mn$; (2) $F(P_{2m+1} \Box C_{2n}) = mn + 1$.

Question 6.2 Find necessary and sufficient conditions for a plane bipartite graph G (with more than 1 perfect matching) to have no gaps in $Spec(G)$.

Known: (Afshani, Hatami, Mahmoodian (2004)) For any finite set A of positive integers, there is a plane bipartite graph G such that $Spec(G) = A$.

Question 6.3 (H. Zhang, Ye, Shiu (2010) [53]):

- Find sharp upper bound for the forcing number $f(G, M)$ of fullerene graphs G.
- Determine all fullerene graphs G with $f(G) = 3$.
- Determine all fullerene graphs G of which all perfect matchings M have the same forcing number $f(G, M)$.

Question 6.4 (Afshani, Hatami, Mahmoodian (2004) [1])

What is the computational complexity of the following problem: Given a planar graph G, find the smallest (or largest) forcing number of G.

Known:

– Finding the smallest forcing set of a perfect matching is NP-complete for bipartite graphs with maximum degree 3. (Adams et al 2004)

– Finding the smallest forcing number of a graph is NP-complete for bipartite graphs with maximum degree 4. (Afshani et al 2004)

Question 6.5 Study forcing for graphs on other closed surfaces: forcing edges, forcing faces, forcing numbers, spectra.

Each closed surface can be constructed from an oriented polygon with an even number of sides, called a fundamental polygon of the surface, by pairwise identification of its edges.

For example, in each polygon below, attaching the sides with matching labels (A with A, B with B), so that the arrows point in the same direction, yields the indicated surface.

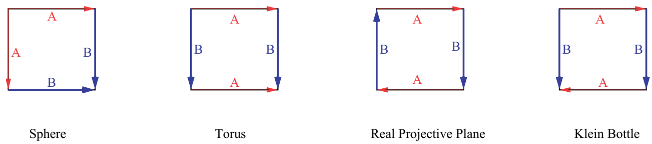

Figure 16. Surfaces.

Question 6.6 How to characterize the graphs G on $2n$ vertices whose forcing number $f(G)$ reaches the largest possible value $n-1$?

Conjecture 6.1 (Pachter and Kim (1998)[29])

For hypercube, $f(Q_n) = 2^{n-2}$.

The case n even was proved by Riddle (2002) It is still open for n odd.

Conjecture 6.2 (Che and Chen) For any fullerene graph G, $Spec(G)$ has no gap.

Conjecture 6.3 (Che and Chen) Every fullerene graph G has a perfect matching M such that G has no M-alternating hexagons.

We note that Conjectures 6.2 and 6.3 are true for C_{20}, C_{60} , C_{70} , and C_{72} from the work of Randić et al.

Acknowledgments

We would like to thank Professor Fuji Zhang for his helpful suggestions. We are also grateful to Professor A. T. Balaban for kindly providing a list of his reference papers which he thought should be and indeed are closely related to our question on the chemical meaning of the forcing hexagons in the molecule structures of benzenoid hydrocarbons.

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