Distribution of forcing and anti-forcing numbers of random perfect matchings on hexagonal chains and crowns

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Abstract

Forcing numbers and anti-forcing numbers were introduced in connection with chemical compound structures. The forcing number of a perfect matching M on a graph G is the smallest cardinality of a subset of M contained in a unique perfect matching on G, and the anti-forcing number of a perfect matching M on G is the smallest number of edges of G whose deletion results in a subgraph with a unique perfect matching M. We study in this paper the distribution of such numbers in random perfect matchings on hexagonal chains and hexagonal crowns. Recurrence relations and precise normal approximations are derived for their distributions.

Keywords: Hexagonal system; perfect matching; forcing number; anti-forcing number; hexagonal chain; hexagonal crown, central limit theorem, innate degree of freedom.

MSC(2010): 05A15; 05C30.

1 Introduction

Given a set of objects in a combinatorial structure, what is the minimum set of substructures to identify an object in this set? Here typical objects include critical sets of Latin squares, block designs, graph colorings, graph orientations, and dominating sets of graphs; see the survey paper [5]. In this paper, we are concerned with the minimum number of edges to identify a perfect matching.

All graphs in this paper are connected and simple. Given a perfect matching M of a graph G, a *forcing set* of M is a subset of M contained in no other perfect matchings on G. The *forcing number* of the perfect matching M, is the cardinality of a forcing set of M with the smallest size.

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The *forcing number* of the graph G is the minimum forcing numbers among all perfect matchings on G.

The concept of forcing number of a perfect matching was first introduced by Harary et al. [8]. The same idea appeared in an earlier chemical paper [11, 15] as innate degree of freedom of a Kekulé structure (equivalent to perfect matching), which plays an important role in the resonance theory in chemistry. Over the past twenty years, the study on forcing sets and forcing numbers has attracted much attention in the mathematical chemistry literature. For more details, we refer the reader to the recent survey paper [3].

Recently, Vukičević and Trinajstić [18] introduced the anti-forcing number, which is opposite to the forcing number. The *anti-forcing number* of a graph G is the cardinality of a subset S of the edge set with the smallest size such that $G - S$ has only one perfect matching. An explicit formula for anti-forcing number of unbranched cata-condensed benzenoids was then derived in [19]. Deng [4] gave an algorithm to compute the anti-forcing number of hexagonal chains, and determined the anti-forcing number of double hexagonal chains, as well as characterizing the extremal graphs. Zhang et al. [20] defined the concept of forcing polynomial and gave the recurrence relations for forcing polynomials of hexagonal chains.

Similar to the forcing number of a perfect matching, the anti-forcing number of a perfect matching can be naturally defined (see [12]): the anti-forcing number of a perfect matching M of G is the smallest number of edges of G whose deletion results in a subgraph with the unique perfect matching M.

Hexagonal chains and hexagonal crowns are significant in organic chemistry; for example, they appear in the molecular graphs of some benzenoid hydrocarbons. In this paper, we examine the distribution of forcing numbers and anti-forcing numbers of random perfect matchings on hexagonal chains and hexagonal crowns, where all possible perfect matchings are assumed to be equally likely. In particular, these numbers behave for large n (the number of hexagons) very close to a normal distribution with linear mean and linear variance. More precisely, random perfect matchings have on average

$$\mathbb{E}(\text{forcing \#}) = \tfrac{1}{\sqrt{5}}\, n + \nu_X + O\left(n\varphi^{-n}\right),$$
$$\mathbb{E}(\text{anti-forcing \#}) = \left(1 - \tfrac{1}{\sqrt{5}}\right) n + \nu_Y + O\left(n\varphi^{-n}\right),$$

the error terms being exponentially small, where $\varphi := \frac{1+\sqrt{5}}{2} \approx 1.618$ denote the golden ratio and

hexagonal systems	ν_X	ν_Y
zig-zag chains	$\frac{9\sqrt{5}-17}{10}$	$\frac{6-2\sqrt{5}}{5}$
crowns	0	0

Only the expected forcing number was previously known; see [20]. These average values are to be compared with the corresponding extremal values.

hexagonal systems	min & max of forcing #	min & max of anti-forcing #
zig-zag chains	$\left\lceil \frac{n}{3} \right\rceil .. \left\lceil \frac{n}{2} \right\rceil$	$\left\lceil \frac{n}{3} \right\rceil ..n$
crowns	n even: $2.. \left\lceil \frac{n}{2} \right\rceil$ n odd: $\left\lceil \frac{n}{3} \right\rceil .. \left\lceil \frac{n}{2} \right\rceil$	n even: $2..n$ n odd: $\left\lceil \frac{n}{3} \right\rceil ..n$

While the minimum (maximum) of the forcing and anti-forcing numbers may be as small (large) as two (n) in the case of hexagonal crowns, the average values $\sim 0.447n$ and $\sim 0.553n$ provide a better description of the typical behavior of these numbers in a random perfect matching. Finer properties such as the variance and convergence rate to the limit law will also be established; see Sections 3 and 4.

This paper is structured as follows. We characterize in the next section the anti-forcing polynomials of hexagonal chains by a general recurrence relation; the corresponding relation for forcing polynomials was already derived in [20]. Then in Section 3 we study the asymptotic distribution of both forcing and anti-forcing numbers of random perfect matchings on zig-zag hexagonal chains. The same study was carried out in Section 4 for hexagonal crowns. Some detailed enumerations related to hexagonal crowns are collected in Appendix.

2 Anti-forcing polynomials of hexagonal chains

We derive in this section a recurrence relation for computing the anti-forcing polynomials of hexagonal chains.

2.1 Preliminaries

Some definitions and useful lemmas are collected here for convenience of reference.

Definition 2.1. *Let G be a graph with a perfect matching, a* forcing set *S of a perfect matching M is a subset of M contained in no other perfect matchings on G. The* forcing number *of the perfect matching M, denoted by $f(G, M)$, is the smallest cardinality among all forcing sets of M.*

Let $P(G)$ denote the set of all perfect matchings on graph G. Given $M \in P(G)$, a cycle C of G is called an *M-alternating cycle* if the edges of C appear alternately in M and $E(G) \setminus M$. The following lemma provides a useful criterion for forcing set.

Lemma 2.2 ([1, 16])**.** *Let M be a perfect matching on a graph G. Then a subset $E \subseteq M$ is a forcing set of M if and only if each M-alternating cycle of G contains at least one edge of E.*

Definition 2.3. *Let G be a graph with a perfect matching. A set S of edges of G is called an* anti-forcing set *of a perfect matching M if $G - S$ has a unique perfect matching, which is M. The* anti-forcing number *of the perfect matching M, denoted by $g(G, M)$, is the smallest cardinality of anti-forcing sets of M.*

A collection of M-alternating cycles A of G is called a *compatible M-alternating set* if any two members of A either are disjoint or intersect only at edges in M.

Lemma 2.4 ([12])**.** *A set $S \subseteq E(G) \setminus M$ is an anti-forcing set of G if and only if S contains at least one edge of every M-alternating cycle of G.*

An immediate consequence of Lemma 2.4 is the following, which will be frequently used below.

Corollary 2.5. *Let $c'(M)$ denote the maximum cardinality of compatible M-alternating sets of G. Then $g(G, M) \geqslant c'(M)$.*

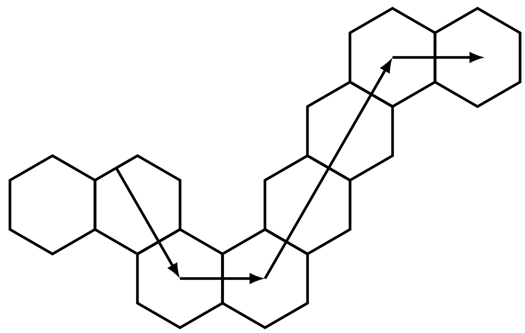


Figure 1: *A hexagonal chain G with $S(G) = (2, 0, 0, 1, 1, 2)$.*

Moreover, in the special case of planar bipartite graphs, the inequality becomes an identity.

Corollary 2.6 ([12]). *Let G be a planar bipartite graph with a perfect matching M. Then $g(G, M) = c'(M)$.*

We define the *forcing polynomial* and *anti-forcing polynomial* of G respectively as

$$f(G,t) := \sum_{M \in P(G)} t^{f(G,M)}, \quad g(G,t) := \sum_{M \in P(G)} t^{g(G,M)}.$$

2.2 Two types of perfect matchings

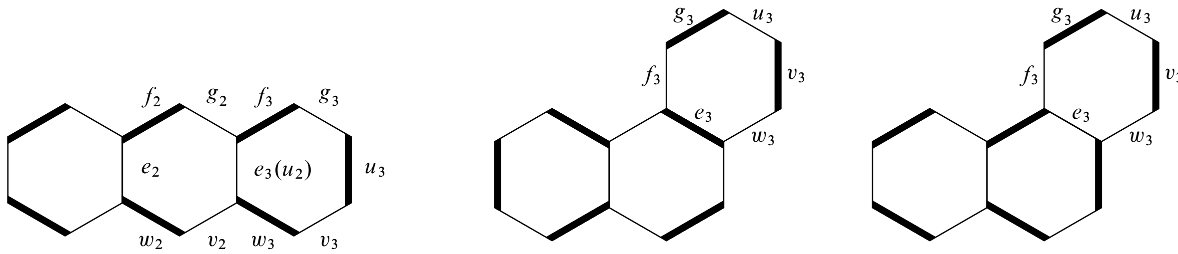
A *hexagonal system* (also called benzenoid system) is a finite 2-connected plane graph in which each interior face is a unit hexagon. A hexagonal system is called *cata-condensed* if it has no interior vertices. A *hexagonal chain* then is a cata-condensed hexagonal system in which no hexagon has more than two neighboring hexagons, i.e. its inner dual is a path.

Let G be a hexagons chain of length n. Then for $n \geqslant 2$, G has exactly 2 terminal hexagons and $n-2$ hexagons each with two neighboring hexagons, and each non-terminal hexagon H has exactly two vertices not shared with any other hexagon.

With each hexagonal chain G with n ($n \geqslant 2$) hexagons, we can associate a $\{0, 1, 2\}$-sequence $S(G) := (a_1, a_2, \ldots, a_{n-2})$ as follows. For $i = 1, 2, \ldots, n-2$, let a_i be the number of vertices on the $(i+1)$st hexagon with degree 2 that lie on the left-hand side when going from the $(i+1)$st hexagon to the $(i+2)$nd hexagon; see Figure 1 for an illustration. If $S(G)$ is an empty sequence, then G has exactly 2 hexagons.

A hexagonal chain is called *linear* if the corresponding sequence is $S(G) = (1, 1, \ldots, 1)$. On the other hand, if $S(G)$ is an alternating sequence of $\{0, 2\}$, then the hexagonal chain is called *zig-zag*. For example, the molecular graph of anthracene is a linear hexagonal chain with three hexagons (see Figure 2), while that of phenanthrene is a zig-zag hexagonal chain with three hexagons (see Figure 2).

We distinguish between two types of perfect matchings on a hexagonal chain G: if the two edges on the rightmost hexagon that are adjacent to the common edge of the last two hexagons are both in M, then M is called Type A perfect matching, otherwise, M is called Type B perfect matching; see Figure 2 for three examples. Let $P_A(G)$ and $P_B(G)$ denote the sets of Type A and Type B perfect matchings on G, respectively. We have $P(G) = P_A(G) \cup P_B(G)$.



Anthracene Phenanthrene

Figure 2: *Perfect matchings drawn with bold lines are of Type A, Type B and Type B, respectively.*

2.3 Bijections

Let G_1 denote the single hexagon, and G_2 denote the hexagon chain of length two. For $3 \leqslant i \leqslant n$, let G_i be the sub-chain of G with $S(G_i) = (a_1, a_2, \ldots, a_{i-2})$.

The number of perfect matchings on G is given by the following recurrence relation due to Gordon and Davison [7]

$$|P(G_k)| = \begin{cases} 2|P(G_{k-1})| - |P(G_{k-2})|, & \text{if } a_{k-2} = 1, \\ |P(G_{k-1})| + |P(G_{k-2})|, & \text{if } a_{k-2} = 0 \text{ or } 2, \end{cases}$$

for $k \geqslant 3$, with the initial conditions

$$|P(G_1)| = 2, \quad \text{and} \quad |P(G_2)| = 3.$$

From this it follows that the number of perfect matchings on a linear hexagonal chain with n hexagons is $n+1$, and that the number of perfect matchings on a zig-zag hexagonal chain with n hexagons is the the $(n+2)$nd Fibonacci number.

For $k \geqslant 2$, denote the common edge of the $(k-1)$th and kth hexagons of G by e_k, and along the clockwise direction the remaining edges of the kth hexagon are denoted by f_k, g_k, u_k, v_k, w_k. Notice that e_{k+1} represents the same edge as g_k, u_k or v_k according as a_{k-1} is 0, 1 or 2. See the first graph of Figure 2 for an example of these notations.

The following three lemmas are immediate from the fact that a perfect matching $M \in P(G_k)$ is of Type A if and only if $\{f_k, u_k, w_k\} \subseteq M$, and is of Type B if and only if $\{g_k, v_k\} \subseteq M$.

Lemma 2.7. *For each $k \in \{1, 2, \ldots, n-1\}$, there is a bijection $\tau_k : P(G_k) \to P_B(G_{k+1})$ given by*

$$\tau_k(M) = M \cup \{g_{k+1}, v_{k+1}\}.$$

Lemma 2.8. *For each $k \in \{2, 3, \ldots, n-1\}$, if $a_{k-1} = 1$, then there is a bijection $\omega_k : P_A(G_k) \to P_A(G_{k+1})$ given by*

$$\omega_k(M) = (M - \{e_{k+1}\}) \cup \{f_{k+1}, u_{k+1}, w_{k+1}\}.$$

Lemma 2.9. *For each $k \in \{2, 3, \ldots, n-1\}$, if $a_{k-1} = 0$ or 2, then there is a bijection $\lambda_k : P_B(G_k) \to P_A(G_{k+1})$ given by*

$$\lambda_k(M) = (M - \{e_{k+1}\}) \cup \{f_{k+1}, u_{k+1}, w_{k+1}\}.$$

See Figure 3 for examples of these bijections.

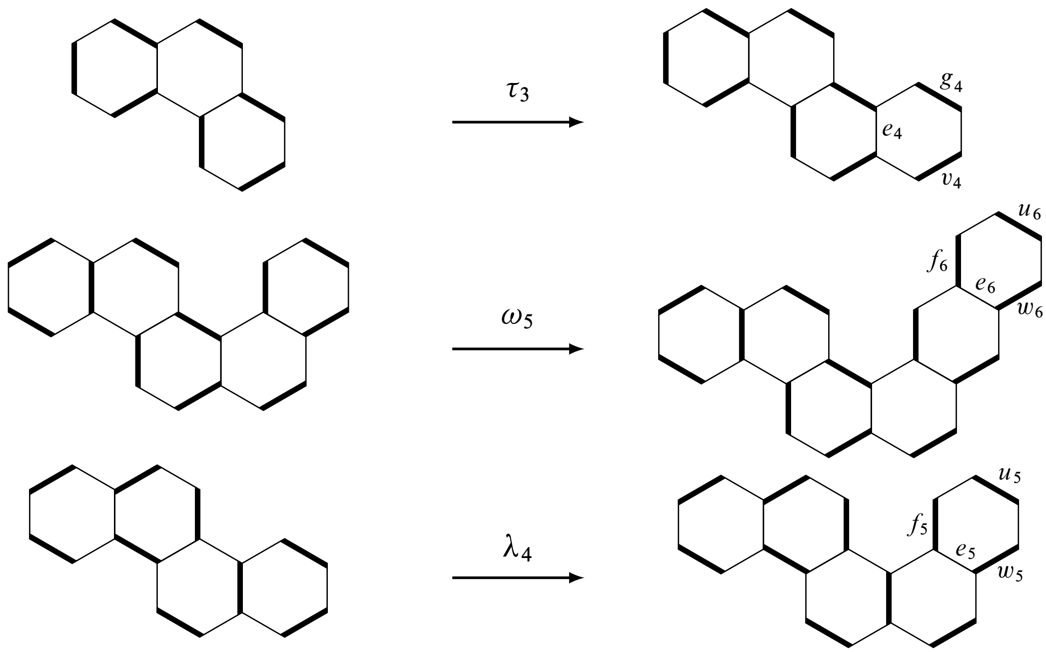


Figure 3: *Examples for the bijections τ_3, ω_5 and λ_4.*

2.4 Anti-forcing polynomials

The following two lemmas show how these bijections change the anti-forcing number of perfect matchings.

Lemma 2.10. *If $a_{k-1} = 1$, then the anti-forcing numbers can be computed as follows.*

1. *Given $M \in P_A(G_k)$, $g(G_{k+1}, \tau_k(M)) = g(G_k, M) + 1$;*
2. *given $M \in P_B(G_k)$, $g(G_{k+1}, \tau_k(M)) = g(G_k, M)$);*
3. *given $M \in P_A(G_k)$, $g(G_{k+1}, \omega_k(M)) = g(G_k, M)$.*

Proof. The proof is elementary but tedious, so we only prove the last part, the proof for the other two parts being similar.

Let A be a maximum compatible M-alternating set of G_k. By Corollary 2.6, $|A| = g(G_k, M)$. Let c_{k+1} denote the $(k + 1)$st hexagon of G_{k+1}, i.e. the hexagon with the edge set

$$\{e_{k+1}, f_{k+1}, g_{k+1}, u_{k+1}, v_{k+1}, w_{k+1}\}.$$

There exists exactly one cycle in A, denoted by c, containing the path $f_k g_k \ldots w_k$. We see that $(A - \{c\}) \cup \{c_{k+1}\}$ is a compatible $\omega_k(M)$-alternating set of G_{k+1}, so that by Corollary 2.5

$$g(G_{k+1}, \omega_k(M)) \geqslant |A| = |(A - \{c\}) \cup \{c_{k+1}\}| = g(G_k, M).$$

On the other hand, the edges $\{f_{k+1}, g_{k+1}, u_{k+1}, v_{k+1}, w_{k+1}\}$ must appear in exactly one cycle of any maximum compatible $\omega_k(M)$-alternating set B of G_{k+1}, denoted by c'. There are two cases.

- If $c' = c_{k+1}$, then the edge u_k $(= e_{k+1})$ is not contained in any other cycle of B; for otherwise, u_k is a common edge of two cycles but $u_k \notin \omega_k(M)$, and this will cause a contradiction. Thus none of the $\{f_k, g_k, v_k, w_k\}$ is contained in the cycle of B. As a consequence, e_k is contained in no cycle of B since that the two edges in c_{k-1} adjacent to e_k are not in M. Then $(B - \{c'\}) \cup \{c_k\}$ is a compatible M-alternating set of G_k, and

$$g(G_{k+1}, \omega_k(M)) = |B| = |(B - \{c_{k+1}\}) \cup \{c_k\}| \leqslant g(G_k, M).$$

- If $c' \neq c_{k+1}$, then $e_{k+1} \notin E(c')$. Accordingly,

$$(B - \{c'\}) \cup \{(c' - \{f_{k+1}, g_{k+1}, u_{k+1}, v_{k+1}, w_{k+1}\}) \cup \{e_{k+1}\}\}$$

  is a compatible M-alternating set of G_k, and $g(G_{k+1}, \omega_k(M)) \leqslant g(G_k, M)$.

It follows that $g(G_{k+1}, \omega_k(M)) = g(G_k, M)$, which proved part 3 of the lemma. ∎

In a similar manner, we have the following lemma.

Lemma 2.11. *If $a_{k-1} = 0$ or 2, then the anti-forcing numbers can be computed as follows.*

1. *Given $M \in P_A(G_k)$, $g(G_{k+1}, \tau_k(M)) = g(G_k, M)$;*
2. *given $M \in P_B(G_k)$, $g(G_{k+1}, \tau_k(M)) = g(G_k, M) + 1$;*
3. *given $M \in P_B(G_k)$, $g(G_{k+1}, \lambda_k(M)) = g(G_{k-1}, \tau_{k-2}^{-1}(M)) + 1$.*

We will compute anti-forcing polynomials according to the types of perfect matchings

$$g(G, t) = g_A(G, t) + g_B(G, t),$$

where

$$g_A(G, t) := \sum_{M \in P_A(G)} t^{g(G,M)} \quad \text{and} \quad g_B(G, t) := \sum_{M \in P_B(G)} t^{g(G,M)}.$$

Lemma 2.12. *If $a_{k-1} = 1$, then*

$$\begin{cases} g_A(G_{k+1}, t) = g_A(G_k, t), \\ g_B(G_{k+1}, t) = t g_A(G_k, t) + g_B(G_k, t). \end{cases}$$

If $a_{k-1} = 0$ or 2, then

$$\begin{cases} g_A(G_{k+1}, t) = t g(G_{k-1}, t), \\ g_B(G_{k+1}, t) = g_A(G_k, t) + t g_B(G_k, t). \end{cases}$$

Proof. If $a_{k-1} = 1$, by Lemmas 2.7–2.10, we have

$$g_A(G_{k+1}, t) = \sum_{M \in P_A(G_{k+1})} t^{g(G_k, \omega_k^{-1}(M))} = g_A(G_k, t),$$

and

$$\begin{aligned} g_B(G_{k+1},t) &= \sum_{\substack{M\in P_B(G_{k+1})\\ \tau_k^{-1}(M)\in P_A(G_k)}} t^{g(G_{k+1},M)} + \sum_{\substack{M\in P_B(G_{k+1})\\ \tau_k^{-1}(M)\in P_B(G_k)}} t^{g(G_{k+1},M)} \\ &= t g_A(G_k,t) + g_B(G_k,t). \end{aligned}$$

The case when $a_{k-1} = 0$ or 2 is similar by using Lemmas 2.7–2.9 and 2.11. ■

Given two hexagonal chains G and G', if the two sequences $S(G)$ and $S(G')$ have identical positions in their occurrences of 1's, then $g(G,t) = g(G',t)$ by Lemma 2.12. We may thus assume that $S(G)$ is a $\{1,2\}$-sequence in the rest of this section.

Given a $\{1,2\}$-sequence $S(G)$ of length n, let k be the number of 2's, r_1 be the number of 1's before the first occurrence of 2 ($r_1 = n$ if $k = 0$), r_{k+1} be the number of 1's after the last occurrence of 2, and r_j be the number of 1's between the $(j-1)$st and the jth occurrence of 2 for $2 \leqslant j \leqslant k$.

$$S(G) = (\overbrace{1,\cdots,1}^{r_1},2,\overbrace{1,\cdots,1}^{r_2},2,\cdots,2,\overbrace{1,\cdots,1}^{r_k},2,\overbrace{1,\cdots,1}^{r_{k+1}}) \qquad (r_1,\ldots,r_{k+1} \geqslant 0).$$

Then we have $r_j \geqslant 0$ and $\sum_{1\leqslant j\leqslant k} r_j = n-k$, i.e. $(r_1,\ldots,r_k)$ is a weak $(k+1)$-composition of $n-k$[1]. It is easy to recover $S(G)$ from $(r_1,\ldots,r_{k+1})$. Actually, this gives a classical bijection between $\{1,2\}$-sequences and weak compositions; see [17]. For convenience, define

$$f(r_1,r_2,\ldots,r_{k+1}) := f(G,t), \quad \text{and} \quad g(r_1,r_2,\ldots,r_{k+1}) := g(G,t).$$

The two polynomials $g_A(r_1,\ldots,r_{k+1})$ and $g_B(r_1,\ldots,r_{k+1})$ are defined similarly. Now we derive a recurrence relation to compute the anti-forcing polynomials of hexagonal chains.

Theorem 2.13. *Let $g(r_1,\ldots,r_k,-1) = g(r_1,\ldots,r_k)$ for $k \geqslant 1$, and $g(-1) = g(G_1,t)$. Then for $k \geqslant 2$*

$$\begin{aligned} g(r_1,\ldots,r_{k+1}) = {} & t g(r_1,\ldots,r_k) + (t + r_{k+1}t^2) g(r_1,\ldots,r_k - 1) \\ & + (t - t^2) g(r_1,\ldots,r_{k-1} - 1), \end{aligned} \tag{1}$$

with the initial conditions $g(r_1) = 2t + (r_1+1)t^2$, and $g(r_1,r_2) = t + 3t^2 + (2r_1 + 2r_2 + 1)t^3 + r_1 r_2 t^4$.

The corresponding recurrence relation for forcing polynomials was derived in [20].

Theorem 2.14 ([20])**.** *Let $f(r_1,\ldots,r_k,-1) = f(r_1,\ldots,r_k)$ for $k \geqslant 1$. The forcing polynomial of a hexagonal chain G satisfies the following recurrence relation*

$$f(r_1,r_2,\ldots,r_{k+1}) = (r_{k+1}+2) t f(r_1,r_2,\ldots,r_k - 1) + t f(r_1,r_2,\ldots,r_{k-1} - 1),$$

with the initial conditions $f(r_1) = (r_1+3)t$ and $f(r_1,r_2) = t + (r_1+2)(r_2+2)t^2$.

[1] A weak (integer) composition of n is an ordered sequence $(j_1,\ldots,j_k)$ with $j_i \geqslant 0$ such that $j_1 + \cdots + j_k = n$.

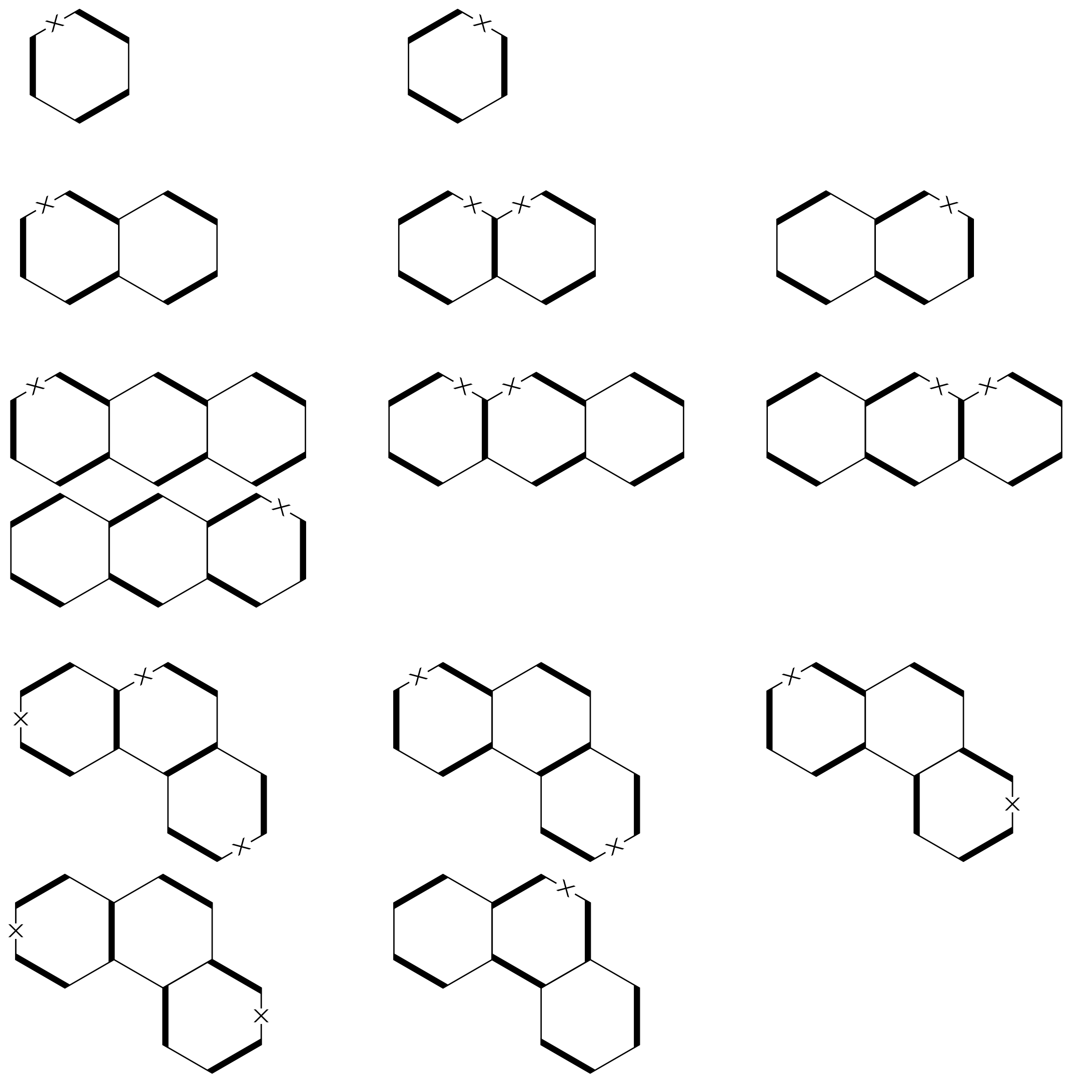


Figure 4: *The perfect matchings are drawn with bond lines; the edges marked by "×" form their smallest anti-forcing sets such that (from top to bottom)* $g(-1) = 2t$, $g(0) = 2t + t^2$, $g(1) = 2t + 2t^2$ *and* $g(0, 0) = t + 3t^2 + t^3$.

When $t = 1$, the values of f and g must coincide. This can be checked by induction although the two recurrences are different.

Proof. (of Theorem 2.13) The proof for small values of r_1 and r_2 is straightforward; see Figure 4. If $k = 0$ and $r_1 \geqslant 1$, then, by Lemma 2.12,

$$g_A(r_1) = g_A(r_1 - 1) = \cdots = g_A(0) = t,$$

and

$$g_B(r_1) = tg_A(r_1 - 1) + g_B(r_1 - 1) = t^2 + g_B(r_1 - 1) = \cdots = t + (r_1 + 1)t^2.$$

Thus

$$g(r_1) = g_A(r_1) + g_B(r_1) = 2t + (r_1 + 1)t^2.$$

When $k \geqslant 1$, we have

$$\begin{aligned} g_A(r_1, \ldots, r_{k+1}) &= g_A(r_1, \ldots, r_{k+1} - 1) = \cdots = g_A(r_1, \ldots, r_k, 0) \\ &= tg(r_1, \ldots, r_k - 1) = \begin{cases} 2t^2 + r_1 t^3, & \text{if } k = 1, \\ tg(r_1, \ldots, r_k - 1), & \text{if } k > 1, \end{cases} \end{aligned} \tag{2}$$

and

$$\begin{aligned} g_B(r_1, \ldots, r_k, 0) &= g_A(r_1, \ldots, r_k) + tg_B(r_1, \ldots, r_k) \\ &= (1 - t)g_A(r_1, \ldots, r_k) + tg(r_1, \ldots, r_k) \\ &= \begin{cases} t + t^2 + (r_1 + 1)t^3, & \text{if } k = 1, \\ (t - t^2)g(r_1, \ldots, r_{k-1} - 1) + tg(r_1, \ldots, r_k), & \text{if } k > 1. \end{cases} \end{aligned}$$

If $r_{k+1} \geqslant 1$

$$\begin{aligned} g_B(r_1, \ldots, r_{k+1}) &= tg_A(r_1, \ldots, r_{k+1} - 1) + g_B(r_1, \ldots, r_{k+1} - 1) \\ &= t^2 g(r_1, \ldots, r_k - 1) + g_B(r_1, \ldots, r_{k+1} - 1) \\ &= \cdots = r_{k+1} t^2 g(r_1, \ldots, r_k - 1) + g_B(r_1, \ldots, r_k, 0). \end{aligned} \tag{3}$$

It is easily checked that these relations also hold when $r_{k+1} = 0$. If $k = 1$, then

$$\begin{aligned} g(r_1, r_2) &= g_A(r_1, r_2) + g_B(r_1, r_2) \\ &= 2t^2 + r_1 t^3 + r_2 t^2 g(r_1 - 1) + g_B(r_1, 0) \\ &= t + 3t^2 + (2r_1 + 2r_2 + 1)t^3 + r_1 r_2 t^4. \end{aligned}$$

If $k \geqslant 2$, the recurrence relation (1) follows from (2) and (3). ■

Example 2.15. *Let G be a hexagonal chain with 6 hexagons and $S(G) = (2, 1, 0, 1)$. Since $g(G, t) = g(G', t)$, where $S(G') = (2, 1, 2, 1)$, we can apply Theorem 2.13 with $k = 2$, $r_1 = 0$, $r_2 = 1$, and $r_3 = 1$, and obtain*

$$\begin{aligned} g(G, t) = g(0, 1, 1) &= tg(0, 1) + (t + t^2)g(0, 0) + (t - t^2)g(-1) \\ &= 4t^2 + 5t^3 + 7t^4 + t^5. \end{aligned}$$

Example 2.16. *For a linear hexagonal chain G_n, we have, by Theorems 2.13 and 2.14,*

$$\begin{cases} f(G_n, t) = (n + 1)t, \\ g(G_n, t) = 2t + (n - 1)t^2. \end{cases}$$

3 Forcing and anti-forcing polynomials of zig-zag hexagonal chains

Forcing and anti-forcing polynomials are useful in describing deeper properties of the perfect matchings such as the innate degree of freedom of a Kekulé structure; see [11]. We study in this section the distribution of forcing and anti-forcing numbers of random perfect matchings on zig-zag hexagonal chains of length n, which, for simplicity, is denoted by $\mathscr{Z}_n$.

The forcing polynomial of a zig-zag chain $\mathscr{Z}_n$ satisfies (see [20])

$$f(\mathscr{Z}_n, t) = \begin{cases} 2t, & \text{if } n = 1, \\ 3t, & \text{if } n = 2, \\ t + 4t^2, & \text{if } n = 3, \\ 2tf(\mathscr{Z}_{n-2}, t) + tf(\mathscr{Z}_{n-3}, t), & \text{if } n \geqslant 4, \end{cases}$$

For convenience, we may assume that $f(\mathscr{Z}_0, t) = 1$. Let $f(z,t) := \sum_{n\geqslant 0} f(\mathscr{Z}_n, t)z^n$. Then the above recurrence leads to the rational form

$$f(z,t) = \frac{1 + 2tz + tz^2}{1 - 2tz^2 - tz^3}. \tag{4}$$

The total number of perfect matchings on zig-zag hexagonal chains of length n is given by the (shifted) Fibonacci number[2]

$$F_n := [z^n]f(z,1) = [z^n]\frac{1+z}{1-z-z^2} = \left(\tfrac{1}{2} + \tfrac{3}{10}\sqrt{5}\right)\varphi^n + \left(\tfrac{1}{2} - \tfrac{3}{10}\sqrt{5}\right)(-\varphi)^{-n},$$

where $\varphi := \frac{1+\sqrt{5}}{2} \approx 1.618$ is the golden ratio.

The corresponding anti-forcing polynomial can be computed by substituting $r_1 = r_2 = \cdots = r_{n+1} = 0$ in Theorem 2.13. Let $g(\mathscr{Z}_0, t) = 1$. The anti-forcing polynomial of a zig-zag chain $\mathscr{Z}_n$ satisfies

$$g(\mathscr{Z}_n, t) = \begin{cases} 2t & \text{if } n = 1, \\ 2t + t^2 & \text{if } n = 2, \\ tg(\mathscr{Z}_{n-1}, t) + tg(\mathscr{Z}_{n-2}, t) + (t - t^2)g(\mathscr{Z}_{n-3}, t) & \text{if } n \geqslant 3. \end{cases} \tag{5}$$

Let $g(z,t) := \sum_{n\geqslant 0} g(\mathscr{Z}_n, t)z^n$. From the recurrence relation (5), it follows that

$$g(z,t) = \frac{1 + tz + (t - t^2)z^2}{1 - tz - tz^2 - (t - t^2)z^3}. \tag{6}$$

Note that $f(z,1) = g(z,1)$.

Assume now that all F_n perfect matchings on zig-zag hexagonal chains of length n are equally likely. Let X_n and Y_n denote the forcing number and anti-forcing numbers, respectively, of a random perfect matching. Then the probability generating function of X_n and that of Y_n satisfy

$$\mathbb{E}(t^{X_n}) = \frac{[z^n]f(z,t)}{[z^n]f(z,1)}, \quad \text{and} \quad \mathbb{E}(t^{Y_n}) = \frac{[z^n]g(z,t)}{[z^n]g(z,1)} \qquad (n \geqslant 0).$$

[2] The symbol $[z^n]f(z)$ represents the coefficient of z^n in the Taylor expansion of f.

These are polynomials of t of degree $\lceil \frac{n}{2} \rceil$ and n, respectively. More precisely, by expanding the two rational forms (4) and (6), we obtain the following closed-form expressions for the coefficients of the polynomials.

Theorem 3.1. *For $n \geqslant 3$, the number $\xi_{n,k}$ of perfect matchings on zig-zag hexagonal chains of length n with forcing number k is given by*

$$\xi_{n,k} = [z^n t^k] f(z,t) = \frac{k! 2^{3k-1-n}(n+2-k)}{(3k-n)!(n+1-2k)!},$$

for $\lceil \frac{n}{3} \rceil \leqslant k \leqslant \lceil \frac{n}{2} \rceil$, and the number $\eta_{n,k}$ of perfect matchings on zig-zag hexagonal chains of length n with anti-forcing number k is given by

$$\eta_{n,k} = [z^n t^k] g(z,t) = \mathbb{1}_{n\ odd} \cdot \mathbb{1}_{k=\frac{n+1}{2}} + \sum_{\lceil \frac{n-k}{2} \rceil \leqslant j \leqslant \min\{k, n-k\}} \binom{j+1}{n+1-k-j} \binom{n-2j}{n-k-j},$$

for $\lceil \frac{n}{3} \rceil \leqslant k \leqslant n$.

Here we use the symbol $\mathbb{1}_{\mathscr{A}}$ to denote the indicator function of the event $\mathscr{A}$.

It was proved in [20] that

$$\mathbb{E}(X_n) \sim \frac{1}{\sqrt{5}} n.$$

We will derive finer distributional results below. Let $\Phi(x) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-u^2/2} \mathrm{d}u$ denote the standard normal distribution function.

Theorem 3.2. *The distributions of the forcing and anti-forcing numbers of random perfect matchings on zig-zag hexagonal chains are asymptotically normal: $W \in \{X, Y\}$*

$$\sup_{x \in \mathbb{R}} \left| \mathbb{P}\left(\frac{W_n - \mu_W n}{\sigma_W \sqrt{n}} \leqslant x \right) - \Phi(x) \right| = O\left(n^{-1/2}\right),$$

with linear mean and linear variance

$$\begin{aligned} \mathbb{E}(W_n) &= \mu_W n + \nu_W + O\left(n\varphi^{-n}\right), \\ \mathbb{V}(W_n) &= \sigma_W^2 n + \varsigma_W + O\left(n\varphi^{-n}\right), \end{aligned} \tag{7}$$

the error terms being exponentially small. All the constants are given in the following table.

μ_X	ν_X	μ_Y	ν_Y
$\frac{1}{\sqrt{5}} \approx 0.447$	$\frac{9\sqrt{5}-17}{10} \approx 0.313$	$1 - \frac{1}{\sqrt{5}} \approx 0.553$	$\frac{6-2\sqrt{5}}{5} \approx 0.306$
σ_X	ς_X	σ_Y	ς_Y
$\sqrt{1 - \frac{11}{25}\sqrt{5}} \approx 0.127$	$\frac{207-92\sqrt{5}}{25} \approx 0.051$	$\sqrt{\frac{24\sqrt{5}}{25} - 2} \approx 0.383$	$\frac{23\sqrt{5}-53}{25} \approx -0.063$

Proof. Since both $f(z,t)$ and $g(z,t)$ are of rational form, the proof follows from standard Quasi-Power arguments; see [2, 10] or [6, §IX.6]. The idea is as follows. Let $t \neq 0$ and $\rho_j(t)$ denote the three zeros of the denominator $1 - 2tz^2 - tz^3$ of $f(z,t)$, $j = 1, 2, 3$. Explicit expressions for $\rho_j(t)$

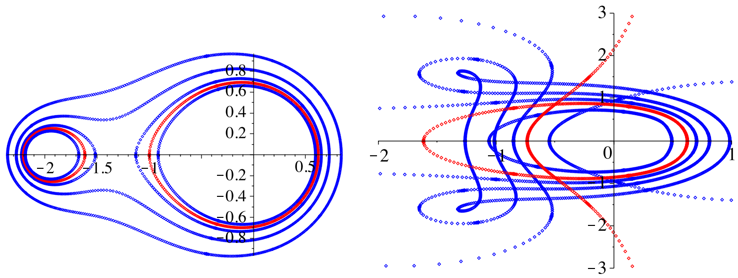


Figure 5: *Distribution of the three zeros of the denominator of* $f(z,t)$ *(left) and* $g(z,t)$ *(right): plotted are the curves* $\rho_j(re^{i\vartheta})$ *for* $-\pi \leqslant \vartheta \leqslant \pi$ *and* $r = 0.5, 0.7, 0.9, 1, 1.1$ *(left) and* $r = 0.4, 0.6, 0.8, 1, 1.5$ *(right). The red curves correspond to* $r = 1$.

are available by classical means but they are messy. We are mainly interested in the behaviors of $\rho_j(t)$ when t lies in a neighborhood of unity. In particular, when $t = 1$, the three zeros are $\varphi^{-1}, -\varphi$ and -1. Assume $\rho_1(1) = \varphi^{-1}$. When t varies in a neighborhood of unity, the zero $\rho_j(t)$, as a function of t, varies smoothly near $\rho_j(1)$; see Figure 5.

We then deduce, by direct partial fraction decomposition, the identity

$$[z^n]f(z,t) = F_n\mathbb{E}(t^{X_n}) = \sum_{1\leqslant j\leqslant 3} R_j(t)\rho_j(t)^{-n}, \tag{8}$$

where

$$R_j(t) := -\frac{1+2t\rho_j(t)+t\rho_j(t)^2}{3-10t\rho_j(t)^2}.$$

This is an identity for all $t \neq 0$ and $n \geqslant 1$. In particular, we have the Quasi-Power Approximation

$$\mathbb{E}\left(e^{X_n s}\right) = \exp\big(\alpha(s)n + \beta(s)\big)\left(1 + O\left((\varphi-\varepsilon)^{-n}\right)\right),$$

where $\varepsilon > 0$ and

$$\alpha(s) := -\log\frac{\rho_1(e^s)}{\rho_1(1)}, \quad \text{and} \quad \beta(s) := \log\frac{R_1(e^s)}{R_1(1)}.$$

The central limit theorem with convergence rate then results from applying the Quasi-Power Theorem; see [6] or [10]. The first two terms of the approximations (7) are obtained by the Taylor expansions

$$\begin{aligned}\alpha(s) &= \mu_X s + \frac{\sigma_X^2}{2}s^2 + O(|s|^3),\\ \beta(s) &= \nu_X s + \frac{\varsigma_X^2}{2}s^2 + O(|s|^3),\end{aligned}$$

as $s \sim 0$, the justification being also part of the Quasi-Power Theorem. The exponential error terms in (7) are worked out by a direct approach: taking derivatives with respective to t, substituting $t = 1$ and then computing the asymptotics of the coefficient of z^n; details are straightforward and omitted here.

The calculations for Y_n are similar, but with one significant difference: the three zeros of the denominator of $g(z,t)$ approach $\varphi^{-1}, -\varphi$ and ∞ as $t \to 1$; see Figure 5. However, this does not change the asymptotic behaviors we are looking for. ■

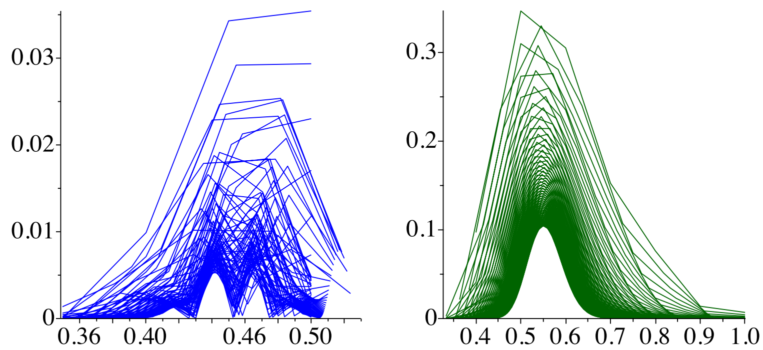


Figure 6: *The histograms of* X_n *and* Y_n *(normalized in the unit interval):* $\left|\mathbb{P}(X_n - k) - \frac{e^{-\frac{(k-\mathbb{E}(X_n))^2}{2\mathbb{V}(X_n)}}}{\sqrt{2\pi\mathbb{V}(X_n)}}\right|$ *(left; see (15)) and* $\mathbb{P}(Y_n = k)$ *for* $n = 10, \dots, 100$.

Note that there is a simplification for the leading term in the asymptotic approximation of $\mathbb{E}(X_n) + \mathbb{E}(Y_n)$

$$\begin{aligned}\mathbb{E}(X_n) + \mathbb{E}(Y_n) &= \frac{nF_n + F_{n-1} - (-1)^n}{F_n} \\ &= n + \varphi - 1 + O\left(\varphi^{-n}\right).\end{aligned}$$

In addition to the simple zig-zag chain with $r_1 = \cdots = r_k = 0$, we can also extend the same study to more general hexagonal chains with $r_1 = \cdots = r_k = r$ ($r \geqslant 1$) and $0 \leqslant r_{k+1} \leqslant r$. We are then led to a system of algebraic equations, and the same set of tools for asymptotic analysis and limit distributions can be extended.

4 Forcing and anti-forcing polynomials of hexagonal crowns

In this section, we consider hexagonal crowns $\mathscr{C}_n$ ($n \geqslant 3$), which are circular versions of spiral hexagonal chains. More precisely, a hexagonal crown is a planar graph obtained by gluing the first and the last hexagons of a spiral hexagonal chain G of length n with $S(G) = (2, 2, \dots, 2)$ such that the exterior face is bounded by a $3n$-cycle. Two typical examples are shown in Figure 7: the molecular graphs of corannulene and coronene, which are $\mathscr{C}_5$ and $\mathscr{C}_6$, respectively.

By similar arguments to those used for hexagonal chains, we can prove that the forcing polynomials $f(\mathscr{C}_n, t)$ of hexagonal crowns satisfy the following relations. For $n \geqslant 3$,

$$f(\mathscr{C}_n, t) = \phi_n(t) + \begin{cases} t^{\lceil \frac{n}{2} \rceil}, & \text{if } n \text{ is odd,} \\ 2t^2 - t^{\lceil \frac{n}{2} \rceil}, & \text{if } n \text{ is even,} \end{cases}$$

where

$$\phi_n(t) = \begin{cases} 3, & \text{if } n = 0, \\ 0, & \text{if } n = 1, \\ 4t, & \text{if } n = 2, \\ 2t\phi_{n-2}(t) + t\phi_{n-3}(t), & \text{if } n \geqslant 3. \end{cases}$$

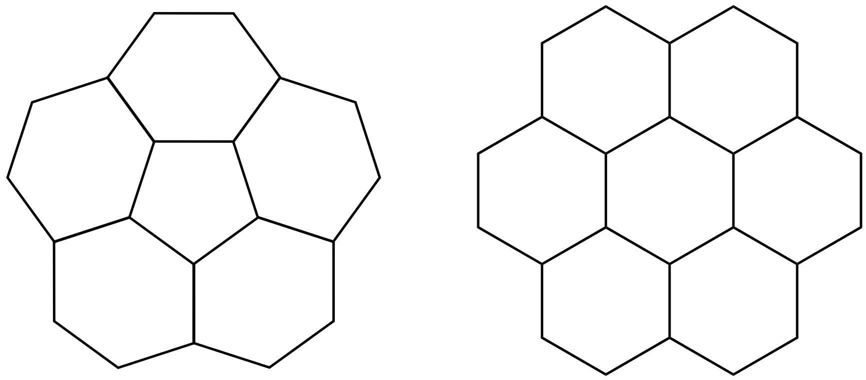


Figure 7: *Two hexagonal crowns: $\mathscr{C}_5$ and $\mathscr{C}_6$.*

(The initial values are defined for $n < 3$ solely for technical convenience.) Similarly, the anti-forcing polynomials $g(\mathscr{C}_n, t)$ satisfy

$$g(\mathscr{C}_n, t) = \psi_n(t) + \begin{cases} 0, & \text{if } n \text{ is odd,} \\ 2t^2 + 2t^{\frac{n}{2}-1}(t-1), & \text{if } n \text{ is even,} \end{cases}$$

for $n \geqslant 3$, where

$$\psi_n(t) = \begin{cases} 3, & \text{if } n = 0, \\ t, & \text{if } n = 1, \\ 2t + t^2, & \text{if } n = 2, \\ t\psi_{n-1}(t) + t\psi_{n-2}(t) + (t - t^2)\psi_{n-3}(t), & \text{if } n \geqslant 3. \end{cases} \tag{9}$$

The corresponding bivariate generating function $f^{[c]}(z,t) := \sum_{n \geqslant 3} f(\mathscr{C}_n, t) z^n$ now has the form

$$f^{[c]}(z,t) = \frac{3 - 2tz^2}{1 - 2tz^2 - tz^3} - \frac{1 - tz}{1 - tz^2} + \frac{2t^2}{1 - z^2} - 2 - 2t^2 - tz - (3t + 2t^2)z^2; \tag{10}$$

and, similarly, $g^{[c]}(z,t) := \sum_{n \geqslant 3} g(\mathscr{C}_n, t) z^n$ satisfies

$$g^{[c]}(z,t) = \frac{3 - 2tz - tz^2}{1 - tz - tz^2 - t(1-t)z^3} + \frac{2t^2}{1 - z^2} + \frac{2(t-1)}{1 - tz^2} - (1 + 2t + 2t^2) - tz - 5t^2z^2. \tag{11}$$

Alternatively, these two rational forms for $f^{[c]}(z,t)$ and $g^{[c]}(z,t)$ can be proved along a different line by enumerating directly the number of perfect matchings with a given forcing and anti-forcing numbers.

Theorem 4.1. *For $n \geqslant 3$*

$$f(\mathscr{C}_n, t) = n \sum_{1 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor} \binom{k}{3k - n} \frac{2^{3k-n}}{k} t^k - (-1)^n t^{\lceil \frac{n}{2} \rceil} + 2t^2 \cdot \mathbb{1}_{n \, even}, \tag{12}$$

and

$$g(\mathscr{C}_n,t) = n\sum_{0\leqslant k\leqslant n} t^k \sum_{r\geqslant 1}\binom{r}{n-k-r}\binom{n-1-2r}{k-r}\frac{1}{r} + t^n + \left(2t^2+2t^{\lfloor\frac{n}{2}\rfloor+1}\right)\cdot \mathbb{1}_{n \text{ even}} \qquad (13)$$

The first few terms of f and g are given as follows.

n	$f(\mathscr{C}_n,t)$	$g(\mathscr{C}_n,t)$
3	$3t+t^2$	$3t+t^3$
4	$9t^2$	$6t^2+2t^3+t^4$
5	$10t^2+t^3$	$5t^2+5t^3+t^5$
6	$5t^2+15t^3$	$5t^2+6t^3+8t^4+t^6$
7	$28t^3+t^4$	$14t^3+7t^4+7t^5+t^7$
8	$2t^2+16t^3+31t^4$	$2t^2+8t^3+20t^4+10t^5+8t^6+t^8$

The proofs are somewhat tedious and will be given in Appendix. Of course, Theorem 4.1 can also be proved by expanding (10) and (11).

The total number of perfect matchings is given by

$$\begin{aligned} L_n &:= [z^n]f^{[c]}(z,1) = [z^n]g^{[c]}(z,1) \\ &= \frac{2-z}{1-z-z^2} + \frac{2}{1-z^2} - 4 - z - 5z^2 \\ &= \varphi^n + (-\varphi)^{-n} + 1 + (-1)^n \qquad (n\geqslant 3), \end{aligned}$$

which are related to the Lucas numbers (A068397 in Sloane's OEIS) and equal $F_n+F_{n-2}+2\cdot\mathbb{1}_{n\text{ even}}$. These numbers also enumerate perfect matchings in the graph $C_n\times P_2$ (C_n being the cycle graph on n vertices and P_2 being the path graph on two vertices); see OEIS's A102081.

Assume that all L_n perfect matchings on hexagonal crowns of length n are equally likely. Let $X_n^{[c]}$ ($Y_n^{[c]}$) denote the forcing number (anti-forcing number) of a random perfect matching.

Theorem 4.2. *The distributions of the forcing and anti-forcing numbers of random perfect matchings on hexagonal crowns are asymptotically normal:* $W^{[c]}\in\{X^{[c]},Y^{[c]}\}$

$$\sup_{x\in\mathbb{R}}\left|\mathbb{P}\left(\frac{W_n^{[c]}-\mu_W n}{\sigma_W\sqrt{n}}\leqslant x\right)-\Phi(x)\right| = O\left(n^{-1/2}\right),$$

with linear mean and linear variance

$$\begin{aligned} \mathbb{E}(W_n^{[c]}) &= \mu_W n + O\left(n\varphi^{-n}\right), \\ \mathbb{V}(W_n^{[c]}) &= \sigma_W^2 n + O\left(n\varphi^{-n}\right), \end{aligned} \qquad (14)$$

the constant terms being both zero. The constants μ_W and σ_W are the same as in Theorem 3.2.

Note specially that

$$[z^n]f^{[c]}(z,t) = \sum_{1\leqslant j\leqslant 3}\rho_j(t)^{-n} - (-1)^n t^{\lceil\frac{n}{2}\rceil} + 2t^2\cdot\mathbb{1}_{n\text{ even}} \qquad (n\geqslant 3),$$

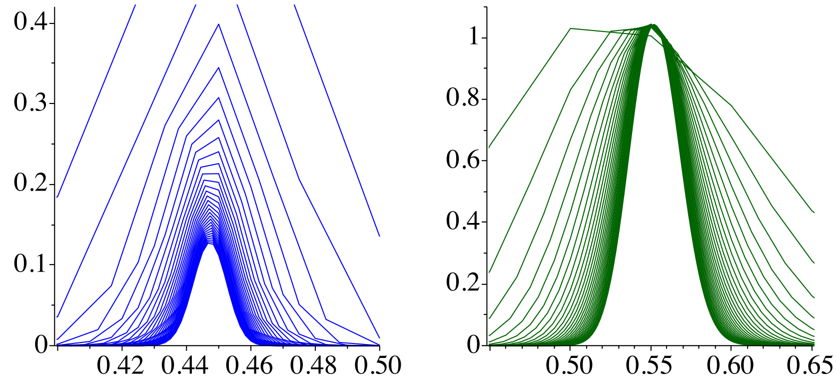


Figure 8: *The histograms of* $X_n^{[c]}$ *and* $Y_n^{[c]}$ *(normalized in the unit interval) for* $n = 20, 40, 60, \cdots, 600$*; the histograms in the right figure are normalized by a factor of* $\sqrt{n}$*.*

where the $\rho_j(t)$'s represent the three zeros of $1-2t^2-tz^3$; cf. (8). The coefficient functions $R_j(t)$ in (8) are all identically 1 here. The same relation holds for the decomposition of $g^{[c]}(z,t)$. These imply that the constant terms in (14) are both zero (cf. (7)), reflecting a better "balancing" property for the forcing and anti-forcing numbers on hexagonal crowns. Numerically, the single term in each of the equation on the right-hand side of (14) provides a very good approximation for small and moderate values of n; see the following table for some instances.

n	$\lvert\mathbb{E}(X_n^{[c]}) - \mu_X n\rvert <$	$\lvert\mathbb{E}(Y_n^{[c]}) - \mu_Y n\rvert <$	$\lvert\mathbb{V}(X_n^{[c]}) - \sigma_X^2 n\rvert <$	$\lvert\mathbb{V}(Y_n^{[c]}) - \sigma_Y^2 n\rvert <$
20	0.00026	0.0011	0.0117	0.0104
30	4.3×10^{-6}	1.5×10^{-5}	2.6×10^{-4}	2.3×10^{-4}
50	5.6×10^{-10}	1.8×10^{-9}	5.3×10^{-8}	4.6×10^{-8}
100	4.5×10^{-20}	1.4×10^{-19}	8.2×10^{-18}	7.2×10^{-18}

Also

$$\mathbb{E}(X_n^{[c]} + Y_n^{[c]}) = n - \frac{n\left(1+\frac{(-1)^n}{2}\right) - \frac{21}{4} - \frac{19}{4}(-1)^n}{L_n},$$

the second-order term on the right-hand side being exponentially small.

The central limit theorems we derived in this paper for forcing and anti-forcing numbers can be enhanced by the corresponding local limit theorems of the form

$$\sup_{x\in\mathbb{R}} \left| \mathbb{P}\left(W_n = \lfloor \mu_W n + x\sigma_W\sqrt{n} \rfloor\right) - \frac{e^{-x^2/2}}{\sqrt{2\pi n}\,\sigma_W} \right| = O\left(n^{-1}\right), \tag{15}$$

where $W \in \{X, Y, X^{[c]}, Y^{[c]}\}$. This can be proved in at least two ways: one via the standard Fourier arguments using the Quasi-power approximations (see [6, §IX.9]), and the other relies directly on the exact forms (12) and (13) using elementary asymptotic approximations.

Acknowledgments

The work of Y.N. Yeh was partially supported by Ministry of Science and Technology under the Grant 101-2115-M-001-013-MY3. The work of H. Zhang was partially supported by NSFC under

the Grant 11371180.

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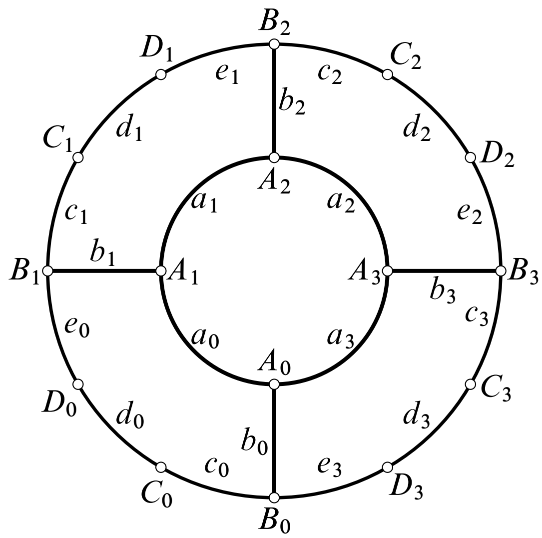

Figure 9: $\mathscr{C}_4$

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Appendix. Forcing and anti-forcing polynomials of hexagonal crowns: a direct enumerative proof

We prove Theorem 4.1 in this Appendix. The method of proof we use here relies on a direct combinatorial enumeration of the number of perfect matchings with a given forcing number or anti-forcing number. While the arguments may be less general than the recursive decompositions we used above, the analysis provides a deeper understanding of the structure of perfect matchings.

4.1 A characterization of perfect matchings

Denote the vertices of $\mathscr{C}_n$ by $\{A_i, B_i, C_i, D_i \mid i \in \mathbb{Z}_n\}$ and the edges by $\{a_i, b_i, c_i, d_i, e_i \mid i \in \mathbb{Z}_n\}$; see Figure 9.

Recall that L_n denote the total number of perfect matchings of a hexagonal crown of length n, which starts with $L_1 = 1$, $L_2 = 5$, and satisfies the Fibonacci type recurrence $L_n = L_{n-1} + L_{n-2} - 2 \cdot \mathbb{1}_{n \text{ odd}}$ for $n \geqslant 3$. On the other hand, the Lucas numbers ℓ_n are related to L_n by $\ell_n = L_n - 1 - (-1)^n$ and satisfies the recurrence $\ell_n = \ell_{n-1} + \ell_{n-2}$ for $n \geqslant 3$ with $\ell_1 = 1$ and $\ell_2 = 3$.

It is known that (see [9]) the number of perfect matchings on the cyclic ladder graph $C_n \times P_2$ equals L_n. Let $V(C_n \times P_2) = \{A'_i, B'_i \mid i \in \mathbb{Z}_n\}$ denote the vertex set and $E(C_n \times P_2) = \{A'_i B'_i, A'_i A'_{i+1}, B'_i B'_{i+1} \mid i \in \mathbb{Z}_n\}$ denote the edge set.

Lemma 4.3. *For $n \geqslant 3$, $|P(\mathscr{C}_n)| = L_n$.*

Proof. Define the mapping $\tau : P(C_n \times P_2) \to P(\mathscr{C}_n)$ as follows. Given $M \in P(C_n \times P_2)$, let

$$\begin{aligned}\tau(M) = &\{a_i \mid A'_i A'_{i+1} \in M \text{ for } i \in \mathbb{Z}_n\} \cup \{b_i \mid A'_i B'_i \in M \text{ for } i \in \mathbb{Z}_n\} \\ &\cup \{c_i,\ e_i \mid B'_i B'_{i+1} \in M \text{ for } i \in \mathbb{Z}_n\} \cup \{d_i \mid B'_i B'_{i+1} \notin M \text{ for } i \in \mathbb{Z}_n\}.\end{aligned}$$

It is easy to check that $\tau(M)$ is a perfect matching on $\mathscr{C}_n$, and τ is injective. For any given perfect matching $M' \in P(\mathscr{C}_n)$, we see that M' contains either both of c_i and e_i or only d_i for each $i \in \mathbb{Z}_n$. Replacing each pair of edges $\{c_i, e_i\}$ in M' by $B'_i B'_{i+1}$, each a_i by $A'_i A'_{i+1}$, each b_i by $A'_i B'_i$, and deleting all d_j's, we get a perfect matching $M \in P(C_n \times P_2)$ such that $\tau(M) = M'$. Thus τ is a bijection. This completes the proof. ■

Let M_0 denote the perfect matching $\{b_i, d_i \mid i \in \mathbb{Z}_n\}$ of $\mathscr{C}_n$ and H_i denote the hexagon with edge set $\{a_i, b_i, c_i, d_i, e_i, b_{i+1}\}$. It is well-known that if C is an M-alternating cycle of a graph G, then the symmetric difference $M \oplus E(C)$ is another perfect matching on G. Consider a sequence $S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1$ such that $i_j \in \mathbb{Z}_n$ and $i_{j+1} - i_j \neq 1$ for $j \in \mathbb{Z}_s$ (the order "$\leqslant$" is induced by their natural ordering as integers, $i_s = i_0 = i_0 + n$ and $i_0 - i_{s-1} \neq 1$). Then

$$M_S := M_0 \oplus H_{i_0} \oplus H_{i_1} \oplus \cdots \oplus H_{i_{s-1}}$$

is a perfect matching on $\mathscr{C}_n$. Note that if S is empty then $M_S = M_0$, and if $S \neq S'$, then $M_S \neq M_{S'}$. For such a sequence S, if each i_j corresponds to an edge $i_j(i_j + 1)$ in the cycle $(0, 1, \ldots, n-1)$, then S corresponds to a matching on the cycle and this is a bijection. Since the number of matchings in n-cycle is the Lucas number ℓ_n, we have

$$\left|\{S \mid S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1, i_{j+1} - i_j \neq 1 \text{ for } j \in \mathbb{Z}_s\}\right| = \ell_n.$$

Moreover, we can determine all the perfect matchings of $\mathscr{C}_n$; see Figure 10 for an illustration.

Lemma 4.4. *If n is odd, then*

$$P(\mathscr{C}_n) = \{M_S \mid S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1,\ i_{j+1} - i_j \neq 1 \text{ for } j \in \mathbb{Z}_s\}.$$

If n is even, then

$$P(\mathscr{C}_n) = \{M_S \mid S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1,\ i_{j+1} - i_j \neq 1 \text{ for } j \in \mathbb{Z}_s\} \cup \{M_1, M_2\},$$

where $M_1 = \{a_{2i}, d_{2i}, c_{2i+1}, e_{2i+1} \mid i = 0, 1, \ldots, \frac{n}{2} - 1\}$, $M_2 = \{a_{2i+1}, d_{2i+1}, c_{2i}, e_{2i} \mid i = 0, 1, \ldots, \frac{n}{2} - 1\}$.

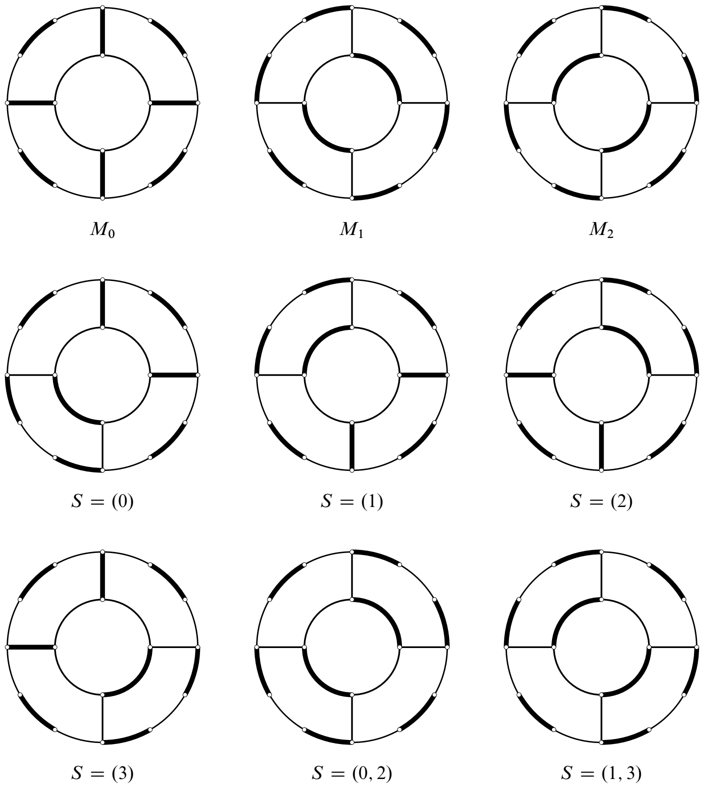

Figure 10: $\mathscr{C}_4$: *The perfect matchings are drawn with bold lines.*

Proof. From the above discussions, we see that

$$\begin{aligned}&\left|\{M_S \mid S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1,\ i_{j+1} - i_j \neq 1 \text{ for } j \in \mathbb{Z}_s\}\right| \\ &\quad= \left|\{S \mid S : 0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1 \mid i_{j+1} - i_j \neq 1 \text{ for } j \in \mathbb{Z}_s\}\right| \\ &\quad= \ell_n.\end{aligned}$$

Since $|\{a_i, d_i\} \cap M_S| = 1$ for $i \in \mathbb{Z}_n$, M_1 and M_2 are both different from M_S for any S, and the proof follows from Lemma 4.3. ∎

4.2 Forcing polynomials

We prove (12) in this subsection by computing the quantity f_k, which equals the number of perfect matchings on $\mathscr{C}_n$ with forcing number k.

By Lemma 2.2 $f(G, M)$, the forcing number of M is at least the maximum number of disjoint M-alternating cycles of G, and if G is a planar bipartite graph, then $f(G, M)$ equals the maximum number of disjoint M-alternating cycles of G; see [14].

When n is even, for the perfect matchings M_1 and M_2 on $\mathscr{C}_n$ (defined in Lemma 4.4), it is straightforward to verify that $\{a_0, d_0\}$ and $\{a_1, d_1\}$ are forcing set of M_1 and M_2, respectively. Since $(a_0, a_1, \ldots, a_{n-1})$ and $(c_0, d_0, e_0, c_1, d_1, \ldots, e_{n-1})$ are disjoint and M_1- and M_2-alternating cycles, by Lemma 2.2, we have

$$f(\mathscr{C}_n, M_1) = f(\mathscr{C}_n, M_2) = 2.$$

To compute f_k, we count the quantities $f_{k,s}$, which represent the number of perfect matchings M_S on $\mathscr{C}_n$ such that the sequence S has s entries and $f(\mathscr{C}_n, M_S) = k$. With these quantities, we then sum over all s and obtain f_k

$$f_k = \begin{cases} \sum\limits_{0 \leqslant s \leqslant \lfloor \frac{n}{2} \rfloor} f_{k,s}, & \text{if } k \neq 2, \\ \sum\limits_{0 \leqslant s \leqslant \lfloor \frac{n}{2} \rfloor} f_{k,s} + (-1)^n + 1, & \text{if } k = 2. \end{cases} \tag{16}$$

For the empty sequence S, $M_S = M_0$. Since $H_0, H_2, \ldots, H_{2\lfloor \frac{n}{2} \rfloor - 2}$ are disjoint M_0-alternating cycles of $\mathscr{C}_n$, by Lemma 2.2, we have $f(\mathscr{C}_n, M_0) \geqslant \lfloor \frac{n}{2} \rfloor$. If n is even, it is straightforward to verify that $\{b_0, b_2, \ldots, b_{n-2}\}$ is a forcing set of M_0. In this case, $f(\mathscr{C}_n, M_0) = \frac{n}{2}$. If n is odd, then $\{b_0, b_2, \ldots, b_{n-1}\}$ is a forcing set of M_0. Suppose there exists a forcing set $\mathscr{I}$ of M_0 with less than $\frac{n+1}{2}$ edges, then there exists an integer $v \in \mathbb{Z}_n$, such that $H_v \cap \mathscr{I} = \emptyset$, a contradiction to Lemma 2.2. Thus $f(\mathscr{C}_n, M_0) = \frac{n+1}{2}$, and it follows that, for an arbitrary $n \geqslant 3$,

$$f(\mathscr{C}_n, M_0) = \lceil \tfrac{n}{2} \rceil .$$

Let now S be a nonempty sequence. Since $H_{i_0}, H_{i_1}, \ldots, H_{i_{s-1}}$ are disjoint M_S-alternating cycles, by Lemma 2.2, we have

$$f(\mathscr{C}_n, M_S) \geqslant s.$$

Let $\Omega_S = \{i_j \mid i_j \in S,\ i_{j+1} - i_j \equiv 1 \pmod 2\}$.

Lemma 4.5. *For $s > 0$, let S be a sequence $0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1$ such that $i_{j+1} - i_j \neq 1$ for $j \in \mathbb{Z}_s$. Then $f(\mathscr{C}_n, M_S) = \frac{1}{2}(n - |\Omega_S|)$.*

Proof. Assume that n is even and $S = (0, 2, \ldots, n-2)$. Let $\mathscr{I} := \{a_0, e_2, e_4, \ldots, e_{n-2}\}$. We see that $\mathscr{I}$ is a forcing set of M_S. Thus $f(\mathscr{C}_n, M_S) \leqslant \frac{n}{2}$. Moreover, the hexagons $H_0, H_2, \ldots, H_{n-2}$ are disjoint and M_S-alternating by Lemma 2.2, and the forcing number of M_S is at least $\frac{n}{2}$. Accordingly, $f(\mathscr{C}_n, M_S) = \frac{n}{2}$. The proof for the other case when n is even and $S = (1, 3, \ldots, n-1)$ is similar.

For the remaining cases, let

$$\mathscr{I} = \bigcup_{i_{j+1} - i_j = 2} \{e_{i_j}\} \bigcup_{\substack{i_{j+1} - i_j \neq 2 \\ i_{j+1} - i_j \equiv 0 \pmod 2}} \{e_{i_j}, d_{i_j+2}, b_{i_j+4}, b_{i_j+6}, \ldots, b_{i_{j+1}-2}\}$$
$$\bigcup_{i_{j+1} - i_j \equiv 1 \pmod 2} \{e_{i_j}, b_{i_j+3}, b_{i_j+5}, \ldots, b_{i_{j+1}-2}\}.$$

We have $|\mathscr{I}| = \frac{1}{2}(n - |\Omega_S|)$, and we prove that $\mathscr{I}$ is a forcing set of M_S. As shown in Figure 11, for each pair of edges $(x_i, y_j) \in \{(x_i, y_j) \mid x, y \in \{b, d, e\}, x_i \in \mathscr{I}, y_j \in \mathscr{I}, j - i \equiv 2 \text{ or } 3 \pmod n\}$, any edge of $H_i, H_{i+1}, \ldots, H_j$ is forced to be in or not in M_S by x_i and y_j except for the edges $a_i, a_{i+1}, \ldots, a_j$ (the case marked (1) in Figure 11). Since there exists at least one pair of edges (x_k, y_l) in $\mathscr{I}$ that is not of case (1) (otherwise, $M_S = M_1$ or M_2), we can determine first $a_k, a_{k+1}, \ldots, a_l$, and then $a_i, a_{i+1}, \ldots, a_j$ of case (1) step by step. Therefore, $\mathscr{I}$ is a forcing set of M_S, and

$$f(\mathscr{C}_n, M_S) \leqslant \tfrac{1}{2}(n - |\Omega_S|).$$

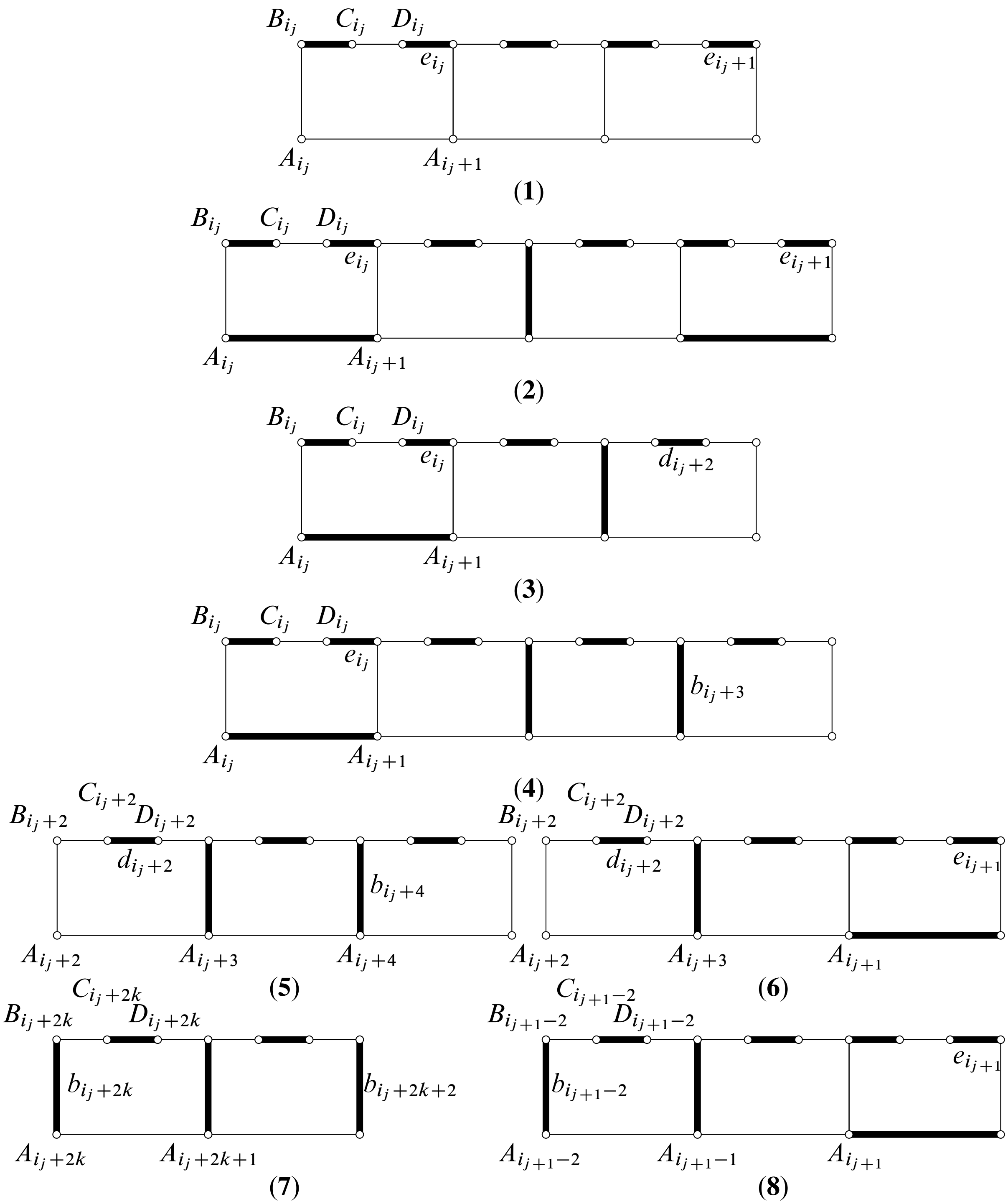

Figure 11: *The edges drawn by bold lines are forced in M_S by the edges labeled in the graphs.*

Moreover, the hexagons $\{H_i \mid |\{a_i, b_i, c_i, d_i, e_i\} \cap \mathscr{I}| = 1\}$ are disjoint M_S-alternating cycles. Thus, by Lemma 2.2,

$$f(\mathscr{C}_n, M_S) \geqslant |\{H_i \mid |\{a_i, b_i, c_i, d_i, e_i\} \cap \mathscr{I}| = 1\}| = \tfrac{1}{2}(n - |\Omega_S|).$$

See Figure 12 for an illustration. This completes the proof. ■

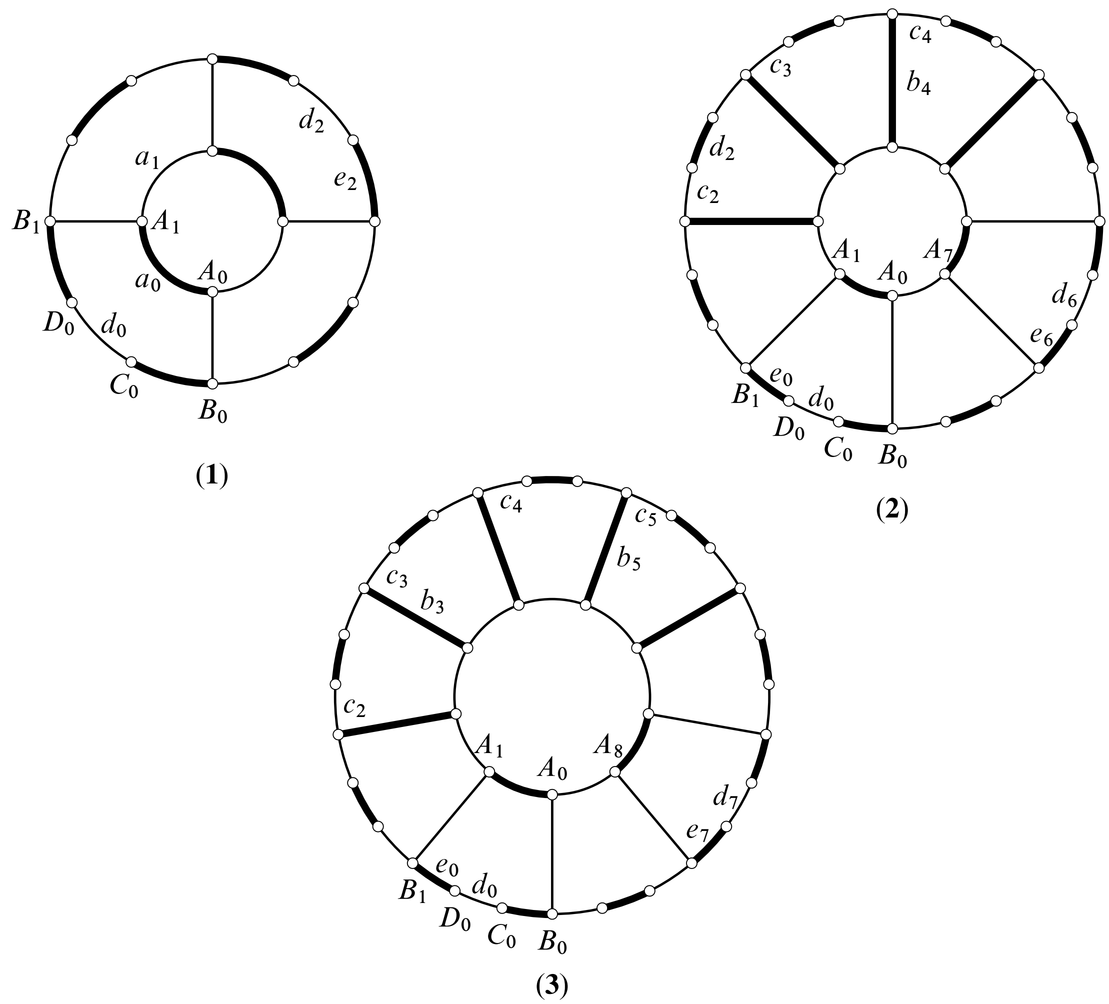

Figure 12: (1). $S = (0, 2)$, $\mathscr{I} = \{a_0, e_2\}$, $f(\mathscr{C}_4, M_S) = 2$; $\mathscr{I}' = \{a_1, d_0, d_2\}$, $g(\mathscr{C}_4, M_S) = 3$. (2). $S = (0, 6)$, $\mathscr{I} = \{e_0, d_2, b_4, e_6\}$, $f(\mathscr{C}_8, M_S) = 4$; $\mathscr{I}' = \{d_0, c_2, c_3, c_4, d_6\}$, $g(\mathscr{C}_8, M_S) = 5$. (3). $S = (0, 7)$, $\mathscr{I} = \{e_0, b_3, b_5, e_7\}$, $f(\mathscr{C}_9, M_S) = 4$; $\mathscr{I}' = \{d_0, c_2, c_3, c_4, c_5, d_7\}$, $g(\mathscr{C}_9, M_S) = 6$.

From the above discussions, we see that $1 \leqslant f(\mathscr{C}_n, M_S) \leqslant \lceil \frac{n}{2} \rceil$ for any perfect matching M on $\mathscr{C}_n$. Hence, the forcing polynomial can be decomposed as

$$f(\mathscr{C}_n, t) = \sum_{1 \leqslant k \leqslant \lceil \frac{n}{2} \rceil} f_k t^k.$$

Recall that f_k is the number of perfect matchings on $\mathscr{C}_n$ with forcing number k and $f_{k,s}$ is the number of perfect matchings M_S of $\mathscr{C}_n$ such that the sequence S has s entries and $f(\mathscr{C}_n, M_S) = k$. Then $k = f(\mathscr{C}_n, M_S) \geqslant s$. Moreover, by Lemma 4.5, $s \geqslant |\Omega_S| = n - 2k$ for $s \neq 0$. Then we obtain the decomposition (16). We now compute $f_{k,s}$.

Lemma 4.6. *If $s \neq 0$, then $f_{k,s} = \frac{n}{k}\binom{k}{n-2k, s+2k-n, k-s}$; if $s = 0$, then $f_{k,0} = \mathbb{1}_{k=\lceil \frac{n}{2} \rceil}$.*

Proof. The method of proof is similar to that used by Moser and Abramson in [13]. For each S: $0 \leqslant i_0 < i_1 < \cdots < i_{s-1} \leqslant n-1$ with $i_{j+1} - i_j \neq 1$ for $j \in \mathbb{Z}_S$ such that $k = \frac{1}{2}(n - |\Omega_S|)$, M_S corresponds to an arrangement of s 1's and $n-s$ 0's in a circle with one of the n entries marked by an asterisk, which we denote by ε_0, and which is followed by $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_{n-1}$ (reading off clockwise), where

$$\varepsilon_i = \begin{cases} 1, & \text{if } i = i_0, i_1, \ldots, i_{s-1}, \\ 0, & \text{otherwise.} \end{cases}$$

The s 1's determine s cells.

Now we count such arrangements. Let $u = \frac{1}{2}(n - 2s - |\Omega_S|)$. We construct the arrangements by the following steps.

- Place s 1's in a circle, forming s cells. Color one cell so that the cells are distinguishable;
- Distribute u groups of two 0's each into the s cells in $\binom{u+s-1}{s-1}$ ways;
- Choose $|\Omega_S|$ cells, and put one 0 into each in $\binom{s}{|\Omega_S|}$ ways;
- Put one 0 into each cell;
- Mark one term, there are n choices.

There are in total $n\binom{u+s-1}{s-1}\binom{s}{|\Omega_S|}$ circular-asterisked-colored arrangements. If we remove the color, then these arrangements fall into sets of s each that are identical by rotation. Then

$$f_{k,s} = \frac{n}{s}\binom{u+s-1}{s-1}\binom{s}{|\Omega_S|} = \frac{n}{k}\binom{k}{n-2k, s+2k-n, k-s}.$$

If $s = 0$, then $k = f(\mathscr{C}_n, M_0) = \lceil \frac{n}{2} \rceil$. ■

Proof of Theorem 4.1, forcing polynomials (12). Assume that n is odd. Then $f_{\frac{n+1}{2},s} = 0$ for $s \neq 0$. Also, by Lemma 4.6,

$$\begin{aligned} f(\mathscr{C}_n, t) &= \sum_{1 \leqslant k \leqslant \frac{n+1}{2}} f_k t^k = \sum_{1 \leqslant k \leqslant \frac{n+1}{2}} t^k \sum_{n-2k \leqslant s \leqslant k} f_{k,s} \\ &= t^{\frac{n+1}{2}} + n \sum_{1 \leqslant k \leqslant \frac{n-1}{2}} \frac{k!}{k(n-2k)!} t^k \sum_{n-2k \leqslant s \leqslant k} \frac{1}{(s+2k-n)!(k-s)!}, \end{aligned}$$

which leads to (12). The proof for the case when n is even is similar. ■

From the closed-form (12), it is easy to derive the rational form (10) for the bivariate generating function $f^{[c]}(z,t)$ by using the following relations. First,

$$f_0(z,t) := \sum_{n\geqslant 0} z^n \sum_{k\geqslant 1} \binom{k}{3k-n} \frac{2^{3k-n}}{k} t^k = \log \frac{1}{1-tz^2(2+z)}.$$

Then

$$\sum_{n\geqslant 0} nz^n \sum_{k\geqslant 1} \binom{k}{3k-n} \frac{2^{3k-n}}{k} t^k = z\frac{\partial}{\partial z} f_0(z,t) = \frac{3-2tz^2}{1-2tz^2-tz^3} - 3,$$

and (10) follows from subtracting the first few terms.

4.3 Anti-forcing polynomials

We prove the exact form (13) for anti-forcing polynomials by an argument similar to that used for proving (12).

Define $\Omega'_S = \{i_j \mid i_j \in S, i_{j+1} - i_j \notin \{1,2\}\}$.

Lemma 4.7. *If $s=0$, then $g(\mathscr{C}_n, M_0) = n$; if $s=1$, then $g(\mathscr{C}_n, M_S) = n-2$; if $n=2s$, then $g(\mathscr{C}_n, M_S) = \frac{n}{2}+1$; for other values of n,*

$$g(\mathscr{C}_n, M_S) = n - s - \left|\Omega'_S\right|. \tag{17}$$

Proof. If $s=0$, then $\{c_0, c_1, \ldots, c_{n-1}\}$ is an anti-forcing set of M_0. Also $\{H_0, H_1, \ldots, H_{n-1}\}$ is a compatible M_0-alternating set of $\mathscr{C}_n$. Thus, by Corollary 2.5, $g(\mathscr{C}_n, M_0) = n$.

If $s=1$, say $S=(i)$, $i\in\mathbb{Z}_n$, then $\{d_i, c_{i+2}, c_{i+3}\ldots, c_{i+n-2}\}$ is an anti-forcing set of M_S, and $\{H_i, H_{i+2}, H_{i+3}, \ldots, H_{i+n-2}\}$ is a compatible M_S-alternating set of $\mathscr{C}_n$. Again, by Corollary 2.5, $g(\mathscr{C}_n, M_S) = n-2$.

Assume now $s>1$. Consider first the case when n is even and $S=(0,2,4,\ldots,n-2)$. Let $\mathscr{I}' = \{a_1, d_0, d_2, \ldots, d_{n-2}\}$. Then $\mathscr{I}'$ is an anti-forcing set of S and $|\mathscr{I}'| = \frac{n}{2}+1$. Since $\{(a_0, a_1, \ldots, a_{n-1}), H_0, H_2, \ldots, H_{n-2}\}$ is a compatible M_S-alternating set of $\mathscr{C}_n$ (whose cardinality is $\frac{n}{2}+1$), we have $g(\mathscr{C}_n, M_S) = \frac{n}{2}+1$ by Corollary 2.5. The case $S=(1,3,\ldots,n-1)$ is similar.

For other cases, let

$$\mathscr{I}' = \bigcup_{i_{j+1}-i_j=2} \{d_{i_j}\} \bigcup_{i_{j+1}-i_j\neq 2} \{d_{i_j}, c_{i_j+2}, c_{i_j+3}, \ldots, c_{i_{j+1}-2}\}.$$

Then $|\mathscr{I}'| = n-s-\left|\Omega'_S\right|$. Analogous to the proof of Lemma 4.5, we see that $\mathscr{I}'$ is an anti-forcing set of M_S. On the other hand, the set of hexagons $\{H_i \mid c_i \text{ or } d_i \in \mathscr{I}'\}$ is a compatible M_S-alternating set. Thus (17) follows from Corollary 2.5. See Figure 12 for illustrative examples. ■

Similarly, for the perfect matchings M_1 and M_2, it is straightforward to verify that $\{a_1, d_1\}$ and $\{a_0, d_0\}$ are anti-forcing sets of M_1 and M_2, respectively. Since the cycles $(a_0, a_1, \ldots, a_{n-1})$ and $(c_0, d_0, e_0, c_1, d_1, \ldots, e_{n-1})$ form a compatible M_1- and M_2-alternating set, we have $g(\mathscr{C}_n, M_1) = g(\mathscr{C}_n, M_2) = 2$ from Corollary 2.5.

Let now

$$g(\mathscr{C}_n,t)=\sum_{1\leqslant k\leqslant n} g_k t^k,$$

where the coefficient g_k represents the number of perfect matchings on $\mathscr{C}_n$ with anti-forcing number k. Let $g_{k,s}$ be the number of perfect matchings M_S of $\mathscr{C}_n$ such that the sequence S has s entries and $g(\mathscr{C}_n, M_S)=k$. Then

$$g_k=\begin{cases}\sum_{0\leqslant s\leqslant \lfloor \frac{n}{2}\rfloor} g_{k,s}, & \text{if } k\neq 2,\\ \sum_{0\leqslant s\leqslant \lfloor \frac{n}{2}\rfloor} g_{k,s}+(-1)^n+1, & \text{if } k=2.\end{cases}$$

Lemma 4.8. *The quantities $g_{k,s}$ satisfy $g_{k,0}=\mathbb{1}_{k=n}$, $g_{k,1}=n\cdot\mathbb{1}_{k=n-2}$,*

$$g_{k,s}=\frac{n}{s}\binom{s}{n-s-k}\binom{n-2s-1}{n-s-k-1},\qquad \left(2\leqslant s<\tfrac{n}{2}\right),$$

and $g_{k,s}=2\cdot\mathbb{1}_{k=\frac{n}{2}+1}$ when $n=2s$.

Sketch of proof. The proofs for the cases $s=0$, $s=1$ and $n=2s$ are immediate from Lemma 4.7. The method of proof for the remaining cases follows from the same idea used in Lemma 4.6, details being omitted here. ∎

Proof of Theorem 4.1, anti-forcing polynomials (13). By Lemma 4.8, if n is even, then

$$\begin{aligned}g(\mathscr{C}_n,t)&=\sum_{1\leqslant k\leqslant n} g_k t^k=2t^2+\sum_{1\leqslant k\leqslant n} t^k\sum_{0\leqslant s\leqslant \frac{n}{2}} g_{k,s}\\ &=2t^2+2t^{\frac{n}{2}+1}+t^n+n\sum_{1\leqslant k\leqslant n} t^k\sum_{1\leqslant s\leqslant \frac{n}{2}-1}\frac{1}{s}\binom{s}{n-s-k}\binom{n-2s-1}{k-s};\end{aligned}$$

The proof for the odd case is similar. This proves (13). ∎

Unlike $f^{[c]}(z,t)$, the passage from the closed-form expression (13) to (11) is less straightforward, so we sketch the major steps as follows. Consider first the sum

$$\begin{aligned}n\sum_{k\geqslant 0} t^k\sum_{s\geqslant 1}\frac{1}{s}\binom{s}{n-s-k}\binom{n-2s-1}{k-s}&=n\sum_{s\geqslant 1}\left(\frac{t^s}{s}[z^{n-2s}](1+z)^s(1+tz)^{n-2s-1}-\mathbb{1}_{n=2s}\right)\\ &=n[z^n](1+tz)^{n-1}\log\frac{1}{1-\frac{tz^2(1+z)}{(1+tz)^2}}-2t^{\frac{n}{2}}\mathbb{1}_{n\text{ is even}}\end{aligned}$$

Let $\Lambda(z):=\log\frac{1}{1-\frac{tz^2(1+z)}{(1+tz)^2}}$. Then

$$n[z^n](1+tz)^{n-1}\Lambda(z)=[z^{n-1}](1+tz)^n\Lambda'(z).$$

By Lagrange inversion formula (see [6]), if $\Upsilon(z)=z\Psi(\Upsilon(z))$, then

$$n[z^n]\Lambda(\Upsilon(z))=[z^{n-1}]\Psi^n(z)\Lambda'(z).$$

So we let $\Psi(z) = 1 + tz$, then $\Upsilon(z) = \frac{z}{1-tz}$, and

$$[z^{n-1}](1+tz)^n \Lambda'(z) = n[z^n]\Lambda\left(\Upsilon(z)\right) = [z^n]z\frac{\partial}{\partial z}\Lambda\left(\Upsilon(z)\right)$$
$$= [z^n]\left(\frac{3-2tz-tz^2}{1-tz-tz^2-t(1-t)z^3} - 2 - \frac{1}{1-tz}\right),$$

from which we deduce (11).