Applied Mathematics and Computation 284 (2016) 209–218

Contents lists available at ScienceDirect

Applied Mathematics and Computation

journal homepage: www.elsevier.com/locate/amc

Forcing polynomials of benzenoid parallelogram and its related benzenoids[☆]

Shuang Zhao, Heping Zhang[*]

School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P.R. China

ARTICLE INFO

Keywords:
Forcing polynomial
Perfect matching
Innate degree of freedom
Forcing number
Benzenoid

ABSTRACT

Klein and Randić introduced the innate degree of freedom (forcing number) of a Kekulé structure (perfect matching) M of a graph G as the smallest cardinality of subsets of M that are contained in no other Kekulé structures of G, and the innate degree of freedom of the entire G as the sum over the forcing numbers of all perfect matchings of G. We proposed the forcing polynomial of G as a counting polynomial for perfect matchings with the same forcing number. In this paper, we obtain recurrence relations of the forcing polynomial for benzenoid parallelogram and its related benzenoids. In particular, for benzenoid parallelogram, we derive explicit expressions of its forcing polynomial and innate degree of freedom by generating functions.

1. Introduction

The forcing number of a perfect matching in benzenoid systems has been introduced by Harary et al. [11] more than twenty years ago. The roots of this concept can be found in an earlier paper by Klein and Randić [12] using the name ‘innate degree of freedom’. The *forcing* concept in Kekulé structures plays an important role in the resonance theory of theoretic chemistry [14,15]. In particular, for all benzenoid systems, recently Xu et al. [22] showed that the maximum forcing number is equal to the Clar number, and Lei et al. [13] showed that the maximum anti-forcing number is equal to the Fries number. Both indices can measure the stability of benzenoid hydrocarbons. We may refer to a survey [2] on this topic.

A *benzenoid system* (*benzenoid*, or *hexagonal system*) is a 2-connected finite plane graph such that every interior face is a regular hexagon of side length one [5]. The study of perfect matching in benzenoid systems is of chemical relevance since a benzenoid system with a perfect matching can be regarded as carbon skeleton of a benzenoid hydrocarbon molecule [5]. Also, many well-known combinatorial problems have been encountered in perfect matching count of benzenoid systems. For example, the number of k-combinations of $k+m$ elements equals perfect matching count of benzenoid parallelogram $L(k, m)$ [7,8], and $(n+1)$-st Catalan number equals perfect matching count of triangular benzenoid $T(n, n; n-1)$ [7,19].

Let G be a graph with a perfect matching M. A *forcing set* S of M is a subset of M such that S is contained in no other perfect matchings of G. The *forcing number of* M, denoted by $f(G, M)$, is the smallest cardinality over all forcing sets of M. The *innate degree of freedom of* G, denoted by $IDF(G)$, is the sum over the forcing numbers of all perfect matchings of G. An edge of G is called *forcing* if it is contained in exactly one perfect matching of G. The maximum and minimum values of

☆ Supported by NSFC (grant no. 11371180) and the Fundamental Research Funds for the Central Universities (grant no. lzujbky-2015-211).
* Corresponding author. Tel.: +86 18993168369; fax: +86 9318912481.
E-mail addresses: zhaosh08@lzu.edu.cn (S. Zhao), zhanghp@lzu.edu.cn (H. Zhang).

http://dx.doi.org/10.1016/j.amc.2016.03.008
0096-3003/

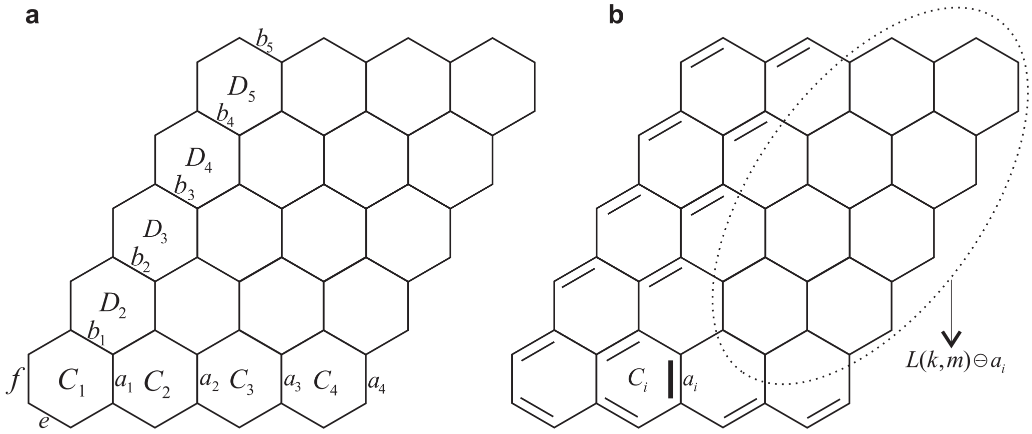

Fig. 1. Illustration of $L(k, m)$ (a) and $L(k, m) \ominus a_i$ (b), for $k = 4, m = 5, i = 2$.

$f(G, M)$ over all perfect matchings M of G are denoted by $F(G)$ and $f(G)$, respectively. For other related concepts we refer the reader to [2,5].

Zhang and Li [23,24], and Hansen and Zheng [10] independently characterized benzenoid systems with a forcing edge, which include the above mentioned benzenoids. Zhang and Zhang [25] gave a novel computation of perfect matching count for such benzenoids, and Zhang and Deng [26] showed that their forcing numbers of all perfect matchings form either the integer interval from 1 to the Clar number or with only the gap 2. In particular, for benzenoid parallelogram, some other indices and properties about forcing were also obtained, such as global forcing number [17], anti-Kekulé number [21], anti-forcing number [21], and Clar cover polynomial [9].

In [27], we proposed the forcing polynomial of a graph to study the number of perfect matchings that have the same forcing number, i.e.

$$F(G,x)=\sum_{M\in\mathcal{M}(G)}x^{f(G,M)}=\sum_{i=f(G)}^{F(G)}w(G,i)x^i, \tag{1}$$

where $\mathcal{M}(G)$ denotes the set of all perfect matchings of G and $w(G,i)$ denotes the number of perfect matchings of G with forcing number i. It is easy to show that

$$F(G,x)|_{x=1}=\Phi(G),\ \text{the perfect matching count of } G, \tag{2}$$

$$\left.\frac{\mathrm{d}}{\mathrm{d}x}F(G,x)\right|_{x=1}=IDF(G),\ \text{the innate degree of freedom of } G. \tag{3}$$

For some other graph polynomials, see a new book [18] and recent papers [3,4,6].

In this paper, we will apply this polynomial to benzenoid parallelogram and its related benzenoid systems. In Section 2, we first derive recurrence relation of the forcing polynomial for benzenoid parallelogram by equivalent definition of forcing set, and then obtain its explicit expression by generating function. As corollaries, we give explicit expressions of its perfect matching count and innate degree of freedom, and asymptotic behavior of its innate degree of freedom as one variable approaches infinity. In the end of this section, we present a new combinational explanation for the coefficients of forcing polynomial for benzenoid parallelogram with (0, 1)-sequence. In Section 3, we get recurrence relation of the forcing polynomial for pentagonal benzenoid, and explicit expressions of the forcing polynomial for benzenoid parallelograms with one additional hexagon.

2. Benzenoid parallelogram

First recall some basic results on forcing set of a perfect matching of a graph. Let G be a graph with a perfect matching M. A cycle of G is called *M-alternating* if its edges appear alternately in M and $E(G)\backslash M$, where $E(G)$ denotes the edge set of G.

Lemma 2.1. [1,16] *Let G be a graph with a perfect matching M. A subset $S \subseteq M$ is a forcing set of M if and only if each M-alternating cycle of G contains at least one edge of S.*

For an edge $e \in M$, let $G \ominus e$ be the subgraph obtained from G by first deleting e with the end vertices, and then deleting recursively pendant edges (with an end of degree one) with the ends until the remaining graph has no pendant edges or is empty (no vertices). We call the deleted edges of M in the above procedure *determined* by e.