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The Numbers of Perfect and Maximal Matchings in Double Hexagonal Chains

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Abstract

A double hexagonal chain is a hexagonal system constructed by successive triple-edge fusions of naphthalenes. Oz and Cangul computed the Merrifield-Simmons index of the double hexagonal chain by utilizing Merrifield-Simmons vector defined at a path of double hexagonal chain. In this paper, inspired by Oz and Cangul's idea, by applying the perfect matching vector and maximal matching vector at a path of double hexagonal chain, we obtain the numbers of perfect matchings and maximal matchings of a double hexagonal chain with n naphthalenes.

1 Introduction

Let G be a graph with vertex set $V(G)$ and edge set $E(G)$. A subset $M \subseteq E(G)$ consisting of independent edges or edges with no common end-vertex is called a *matching* of G. If a vertex of G is incident with an edge in M, then we say that the vertex is *covered* by M, otherwise, *uncovered*

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by M. In general, we are interested in matchings with the largest size. A matching M of G is called a *maximum matching* if it has the maximum size over all matchings in G. If each vertex of G is covered by M, then M is called *perfect matching*. Obviously, perfect matchings must be maximum matchings, but not vice versa. The perfect matching corresponds to the Kekulé structure in organic chemistry, its enumeration plays an important role in the study of benzenoid hydrocarbons [3, 11]. For some backgrounds on matching theory we refer the reader to the famous book by Lovász and Plummer [13].

Another way to characterize large matchings is based on set inclusion. A matching M in a graph G is *maximal* if it is not contained in any other matchings of G. A maximum matching is obviously also maximal, but the converse is generally not true. Maximal matchings are much less known and researched than their maximum and perfect counterparts. The structures of maximal matchings have been studied for benzenoids [7], fullerenes [2, 5], nanocones and nanotubes [22, 23]. We also refer the interested reader to papers [9, 12, 24] etc. In a sense, maximal matchings are feasible models to solve several physical and technical problems such as the block-allocation of a sequential resource and adsorption of dimers on a structured substrate or a molecule. The enumeration of maximal matchings plays a crucial role in the application of these models [8]. Recently, the number of maximal matchings in benzenoid chains, polyspiro and linear polymers have been researched, see [6, 8, 21].

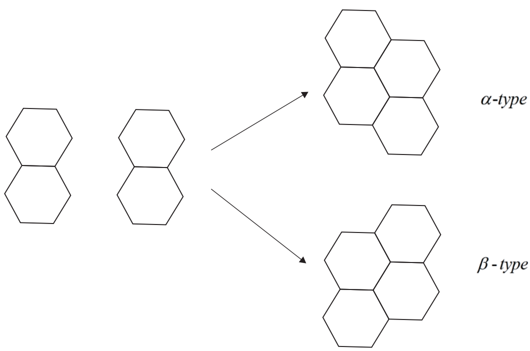


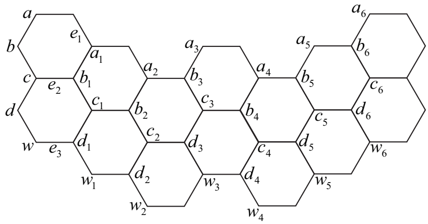
Figure 1. Two types of triple-edge fusion of two naphthalenes.

A 2-connected plane graph with every interior face bounded by a regular hexagon of side length one is called a *hexagonal system* or *benzenoid system.* Hexagonal systems are of great importance for theoretical chemistry since they are the graphs representing the carbon-atom skeleton of benzenoid hydrocarbons [3, 11]. A vertex of a hexagonal system belongs to at most three hexagons. For a hexagonal system H, if there exist three hexagons sharing a common vertex, then H is called *peri-condensed*, otherwise, H is called *cata-condensed.* A *hexagonal chain* is a cata-condensed hexagonal system in which every hexagon is adjacent to at most two hexagons. A *double hexagonal chain* is a peri-condensed hexagonal system which is constructed by successive triple-edge fusions of naphthalenes. There are two types of triple-edge fusion of two naphthalenes as depicted in Fig. 1, that are called α-type fusing and β-type fusing respectively. The double hexagonal chains have been much studied in other areas of mathematical chemistry, we refer the reader to see [1,4,17–20,25]. Recently, Oz and Cangul [16] computed the Merrifield-Simmons index of the double hexagonal chain by introducing the Merrifield-Simmons vector defined at a path of double hexagonal chain. Inspired by their methods, in this paper, by utilizing the perfect matching vector and maximal matching vector at a path, we obtain the numbers of perfect matchings and maximal matchings of a double hexagonal chain with n naphthalenes.

2 Counting perfect matchings in double hexagonal chains

A double hexagonal chain with n naphthalene units, denoted by D_n^2, can be obtained from a naphthalene by a stepwise triple-edge fusion of new naphthalenes, and each type of fusion is α-type or β-type fusing. For convenience, we write $D_n^2 := \theta_1\theta_2\theta_3\cdots\theta_{n-1}$, where θ_i denotes α-type or β-type fusing, according to the fusion process of naphthalenes (see Fig. 2 (a) for D_7^2).

Note that a naphthalene has five vertices on the left sides and five on the right sides. See Fig. 2 (a), starting from the first naphthalene unite



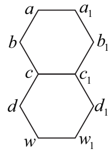


Figure 2. (a) $D_7^2 := \alpha\alpha\beta\alpha\beta\beta$ with 7 naphthalenes, (b) D_1^2.

on the left in D_n^2, we label the five vertices on its left sides by a, b, c, d, w respectively. For the i-th ($i \in \{2, 3, \cdots, n\}$) naphthalene unite in D_n^2, we label the five vertices on its left sides by $a_{i-1}, b_{i-1}, c_{i-1}, d_{i-1}, w_{i-1}$ successively. In particular, the vertices of D_1^2 are labeled as depicted in Fig. 2 (b).

For $X = \{x_1, \cdots, x_k\} \subseteq V(G)$, let $G - X$ or $G - x_1 - \cdots - x_k$ be the graph obtained by deleting all vertices $x_1, \cdots, x_k$ from graph G. Let $\Phi(G)$ denote the number of perfect matchings of G.

Definition 1. For the path *abcdw* in D_n^2 (see Fig. 2), the following vector

$$\Phi_{abcdw}(D_n^2) = \begin{pmatrix} \Phi(D_n^2) \\ \Phi(D_n^2 - a - b) \\ \Phi(D_n^2 - a - d) \\ \Phi(D_n^2 - d - w) \\ \Phi(D_n^2 - b - w) \end{pmatrix}$$

is called the perfect matching vector of D_n^2.

Proposition 1. $\Phi_{abcdw}(D_1^2) = (3, 2, 1, 2, 1)^T$.

Proof. As shown in Fig. 2 (b), D_1^2 is a hexagonal chain with exactly two hexagons. It is easy to check that $\Phi(D_1^2) = 3$. By the symmetry, it is not difficult to verify that $\Phi(D_1^2 - a - b) = \Phi(D_1^2 - d - w) = 2$ and $\Phi(D_1^2 - a - d) = \Phi(D_1^2 - b - w) = 1$. ■

The following two 5×5 matrices play an important role in the sequel discussion.

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Theorem 2. *Let $D_n^2 := \theta_1\theta_2\theta_3\cdots\theta_{n-1}$ be a double hexagonal chain with $n \geq 2$ naphthalene units. Then*

$$\Phi_{abcdw}(D_n^2) = \begin{cases} A \cdot \Phi_{a_1b_1c_1d_1w_1}(D_{n-1}^2), & \theta_1 = \alpha; \\ P \cdot A \cdot P \cdot \Phi_{a_1b_1c_1d_1w_1}(D_{n-1}^2), & \theta_1 = \beta. \end{cases}$$

Proof. We first show the case when $\theta_1 = \alpha$. Note that there are three edges e_1, e_2, e_3 in the first naphthalene unit on the left side of D_n^2 (see Fig. 2 (a)), and all the perfect matchings of D_n^2 can be divided into three categories: $\mathcal{M}_1 = \{M|M$ is a perfect matching of D_n^2, and $e_1, e_2, e_3 \notin M\}$, $\mathcal{M}_2 = \{M|M$ is a perfect matching of D_n^2, and $e_1, e_2 \in M$ and $e_3 \notin M\}$, $\mathcal{M}_3 = \{M|M$ is a perfect matching of D_n^2, and $e_1, e_3 \in M$ and $e_2 \notin M\}$. We have

$$\begin{aligned} \Phi(D_n^2) =& |\mathcal{M}_1| + |\mathcal{M}_2| + |\mathcal{M}_3| \\ =& \Phi(D_{n-1}^2) + \Phi(D_{n-1}^2 - a_1 - b_1) + \Phi(D_{n-1}^2 - a_1 - d_1) \\ =& (1,1,1,0,0) \times \Phi_{a_1b_1c_1d_1w_1}(D_{n-1}^2). \end{aligned}$$

Since edge e_1 belongs to each perfect matching of $D_n^2 - a - b$, all the perfect matchings of $D_n^2 - a - b$ can be divided into two categories according to whether including edge e_2. If e_2 is contained in a perfect matching M of $D_n^2 - a - b$, then $dw \in M$ and the number of such perfect matchings in $D_n^2 - a - b$ is $\Phi(D_{n-1}^2 - a_1 - b_1)$. If e_2 is not contained in a perfect matching M of $D_n^2 - a - b$, then $cd, e_3 \in M$ and the number of such perfect matchings in $D_n^2 - a - b$ is $\Phi(D_{n-1}^2 - a_1 - d_1)$. Hence

$$\Phi(D_n^2 - a - b) = \Phi(D_{n-1}^2 - a_1 - b_1) + \Phi(D_{n-1}^2 - a_1 - d_1)$$

$$= (0,1,1,0,0) \times \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1}).$$

Similarily, we have

$$\begin{aligned}\Phi(D^2_n - a - d) =& \Phi(D^2_{n-1} - a_1 - d_1) = (0,0,1,0,0) \times \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1}),\\ \Phi(D^2_n - d - w) =& \Phi(D^2_{n-1}) + \Phi(D^2_{n-1} - a_1 - b_1)\\ =& (1,1,0,0,0) \times \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1}),\\ \Phi(D^2_n - b - w) =& \Phi(D^2_{n-1}) = (1,0,0,0,0) \times \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1}).\end{aligned}$$

To sum up, we have $\Phi_{abcdw}(D^2_n) = A \cdot \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1})$ if $\theta_1 = \alpha$.

For the case $\theta_1 = \beta$, according to Definition 1 and the symmetry of D^2_n, we have $\Phi_{abcdw}(D^2_n) = P \cdot \Phi_{wdcba}(D^2_n) = P \cdot A \cdot \Phi_{w_1d_1c_1b_1a_1}(D^2_{n-1}) = P \cdot A \cdot P \cdot \Phi_{a_1b_1c_1d_1w_1}(D^2_{n-1})$. ■

Theorem 3. *Let $D^2_n := \theta_1\theta_2\theta_3\cdots\theta_{n-1}$ be a double hexagonal chain with $n \geq 2$ naphthalene units. Then*

$$\Phi(D^2_n) = (1,0,0,0,0) \cdot X_1 \cdot X_2 \cdot \cdots \cdot X_{n-1} \cdot (3,2,1,2,1)^T,$$

where $X_i = A$ if $\theta_i = \alpha$ and $X_i = P \cdot A \cdot P$ if $\theta_i = \beta$, $i = 1,2,\ldots,n-1$.

Proof. By Definition 1, $\Phi(D^2_n) = (1,0,0,0,0) \cdot \Phi_{abcdw}(D^2_n)$. Applying Theorem 2 repeatedly, and by Proposition 1, we get

$$\Phi_{abcdw}(D^2_n) = X_1 \cdot X_2 \cdot \cdots \cdot X_{n-1} \cdot (3,2,1,2,1)^T,$$

where $X_i = A$ if $\theta_i = \alpha$ and $X_i = P \cdot A \cdot P$ if $\theta_i = \beta$, $i = 1,2,\ldots,n-1$. Hence the conclusion holds. ■

Example 1. Let $D^2_n := \theta_1\theta_2\theta_3\cdots\theta_{n-1}$ be a double hexagonal chain with $n \geq 2$ naphthalene units, where $\theta_1 = \theta_2 = \cdots = \theta_{n-1} = \alpha$. Then now D^2_n denotes a benzenoid parallelogram with $2 \times n$ hexagons, and $\Phi(D^2_n) = \frac{(n+1)(n+2)}{2}$.

Proof. According to Theorem 3,

$$\Phi(D^2_n) = (1,0,0,0,0) \cdot A^{n-1} \cdot (3,2,1,2,1)^T$$

$$= (1,0,0,0,0) \cdot \begin{pmatrix} 1 & n-1 & \frac{(n-1)n}{2} & 0 & 0 \\ 0 & 1 & n-1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & n-1 & \frac{(n-2)(n+1)}{2} & 0 & 0 \\ 1 & n-2 & \frac{(n-2)(n-1)}{2} & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 3 \\ 2 \\ 1 \\ 2 \\ 1 \end{pmatrix}$$

$$= \frac{(n+1)(n+2)}{2}. \qquad \blacksquare$$

The above conclusion is coincident with the result given by Gutman [10].

Example 2. Let $D_n^2 := \theta_1\theta_2\theta_3\cdots\theta_{n-1}$ be a double hexagonal chain with $n \geq 4$ naphthalene units, where $\theta_i = \alpha$ if i is odd, otherwise $\theta_i = \beta$, $i = 1, 2, \ldots, n-1$. Then now D_n^2 denotes a double zigzag chain with $2 \times n$ hexagons, and

$$\Phi(D_n^2) = \begin{cases} 3a_{11}(n-1) + 2a_{14}(n-1) + a_{15}(n-1), & n \text{ is odd}; \\ 6a_{11}(n-2) + 5a_{14}(n-2) + 3a_{15}(n-2), & n \text{ is even}. \end{cases}$$

Here the sequence $a_{1j}(n)(j = 1, 4, 5)$ has the recursion relation $a_{1j}(n) = 2a_{1j}(n-1) + a_{1j}(n-2) - a_{1j}(n-3)$ with the initial values $a_{11}(1) = 1, a_{11}(2) = 3, a_{11}(3) = 6$, $a_{14}(1) = 1, a_{14}(2) = 2, a_{14}(3) = 5$ and $a_{15}(1) = 1, a_{15}(2) = 1, a_{15}(3) = 3$.

Proof. We can check that

$$(AP)^n = 2(AP)^{n-1} + (AP)^{n-2} - (AP)^{n-3}$$

with the initial conditions $AP = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}$, $(AP)^2 = \begin{pmatrix} 3 & 0 & 0 & 2 & 1 \\ 2 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 2 & 1 \\ 1 & 0 & 0 & 1 & 1 \end{pmatrix}$, $(AP)^3 = \begin{pmatrix} 6 & 0 & 0 & 5 & 3 \\ 3 & 0 & 0 & 3 & 2 \\ 1 & 0 & 0 & 1 & 1 \\ 5 & 0 & 0 & 4 & 2 \\ 3 & 0 & 0 & 2 & 1 \end{pmatrix}$.

Let

$$(AP)^n = \begin{pmatrix} a_{11}(n) & 0 & 0 & a_{14}(n) & a_{15}(n) \\ a_{21}(n) & 0 & 0 & a_{24}(n) & a_{25}(n) \\ a_{31}(n) & 0 & 0 & a_{34}(n) & a_{35}(n) \\ a_{41}(n) & 0 & 0 & a_{44}(n) & a_{45}(n) \\ a_{51}(n) & 0 & 0 & a_{54}(n) & a_{55}(n) \end{pmatrix}.$$

By Theorem 3, if n is odd, then

$$\begin{aligned} \Phi(D_n^2) &= (1,0,0,0,0) \cdot (AP)^{n-1} \cdot (3,2,1,2,1)^T \\ &= 3a_{11}(n-1) + 2a_{14}(n-1) + a_{15}(n-1). \end{aligned}$$

If n is even, then

$$\begin{aligned} \Phi(D_n^2) &= (1,0,0,0,0) \cdot (AP)^{n-2} A \cdot (3,2,1,2,1)^T \\ &= 6a_{11}(n-2) + 5a_{14}(n-2) + 3a_{15}(n-2). \end{aligned}$$

Hence the conclusion holds. ■

Table 1. The number of perfect matchings of double zigzag chains.

n	1	2	3	4	5	6	7	8	9	$\cdots$
$\Phi(D_n^2)$	3	6	14	31	70	157	353	793	1782	$\cdots$

The above recurrence relation is in accordance with the result given by Ohkami and Hosoya [14]. Table 1 displays some initial values of the number of perfect matchings of $2 \times n$ double zigzag chains as the n entries, which is the sequence A006356 on OEIS [15]. In fact, Cyvin and Gutman [3] had already provided an effective algorithm for counting the number of perfect matchings of double hexagonal chains in early years.

3 Counting maximal matchings in double hexagonal chains

The number of maximal matchings of a graph G is denoted by $\Psi(G)$. If G has two connected components G_1 and G_2, then $\Psi(G) = \Psi(G_1) \times \Psi(G_2)$

since any maximal matching of G consists of a maximal matching of G_1 and a maximal matching of G_2. In general, we have the following result.

Proposition 4. [8] *Let G be a graph consisting of k connected components $G_1, G_2, \cdots, G_k$. Then $\Psi(G) = \Psi(G_1) \times \Psi(G_2) \times \cdots \times \Psi(G_k)$.*

By the definition of maximal matching, the following useful result is obvious.

Proposition 5. *Let G be a graph with a 1-degree vertex v and $uv \in E(G)$. Then u is covered by any maximal matching of G.*

For the special case when G is a path, we have the following conclusion.

Proposition 6. [8] *Let P_n be a path with $n \geq 4$ vertices. Then $\Psi(P_n) = \Psi(P_{n-2}) + \Psi(P_{n-3})$ with initial values $\Psi(P_1) = \Psi(P_2) = 1, \Psi(P_3) = 2$.*

For $x_1, \cdots, x_k \in V(G)$, we use $\Psi(G|x_1, \cdots, x_k)$ to denote the number of maximal matchings of G with $x_1, \cdots, x_k$ all covered. For $S \subseteq E(G)$, $\Psi^{-S}(G)$ denotes the number of maximal matchings of G with all edges in S avoided. If S contains only one edge, say xy, then $\Psi^{-S}(G)$ can be written as $\Psi^{-xy}(G)$. In order to count the number of maximal matchings in double hexagonal chains, we introduce the following novel vector.

Definition 2. For the path $abcdw$ in D_n^2 (see Fig. 2), the vector

$$\Psi_{abcdw}(D_n^2) = \begin{pmatrix} \Psi_{bd}^*(D_n^2) \\ \Psi_{bd}^*(D_n^2 - a) \\ \Psi_{bd}^*(D_n^2|a) \\ \Psi_{db}^*(D_n^2 - w) \\ \Psi_{db}^*(D_n^2|w) \end{pmatrix}$$

is called the maximal matching vector of D_n^2, where

$$\Psi_{bd}^*(D_n^2) = \big(\Psi(D_n^2), \Psi(D_n^2 - b), \Psi(D_n^2 - d), \Psi(D_n^2 - b - d), \Psi(D_n^2|b), \\ \Psi(D_n^2|d), \Psi(D_n^2|b, d), \Psi(D_n^2 - b|d), \Psi(D_n^2 - d|b)\big)^T,$$

$$\Psi_{bd}^*(D_n^2 - a) = \big(\Psi(D_n^2 - a), \Psi(D_n^2 - a - b), \Psi(D_n^2 - a - d),$$

$$\Psi(D_n^2-a-b-d),\Psi(D_n^2-a|b),\Psi(D_n^2-a|d),$$
$$\Psi(D_n^2-a|b,d),\Psi(D_n^2-a-b|d),\Psi(D_n^2-a-d|b)\big)^T,$$
$$\Psi^*_{bd}(D_n^2|a)=\big(\Psi(D_n^2|a),\Psi(D_n^2-b|a),\Psi(D_n^2-d|a),\Psi(D_n^2-b-d|a),$$
$$\Psi(D_n^2|a,b),\Psi(D_n^2|a,d),\Psi(D_n^2|a,b,d),\Psi(D_n^2-b|a,d),$$
$$\Psi(D_n^2-d|a,b)\big)^T,$$
$$\Psi^*_{db}(D_n^2-w)=\big(\Psi(D_n^2-w),\Psi(D_n^2-w-d),\Psi(D_n^2-w-b),$$
$$\Psi(D_n^2-w-d-b),\Psi(D_n^2-w|d),\Psi(D_n^2-w|b),$$
$$\Psi(D_n^2-w|d,b),\Psi(D_n^2-w-d|b),\Psi(D_n^2-w-b|d)\big)^T,$$
$$\Psi^*_{db}(D_n^2|w)=\big(\Psi(D_n^2|w),\Psi(D_n^2-d|w),\Psi(D_n^2-b|w),\Psi(D_n^2-d-b|w),$$
$$\Psi(D_n^2|w,d),\Psi(D_n^2|w,b),\Psi(D_n^2|w,d,b),\Psi(D_n^2-d|w,b),$$
$$\Psi(D_n^2-b|w,d)\big)^T.$$

Proposition 7. *For the double hexagonal chain D_1^2 (see Fig. 2 (b)), we have* $\Psi_{abcdw}(D_1^2)=(20,12,12,8,15,15,11,10,10,11,8,6,5,5,8,3,7,4,17,7,10,5,12,13,9,6,8,11,8,6,5,5,8,3,7,4,17,7,10,5,12,13,9,6,8)^T$.

Proof. By the Definition 2, we first calculate $\Psi^*_{bd}(D_1^2)$. Since D_1^2 is a hexagonal chain with two hexagons (see Fig.2 (b)), by the conclusions in papers [6] and [21], $\Psi(D_1^2)=20$.

The maximal matchings in D_1^2-b can be classified into two classes according to containing edge b_1c_1 or not. Let M_1 be a maximal matching in D_1^2-b. If $b_1c_1\in M_1$, then $aa_1\in M_1$ and $M_1\backslash\{aa_1,b_1c_1\}$ is a maximal matching of the path $cdww_1d_1$. By Proposition 6, D_1^2-b has three such maximal matchings. If $b_1c_1\notin M_1$, by Proposition 5, then $\Psi^{-b_1c_1}(D_1^2-b)=\Psi^{-b_1c_1}(D_1^2-b-a-a_1)+\Psi^{-b_1c_1}(D_1^2-b-a_1-b_1)=\Psi(D_1^2-b-a-a_1-b_1|c_1)+\Psi(D_1^2-b-a-a_1-b_1)=4+5=9$. So $\Psi(D_1^2-b)=3+9=12$. By the symmetry of b and d in D_1^2, we have $\Psi(D_1^2-d)=\Psi(D_1^2-b)=12$.

By Proposition 5, the maximal matchings in D_1^2-b-d can be classified into three classes according to how the vertex c_1 is covered. Let M_2 be a maximal matching in D_1^2-b-d. If $cc_1\in M_2$, then the number of such maximal matchings is equal to $\Psi(D_1^2-b-d-c-c_1)$. Note that $D_1^2-b-d-c-c_1$ is a graph consisting of two disjoint paths aa_1b_1 and

ww_1d_1, by Propositions 4 and 6, $\Psi(D_1^2-b-d-c-c_1)=\Psi(P_3)\times\Psi(P_3)=2\times 2=4$. If $b_1c_1\in M_2$, then the number of such maximal matchings is equal to $\Psi(D_1^2-b-d-b_1-c_1)=\Psi(aa_1)\times\Psi(ww_1d_1)\times\Psi(c)=1\times 2\times 1=2$. If $d_1c_1\in M_2$, then the number of such maximal matchings is equal to $\Psi(D_1^2-b-d-d_1-c_1)=2$. Hence $\Psi(D_1^2-b-d)=4+2+2=8$.

The maximal matchings of D_1^2 covering b can be divided into two types according to containing edge ba or bc. So $\Psi(D_1^2|b)=\Psi(D_1^2-b-a)+\Psi(D_1^2-b-c)=8+\Psi(P_8)=15$. By the symmetry of b and d in D_1^2, then $\Psi(D_1^2|d)=15$. Similarly, we can obtain that $\Psi(D_1^2|b,d)=11$, $\Psi(D_1^2-b|d)=\Psi(D_1^2-d|b)=10$. Hence $\Psi^*_{bd}(D_1^2)=(20,12,12,8,15,15,11,10,10)^T$.

As above, we can compute $\Psi^*_{bd}(D_1^2-a)$ and $\Psi^*_{bd}(D_n^2|a)$ as follows.

$\Psi(D_1^2-a)=\Psi(D_1^2-a-c-b)+\Psi(D_1^2-a-c-c_1)+\Psi(D_1^2-a-c-d)=5+2+4=11$.

$\Psi(D_1^2-a-b)=\Psi(D_1^2-a-b-b_1-a_1)+\Psi(D_1^2-a-b-b_1-c_1)=5+3=8$.

$\Psi(D_1^2-a-d)=\Psi(D_1^2-a-d-b_1-a_1)+\Psi(D_1^2-a-d-b_1-c_1)=4+2=6$.

$\Psi(D_1^2-a-b-d)=\Psi(D_1^2-a-b-d-b_1-a_1)+\Psi(D_1^2-a-b-d-b_1-c_1)=3+2=5$.

$\Psi(D_1^2-a|b)=\Psi(D_1^2-a-b-c)=\Psi(P_7)=5$.

$\Psi(D_1^2-a|d)=\Psi(D_1^2-a-d-c)+\Psi(D_1^2-a-d-w)=8$.

$\Psi(D_1^2-a|b,d)=\Psi(D_1^2-a-b-c-d-w)=\Psi(P_5)=3$.

$\Psi(D_1^2-a-b|d)=\Psi(D_1^2-a-b-d-c)+\Psi(D_1^2-a-b-d-w)=7$.

$\Psi(D_1^2-a-d|b)=\Psi(D_1^2-a-d-b-c)=\Psi(P_6)=4$.

$\Psi(D_1^2|a)=\Psi(D_1^2-a-b)+\Psi(D_1^2-a-a_1)=8+9=17$.

$\Psi(D_1^2-b|a)=\Psi(D_1^2-b-a-a_1)=7$.

$\Psi(D_1^2-d|a)=\Psi(D_1^2-d-a-a_1)+\Psi(D_1^2-d-a-b)=10$.

$\Psi(D_1^2-b-d|a)=\Psi(D_1^2-b-d-a-a_1)=5$.

$\Psi(D_1^2|a,b)=\Psi(D_1^2-a-b)+\Psi(D_1^2-a-a_1-b-c)=8+4=12$.

$\Psi(D_1^2|a,d)=\Psi(D_1^2-a-a_1-d-w)+\Psi(D_1^2-a-a_1-d-c)+\Psi(D_1^2-a-b-d-c)+\Psi(D_1^2-a-b-d-w)=13$.

$\Psi(D_1^2|a,b,d)=\Psi(D_1^2-a-a_1-b-c-d-w)+\Psi(D_1^2-a-b-d-c)+\Psi(D_1^2-a-b-d-w)=9$.

$\Psi(D_1^2-b|a,d)=\Psi(D_1^2-b-a-a_1-d-c)+\Psi(D_1^2-b-a-a_1-d-w)=6$.

$\Psi(D_1^2-d|a,b)=\Psi(D_1^2-d-a-b)+\Psi(D_1^2-d-a-a_1-b-c)=8$.

Therefore $\Psi^*_{bd}(D_1^2 - a) = (11, 8, 6, 5, 5, 8, 3, 7, 4)^T$ and $\Psi^*_{bd}(D_1^2|a) = (17, 7, 10, 5, 12, 13, 9, 6, 8)^T$.

By the symmetry of a and w, b and d in D_1^2, we have $\Psi^*_{db}(D_1^2 - w) = \Psi^*_{bd}(D_1^2 - a)$ and $\Psi^*_{db}(D_1^2|w) = \Psi^*_{bd}(D_1^2|a)$. Thus the conclusion holds. ■

Let

$$B = \begin{pmatrix} B_{11} & B_{12} & B_{13} & 0 & 0 \\ B_{21} & B_{22} & B_{23} & 0 & 0 \\ B_{31} & B_{32} & B_{33} & 0 & 0 \\ B_{41} & B_{42} & B_{43} & 0 & 0 \\ B_{51} & B_{52} & B_{53} & 0 & 0 \end{pmatrix}, \quad Q = \begin{pmatrix} Q_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_9 & 0 \\ 0 & 0 & 0 & 0 & I_9 \\ 0 & I_9 & 0 & 0 & 0 \\ 0 & 0 & I_9 & 0 & 0 \end{pmatrix}.$$

Here I_9 is an identity matrix of order 9, Q_1 and $B_{ij}(i = 1, 2, 3, 4, 5, j = 1, 2, 3)$ are all square matrices of order 9 (see Appendix). B and Q are essential in the following discussions.

Theorem 8. *Let $D_n^2 := \theta_1\theta_2\theta_3 \cdots \theta_{n-1}$ be a double hexagonal chain with $n \geq 2$ naphthalene units. Then*

$$\Psi_{abcdw}(D_n^2) = \begin{cases} B \cdot \Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2), & \theta_1 = \alpha; \\ Q \cdot B \cdot Q \cdot \Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2), & \theta_1 = \beta. \end{cases}$$

Proof. Suppose $\theta_1 = \alpha$. Then all the maximal matchings of D_n^2 can be classified into eight categories according to the way that they containing the three edges e_1, e_2 and e_3 (seeing Fig. 2 (a)). So

$$\begin{aligned} \Psi(D_n^2) =& \Psi^{-\{e_1,e_2,e_3\}}(D_n^2) + \Psi^{-\{e_1,e_2\}}(D_n^2 - V(e_3)) + \Psi^{-\{e_1,e_3\}}(D_n^2 - \\ & V(e_2)) + \Psi^{-\{e_2,e_3\}}(D_n^2 - V(e_1)) + \Psi^{-e_1}(D_n^2 - V(e_2) - V(e_3)) \\ & + \Psi^{-e_2}(D_n^2 - V(e_1) - V(e_3)) + \Psi^{-e_3}(D_n^2 - V(e_1) - V(e_2)) + \\ & \Psi(D_n^2 - V(e_1) - V(e_2) - V(e_3)). \end{aligned} \tag{1}$$

Let $\mathcal{M}_1 = \{M \mid M$ is a maximal matching of D_n^2, and $e_1, e_2, e_3 \notin M\}$. Then $\Psi^{-\{e_1,e_2,e_3\}}(D_n^2) =| \mathcal{M}_1 |$. Note that $D_n^2 - e_1 - e_2 - e_3$ has exactly two connected components, one is a path P_6 with six vertices, another is D_{n-1}^2. Let $M \in \mathcal{M}_1$. Then $M \cap E(P_6)$ is a maximal matching in P_6 and $M \cap E(D_{n-1}^2)$ is a maximal matching in D_{n-1}^2. However, the union of a maximal matching in P_6 and a maximal matching in D^2_{n-1} may be not a maximal matching of D^2_n. According to the structures of the four maximal matchings of P_6, we have $\Psi^{-\{e_1,e_2,e_3\}}(D^2_n) = \Psi(D^2_{n-1}) + \Psi(D^2_{n-1}|d_1) + \Psi(D^2_{n-1}|a_1, b_1) + \Psi(D^2_{n-1}|a_1, d_1)$.

Similar to the discussions of $\Psi^{-\{e_1,e_2,e_3\}}(D^2_n)$, we can compute that
$\Psi^{-\{e_1,e_2\}}(D^2_n - V(e_3)) = 2\Psi(D^2_{n-1} - d_1) + \Psi(D^2_{n-1} - d_1|a_1)$,
$\Psi^{-\{e_1,e_3\}}(D^2_n - V(e_2)) = \Psi(D^2_{n-1} - b_1) + \Psi(D^2_{n-1} - b_1|a_1)$,
$\Psi^{-\{e_2,e_3\}}(D^2_n - V(e_1)) = \Psi(D^2_{n-1} - a_1|d_1) + \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - a_1)$,
$\Psi^{-e_1}(D^2_n - V(e_2) - V(e_3)) = \Psi(D^2_{n-1} - b_1 - d_1|a_1) + \Psi(D^2_{n-1} - b_1 - d_1)$,
$\Psi^{-e_2}(D^2_n - V(e_1) - V(e_3)) = 2\Psi(D^2_{n-1} - a_1 - d_1)$,
$\Psi^{-e_3}(D^2_n - V(e_1) - V(e_2)) = \Psi(D^2_{n-1} - a_1 - b_1)$,
$\Psi(D^2_n - V(e_1) - V(e_2) - V(e_3)) = \Psi(D^2_{n-1} - a_1 - b_1 - d_1)$.
According to Eq. (1) and Definition 2, we have

$$\begin{aligned}\Psi(D^2_n) =& \big(\Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - b_1) + 2\Psi(D^2_{n-1} - d_1) + \Psi(D^2_{n-1} - b_1 - d_1)\\ &+ \Psi(D^2_{n-1}|d_1)\big) + \big(\Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1} - a_1 - b_1)\\ &+ 2\Psi(D^2_{n-1} - a_1 - d_1) + \Psi(D^2_{n-1} - a_1 - b_1 - d_1)\\ &+ \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - a_1|d_1)\big) + \big(\Psi(D^2_{n-1} - b_1|a_1)\\ &+ \Psi(D^2_{n-1} - d_1|a_1) + \Psi(D^2_{n-1} - b_1 - d_1|a_1) + \Psi(D^2_{n-1}|a_1, b_1)\\ &+ \Psi(D^2_{n-1}|a_1, d_1)\big) = (1, 1, 2, 1, 0, 1, 0, 0, 0) \times \Psi^*_{b_1 d_1}(D^2_{n-1})\\ &+ (1, 1, 2, 1, 1, 1, 0, 0, 0) \times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1)\\ &+ (0, 1, 1, 1, 1, 1, 0, 0, 0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1).\end{aligned}$$

Similar as the above computation of $\Psi(D^2_n)$, we can obtain the other components of $\Psi^*_{bd}(D^2_n)$ as follows.

$$\begin{aligned}\Psi(D^2_n - b) =& \Psi^{-\{e_1,e_2,e_3\}}(D^2_n - b)\\ &+ \Psi^{-\{e_1,e_2\}}(D^2_n - b - V(e_3)) + \Psi^{-\{e_1,e_3\}}(D^2_n - b - V(e_2))\\ &+ \Psi^{-\{e_2,e_3\}}(D^2_n - b - V(e_1)) + \Psi^{-e_1}(D^2_n - b - V(e_2) - V(e_3))\\ &+ \Psi^{-e_2}(D^2_n - b - V(e_1) - V(e_3)) + \Psi^{-e_3}(D^2_n - b - V(e_1)\\ &- V(e_2)) + \Psi(D^2_n - b - V(e_1) - V(e_2) - V(e_3))\\ =& \Psi(D^2_{n-1}|d_1) + \Psi(D^2_{n-1}|b_1) + \Psi(D^2_{n-1} - d_1) + \Psi(D^2_{n-1} - b_1)\\ &+ \Psi(D^2_{n-1} - a_1|d_1) + \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - b_1 - d_1)\\ &+ \Psi(D^2_{n-1} - a_1 - d_1) + \Psi(D^2_{n-1} - a_1 - b_1)\end{aligned}$$

$$
\begin{aligned}
&+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
=&(0,1,1,1,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,1,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1). \qquad (2)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-d)=&\Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-d_1)\\
&+\Psi(D_{n-1}^2-d_1|a_1,b_1)+\Psi(D_{n-1}^2-b_1|a_1)+\Psi(D_{n-1}^2-b_1)\\
&+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-a_1|b_1,d_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1|a_1)+\Psi(D_{n-1}^2-b_1-d_1)\\
&+\Psi(D_{n-1}^2-a_1-d_1|b_1)+\Psi(D_{n-1}^2-a_1-d_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
=&(0,1,1,1,0,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(0,0,1,1,0,1,1,1,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(0,1,0,1,0,0,1,0,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (3)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-b-d)=&\Psi(D_{n-1}^2|b_1,d_1)+\Psi(D_{n-1}^2-d_1|b_1)+\Psi(D_{n-1}^2-b_1|d_1)+\\
&\Psi(D_{n-1}^2-a_1|b_1,d_1)+\Psi(D_{n-1}^2-b_1-d_1)+\Psi(D_{n-1}^2-a_1\\
&-d_1|b_1)+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
=&(0,0,0,1,0,0,1,1,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(0,0,0,1,0,0,1,1,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1). \qquad (4)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2|b)=&\Psi(D_n^2-a-b)+\Psi(D_n^2-b-c)\\
=&\Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-d_1|a_1)\\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-a_1|b_1)\\
&+\Psi(D_{n-1}^2|a_1)+\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2-a_1-b_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1-d_1)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-d_1)\\
&+\Psi(D_{n-1}^2-a_1)+\Psi(D_{n-1}^2-a_1-d_1)\\
=&(1,1,1,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(1,1,2,1,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+v(1,0,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (5)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2|d)=&\Psi(D_n^2-d-c)+\Psi(D_n^2-d-w)\\
=&\Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-d_1|a_1)\\
&+\Psi(D_{n-1}^2-d_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-a_1-d_1)\\
&+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-b_1|a_1)
\end{aligned}
$$

$$
\begin{aligned}
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1)+\Psi(D_{n-1}^2-a_1|b_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1) \qquad (6)\\
=&(1,1,1,0,0,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(1,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(0,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (7)\\
\Psi(D_n^2|b,d)=&\Psi(D_n^2-b-a-d-c)+\Psi(D_n^2-b-a-d-w)\\
&+\Psi(D_n^2-b-c-d-w)=\Psi(D_{n-1}^2|a_1,d_1)\\
&+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-d_1|a_1)+\Psi(D_{n-1}^2-a_1-d_1)\\
&+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-a_1|b_1)+\Psi(D_{n-1}^2-b_1|a_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-b_1)\\
&+\Psi(D_{n-1}^2-a_1)=(1,0,0,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(1,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(0,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (8)\\
\Psi(D_n^2-b|d)=&\Psi(D_n^2-b-d-c)+\Psi(D_n^2-b-d-w)\\
=&\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-d_1)+\Psi(D_{n-1}^2-a_1|d_1)\\
&+\Psi(D_{n-1}^2-a_1-d_1v)+\Psi(D_{n-1}^2|b_1)+\Psi(D_{n-1}^2-a_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1-b_1)\\
=&(0,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,0,1,1,0,0,0)\times\\
&\Psi_{b_1d_1}^*(D_{n-1}^2-a_1). \qquad (9)\\
\Psi(D_n^2-d|b)=&\Psi(D_n^2-d-b-a)+\Psi(D_n^2-d-b-c)\\
=&\Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2-d_1|a_1,b_1)\\
&+\Psi(D_{n-1}^2-b_1|a_1,d_1)+\Psi(D_{n-1}^2-a_1|b_1,d_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-d_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1|a_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
&+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-d_1)\\
&+\Psi(D_{n-1}^2-a_1-d_1)=(0,0,1,0,0,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(0,0,1,1,0,1,1,1,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(0,0,0,1,0,0,1,1,1)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (10)
\end{aligned}
$$

By Eqs. (2-10), we have $\Psi_{bd}^*(D_n^2)=(B_{11},B_{12},B_{13},0,0)\times\Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2)$.

Similarly, we can compute the other components of $\Psi_{abcdw}(D_n^2)$ as follows.

$$
\begin{aligned}
\Psi(D_n^2-a) =& \Psi(D_{n-1}^2|a_1)+\Psi(D_{n-1}^2|a_1,d_1)+2\Psi(D_{n-1}^2-d_1|a_1) \\
&+\Psi(D_{n-1}^2-b_1|a_1)+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1) \\
&+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-b_1-d_1|a_1) \\
&+2\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2-a_1-b_1) \\
&+\Psi(D_{n-1}^2-a_1-b_1-d_1)=(0,1,0,0,0,0,0,0,0) \\
&\times \Psi_{b_1d_1}^*(D_{n-1}^2)+(1,1,2,1,0,1,0,0,0)\times \\
&\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(1,1,2,1,0,1,0,0,0) \\
&\times \Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (11)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-a-b) =& \Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-d_1|a_1) \\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2v-a_1|b_1) \\
&+\Psi(D_{n-1}^2|a_1)+\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2-a_1-b_1) \\
&+\Psi(D_{n-1}^2-a_1-b_1-d_1)=(0,1,0,0,0,0,0,0,0)\times \\
&\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,1,1,1,0,0,0)\times \\
&\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(1,0,1,0,1,1,0,0,0) \\
&\times \Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (12)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-a-d) =& \Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2-d_1|a_1) \\
&+\Psi(D_{n-1}^2-b_1|a_1,d_1)+\Psi(D_{n-1}^2-a_1|d_1) \\
&+\Psi(D_{n-1}^2-b_1-d_1|a_1)+\Psi(D_{n-1}^2-a_1-d_1)+ \\
&\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1) \\
=&(0,0,1,1,0,1,0,1,0)\times \Psi_{b_1d_1}^*(D_{n-1}^2-a_1) \\
&+(0,0,1,1,0,0,1,1,0)\times \Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (13)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-a-b-d) =& \Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2-a_1-d_1|b_1) \\
&+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1) \\
&+\Psi(D_{n-1}^2-d_1|a_1,b_1)+\Psi(D_{n-1}^2-b_1|a_1,d_1) \\
&+\Psi(D_{n-1}^2-a_1|b_1,d_1)+\Psi(D_{n-1}^2-b_1-d_1|a_1) \\
=&(0,0,0,1,0,0,1,1,1)\times \Psi_{b_1d_1}^*(D_{n-1}^2-a_1) \\
&+(0,0,0,1,0,0,1,1,1)\times \Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (14)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-a|b) =& \Psi(D_n^2-a-b-c)=\Psi(D_{n-1}^2|a_1)+\Psi(D_{n-1}^2-d_1|a_1) \\
&+\Psi(D_{n-1}^2-a_1)+\Psi(D_{n-1}^2-a_1-d_1)
\end{aligned}
$$

$$
\begin{aligned}
&=(1,0,1,0,0,0,0,0,0)\times\Psi^*_{b_1d_1}(D^2_{n-1}-a_1)\\
&\quad+(1,0,1,0,0,0,0,0,0)\times\Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \qquad (15)\\
\Psi(D^2_n-a|d)&=\Psi(D^2_n-a-d-c)+\Psi(D^2_n-a-d-w)\\
&=\Psi(D^2_{n-1}|a_1,d_1)+\Psi(D^2_{n-1}-a_1|d_1)+\Psi(D^2_{n-1}-d_1|a_1)\\
&\quad+\Psi(D^2_{n-1}-a_1-d_1)+\Psi(D^2_{n-1}|a_1)+\Psi(D^2_{n-1}-a_1)\\
&\quad+\Psi(D^2_{n-1}-b_1|a_1)+\Psi(D^2_{n-1}-a_1-b_1)\\
&=(1,1,1,0,0,1,0,0,0)\times\Psi^*_{b_1d_1}(D^2_{n-1}-a_1)\\
&\quad+(1,1,1,0,0,1,0,0,0)\times\Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \qquad (16)\\
\Psi(D^2_n-a|b,d)&=\Psi(D^2_n-a-b-c-d-w)=\Psi(D^2_{n-1}-a_1)\\
&\quad+\Psi(D^2_{n-1}-|a_1)=(1,0,0,0,0,0,0,0,0)\\
&\quad\times\Psi^*_{b_1d_1}(D^2_{n-1}-a_1)+(1,0,0,0,0,0,0,0,0)\times\\
&\quad\Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \qquad (17)\\
\Psi(D^2_n-a-b|d)&=\Psi(D^2_n-a-b-d-c)+\Psi(D^2_n-a-b-d-w)\\
&=\Psi(D^2_{n-1}|a_1,d_1)+\Psi(D^2_{n-1}-a_1|d_1)+\Psi(D^2_{n-1}-d_1|a_1)\\
&\quad+\Psi(D^2_{n-1}-a_1-d_1)+\Psi(D^2_{n-1}|a_1,b_1)\\
&\quad+\Psi(D^2_{n-1}-a_1|b_1)+\Psi(D^2_{n-1}-b_1|a_1)\\
&\quad+\Psi(D^2_{n-1}-a_1-b_1)=(0,1,1,0,1,1,0,0,0)\\
&\quad\times\Psi^*_{b_1d_1}(D^2_{n-1}-a_1)+(0,1,1,0,1,1,0,0,0)\\
&\quad\times\Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \qquad (18)\\
\Psi(D^2_n-a-d|b)&=\Psi(D^2_n-a-d-b-c)=\Psi(D^2_{n-1}|a_1,d_1)\\
&\quad+\Psi(D^2_{n-1}-a_1|d_1)+\Psi(D^2_{n-1}-d_1|a_1)\\
&\quad+\Psi(D^2_{n-1}-a_1-d_1)=(0,0,1,0,0,1,0,0,0)\\
&\quad\times\Psi^*_{b_1d_1}(D^2_{n-1}-a_1)+(0,0,1,0,0,1,0,0,0)\\
&\quad\times\Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \qquad (19)
\end{aligned}
$$

By Eqs. (11-19), we obtain $\Psi^*_{bd}(D^2_n-a)=(B_{21},B_{22},B_{23},0,0)$ $\times\Psi_{a_1b_1c_1d_1w_1}(D^2_{n-1})$.

$$
\begin{aligned}
\Psi(D^2_n|a)=&\Psi(D^2_{n-1})+\Psi(D^2_{n-1}|d_1)+2\Psi(D^2_{n-1}-d_1)+\Psi(D^2_{n-1}-b_1)\\
&+\Psi(D^2_{n-1}-b_1-d_1)+\Psi(D^2_{n-1}|a_1,d_1)+\Psi(D^2_{n-1}|a_1,b_1)\\
&+\Psi(D^2_{n-1}-d_1|a_1)+\Psi(D^2_{n-1}-b_1)+\Psi(D^2_{n-1}-a_1|d_1)\\
&+\Psi(D^2_{n-1}-a_1|b_1)+\Psi(D^2_{n-1}|a_1)+\Psi(D^2_{n-1}-a_1-d_1)
\end{aligned}
$$

$$
\begin{aligned}
&+\Psi(D_{n-1}^2-a_1-b_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
=&(1,2,2,0,0,1,0,1,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(0,1,1,1,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(1,0,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (20)\\
\Psi(D_n^2-b|a)=&\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2|b_1)+\Psi(D_{n-1}^2-d_1)\\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-b_1-d_1)\\
=&(0,1,1,1,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2). \qquad (21)\\
\Psi(D_n^2-d|a)=&\Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2-d_1|a_1,b_1)\\
&+\Psi(D_{n-1}^2-b_1|a_1,d_1)+\Psi(D_{n-1}^2-a_1|b_1,d_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-d_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1|a_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
&+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-b_1|d_1)+\Psi(D_{n-1}^2-d_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1)=(0,0,1,1,0,1,0,1,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,0,0,1,0,0,1,1,1)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(0,0,0,1,0,0,1,1,1)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (22)\\
\Psi(D_n^2-b-d|a)=&\Psi(D_{n-1}^2|b_1,d_1)+\Psi(D_{n-1}^2-b_1|d_1)+\Psi(D_{n-1}^2-d_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1)=(0,0,0,1,0,0,1,1,1)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2). \qquad (23)\\
\Psi(D_n^2|a,b)=&\Psi(D_n^2-a-b)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-d_1)\\
=&\Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-d_1|a_1)\\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-a_1|b_1)\\
&+\Psi(D_{n-1}^2|a_1)+\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2-a_1-b_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1-d_1)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-d_1)\\
=&(1,1,1,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,1,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(1,0,1,0,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (24)\\
\Psi(D_n^2|a,d)=&\Psi(D_{n-1}^2-d_1)+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2-b_1)\\
&+\Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2-d_1|a_1)+\Psi(D_{n-1}^2-a_1|d_1)\\
&+\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-a_1|b_1)
\end{aligned}
$$

$$
\begin{aligned}
&+\Psi(D_{n-1}^2-b_1|a_1)+\Psi(D_{n-1}^2-a_1-b_1)\\
=&(1,1,1,0,0,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,0,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(0,1,1,0,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (25)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2|a,b,d)=&\Psi(D_{n-1}^2|a_1,d_1)+\Psi(D_{n-1}^2-a_1|d_1)+\Psi(D_{n-1}^2-d_1|a_1)\\
&+\Psi(D_{n-1}^2-a_1-d_1)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-a_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1|a_1)+\Psi(D_{n-1}^2-a_1-b_1)+\Psi(D_{n-1}^2)\\
=&(1,0,0,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,1,1,0,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(0,1,1,0,1,1,0,0,0)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (26)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-b|a,d)=&\Psi(D_{n-1}^2-d_1)+\Psi(D_{n-1}^2|d_1)+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2|b_1)\\
=&(0,1,1,0,1,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2). \qquad (27)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-d|a,b)=&\Psi(D_{n-1}^2|a_1,b_1,d_1)+\Psi(D_{n-1}^2-d_1|a_1,b_1)\\
&+\Psi(D_{n-1}^2-b_1|a_1,d_1)+\Psi(D_{n-1}^2-a_1|b_1,d_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1|d_1)+\Psi(D_{n-1}^2-a_1-d_1|b_1)\\
&+\Psi(D_{n-1}^2-b_1-d_1|a_1)+\Psi(D_{n-1}^2-a_1-b_1-d_1)\\
&+\Psi(D_{n-1}^2d_1)+\Psi(D_{n-1}^2|d_1)\\
=&(0,0,1,0,0,1,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)+(0,0,0,1,0,0,1,1,1)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)+(0,0,0,1,0,0,1,1,1)\\
&\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (28)
\end{aligned}
$$

By Eqs. (20-28), we have $\Psi_{bd}^*(D_n^2|a)=(B_{31},B_{32},B_{33},0,0)\times\Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2)$.

$$
\begin{aligned}
\Psi(D_n^2-w)=&\Psi(D_{n-1}^2|a_1)+2\Psi(D_{n-1}^2)+2\Psi(D_{n-1}^2-a_1)\\
&+\Psi(D_{n-1}^2-b_1|a_1)+\Psi(D_{n-1}^2-b_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1)\\
=&(2,1,0,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2)\\
&+(2,1,0,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2-a_1)\\
&+(1,1,0,0,0,0,0,0,0)\times\Psi_{b_1d_1}^*(D_{n-1}^2|a_1). \qquad (29)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2-w-d)=&\Psi(D_{n-1}^2)+\Psi(D_{n-1}^2|a_1,b_1)+\Psi(D_{n-1}^2-b_1|a_1)\\
&+\Psi(D_{n-1}^2-b_1)+\Psi(D_{n-1}^2-a_1|b_1)+\Psi(D_{n-1}^2-a_1)\\
&+\Psi(D_{n-1}^2-a_1-b_1)=(1,1,0,0,0,0,0,0,0)
\end{aligned}
$$

$$\times \Psi^*_{b_1d_1}(D^2_{n-1}) + (1,1,0,0,1,0,0,0,0)$$
$$\times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1) + (0,1,0,0,1,0,0,0,0)$$
$$\times \Psi^*_{b_1d_1}(D^2_{n-1}|a_1). \tag{30}$$

$$\begin{aligned}\Psi(D^2_n - w - b) =& \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - b_1) + \Psi(D^2_{n-1} - a_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) = (1,1,0,0,0,0,0,0,0)\\ &\times \Psi^*_{b_1d_1}(D^2_{n-1}) + (1,1,0,0,0,0,0,0,0)\\ &\times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1).\end{aligned} \tag{31}$$

$$\begin{aligned}\Psi(D^2_n - w - b - d) =& \Psi(D^2_{n-1}|b_1) + \Psi(D^2_{n-1} - b_1) + \Psi(D^2_{n-1} - a_1|b_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) = (0,1,0,0,1,0,0,0,0)\\ &\times \Psi^*_{b_1d_1}(D^2_{n-1}) + (0,1,0,0,1,0,0,0,0)\\ &\times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1).\end{aligned} \tag{32}$$

$$\begin{aligned}\Psi(D^2_n - w|d) =& \Psi(D^2_{n-1}|a_1) + \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - a_1)\\ =& (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1})\\ &+ (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1)\\ &+ (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1}|a_1).\end{aligned} \tag{33}$$

$$\begin{aligned}\Psi(D^2_n - w|b) =& \Psi(D^2_n - b - a) + \Psi(D^2_n - b - c) = \Psi(D^2_{n-1}|a_1)\\ &+ \Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1} - b_1|a_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1})\\ =& (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1})\\ &+ (2,1,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1)\\ &+ (1,1,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1}|a_1).\end{aligned} \tag{34}$$

$$\begin{aligned}\Psi(D^2_n - w|b,d) =& \Psi(D^2_n - w - d - c - b - a)\\ =& \Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1}|a_1)\\ =& (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1)\\ &+ (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1}|a_1).\end{aligned} \tag{35}$$

$$\begin{aligned}\Psi(D^2_n - w - d|b) =& \Psi(D^2_n - w - d - b - c) + \Psi(D^2_n - w - d - b - a)\\ =& \Psi(D^2_{n-1}|a_1, b_1) + \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - b_1|a_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - a_1)\\ =& (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1})\\ &+ (1,1,0,0,1,0,0,0,0) \times \Psi^*_{b_1d_1}(D^2_{n-1} - a_1)\end{aligned}$$

$$+ (0,1,0,0,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1). \tag{36}$$

$$\begin{aligned}\Psi(D^2_n - w - b|d) =& \Psi(D^2_n - w - b - d - c) = \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - a_1)\\ =&(1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1})\\ &+ (1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1).\end{aligned} \tag{37}$$

By Eqs. (29-37), we obtain $\Psi^*_{db}(D^2_n - w) = (B_{41}, B_{42}, B_{43}, 0, 0)$ $\times \Psi_{a_1 b_1 c_1 d_1 w_1}(D^2_{n-1})$.

$$\begin{aligned}\Psi(D^2_n|w) =& \Psi(D^2_n - w - d) + \Psi(D^2_n - w - d_1)\\ =&\Psi(D^2_{n-1}|a_1, b_1) + \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - b_1|a_1)\\ &+ \Psi(D^2_{n-1} - b_1) + \Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1} - a_1|b_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1} - d_1)\\ &+ \Psi(D^2_{n-1} - d_1|a_1) + \Psi(D^2_{n-1} - d_1)\\ &+ \Psi(D^2_{n-1} - b_1 - d_1|a_1)\\ &+ \Psi(D^2_{n-1} - b_1 - d_1) + 2\Psi(D^2_{n-1} - a_1 - d_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1 - d_1) = (1,1,2,1,0,0,0,0,0)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1}) + (1,1,2,1,1,0,0,0,0)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1) + (0,1,1,1,1,0,0,0,0)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1).\end{aligned} \tag{38}$$

$$\begin{aligned}\Psi(D^2_n - d|w) =& \Psi(D^2_n - d - w - d_1) = \Psi(D^2_{n-1} - d_1|a_1, b_1) + \Psi(D^2_{n-1} - d_1)\\ &+ \Psi(D^2_{n-1} - b_1 - d_1|a_1) + \Psi(D^2_{n-1} - b_1 - d_1)\\ &+ \Psi(D^2_{n-1} - a_1 - d_1) + \Psi(D^2_{n-1} - a_1 - d_1|b_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1 - d_1) = (0,0,1,1,0,0,0,0,0)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1}) + (0,0,1,1,0,0,0,0,1)\times\\ &\Psi^*_{b_1 d_1}(D^2_{n-1} - a_1) + (0,0,0,1,0,0,0,0,1)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1).\end{aligned} \tag{39}$$

$$\begin{aligned}\Psi(D^2_n - b|w) =& \Psi(D^2_n - b - w - d) + \Psi(D^2_n - b - w - d_1)\\ =&\Psi(D^2_{n-1}|b_1) + \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - b_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1} - d_1)\\ &+ \Psi(D^2_{n-1} - a_1 - d_1) + \Psi(D^2_{n-1} - b_1 - d_1)\\ &+ \Psi(D^2_{n-1} - a_1 - b_1 - d_1) = (0,1,1,1,1,0,0,0,0)\\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1}) + (0,1,1,1,1,0,0,0,0)\end{aligned}$$

$$\times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1). \quad (40)$$

$$\begin{aligned}\Psi(D^2_n - b - d|w) =& \Psi(D^2_{n-1} - d_1|b_1) + \Psi(D^2_{n-1} - d_1 - b_1) \\ &+ \Psi(D^2_{n-1} - d_1 - a_1|b_1) + \Psi(D^2_{n-1} - a_1 - b_1 - d_1) \\ =&(0,0,0,1,0,0,0,0,1) \times \Psi^*_{b_1 d_1}(D^2_{n-1}) + (0,0,0,1,0,0,0,0,1) \\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1). \quad (41)\end{aligned}$$

$$\begin{aligned}\Psi(D^2_n|w,d) =& \Psi(D^2_{n-1}|a_1,b_1) + \Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - b_1|a_1) \\ &+ \Psi(D^2_{n-1} - b_1) + \Psi(D^2_{n-1} - a_1) + \Psi(D^2_{n-1} - a_1|b_1) \\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1} - a_1 - d_1) \\ &+ \Psi(D^2_{n-1} - d_1|a_1) + \Psi(D^2_{n-1} - d_1) \\ =&(1,1,1,0,0,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}) + (1,1,1,0,1,0,0,0,0) \\ &\times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1) \\ &+ (0,1,1,0,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1). \quad (42)\end{aligned}$$

$$\begin{aligned}\Psi(D^2_n|w,b) =& \Psi(D^2_n - b - a - w - d) + \Psi(D^2_n - b - a - w - d_1) \\ &+ \Psi(D^2_n - b - c - w - d) + \Psi(D^2_n - b - c - w - d_1) \\ =& \Psi(D^2_{n-1}|a_1,b_1) + \Psi(D^2_{n-1} - a_1|b_1) + \Psi(D^2_{n-1} - b_1|a_1) \\ &+ \Psi(D^2_{n-1} - a_1 - b_1) + \Psi(D^2_{n-1} - d_1|a_1) \\ &+ \Psi(D^2_{n-1} - a_1 - d_1) + \Psi(D^2_{n-1} - b_1 - d_1|a_1) \\ &+ \Psi(D^2_{n-1} - a_1 - b_1 - d_1) + \Psi(D^2_{n-1} - a_1) + \\ &\Psi(D^2_{n-1}) + \Psi(D^2_{n-1} - d_1) + \Psi(D^2_{n-1} - a_1 - d_1) \\ =&(1,0,1,0,0,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}) \\ &+ (1,1,2,1,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1) \\ &+ (0,1,1,1,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1). \quad (43)\end{aligned}$$

$$\begin{aligned}\Psi(D^2_n|w,b,d) =& \Psi(D^2_n - b - c - d - w) + \Psi(D^2_n - b - a - d - w) \\ &+ \Psi(D^2_n - b - a - d - c - w - d_1) = \Psi(D^2_{n-1} - a_1) \\ &+ \Psi(D^2_{n-1}) + \Psi(D^2_{n-1}|a_1,b_1) + \Psi(D^2_{n-1} - a_1|b_1) \\ &+ \Psi(D^2_{n-1} - b_1|a_1) + \Psi(D^2_{n-1} - a_1 - b_1) \\ &+ \Psi(D^2_{n-1} - d_1|a_1) + \Psi(D^2_{n-1} - a_1 - d_1) \\ =&(1,0,0,0,0,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}) \\ &+ (1,1,1,0,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1} - a_1) \\ &+ (0,1,1,0,1,0,0,0,0) \times \Psi^*_{b_1 d_1}(D^2_{n-1}|a_1). \quad (44)\end{aligned}$$

$$
\begin{aligned}
\Psi(D_n^2 - d|w,b) =& \Psi(D_n^2 - b - c - w - d_1) + \Psi(D_n^2 - b - a - w - d_1)\\
=& \Psi(D_{n-1}^2 - d_1) + \Psi(D_{n-1}^2 - d_1 - a_1) + \Psi(D_{n-1}^2 - d_1|a_1,b_1)\\
&+ \Psi(D_{n-1}^2 - d_1 - a_1|b_1) + \Psi(D_{n-1}^2 - d_1 - b_1|a_1)\\
&+ \Psi(D_{n-1}^2 - a_1 - b_1 - d_1)\\
=& (0,0,1,0,0,0,0,0,0) \times \Psi^*_{b_1d_1}(D_{n-1}^2)\\
&+ (0,0,1,1,0,0,0,0,1) \times \Psi^*_{b_1d_1}(D_{n-1}^2 - a_1)\\
&+ (0,0,0,1,0,0,0,0,1) \times \Psi^*_{b_1d_1}(D_{n-1}^2|a_1). \qquad (45)
\end{aligned}
$$

$$
\begin{aligned}
\Psi(D_n^2 - b|w,d) =& \Psi(D_n^2 - b - d - w) + \Psi(D_n^2 - b - d - c - w - d_1)\\
=& \Psi(D_{n-1}^2|b_1) + \Psi(D_{n-1}^2 - a_1|b_1) + \Psi(D_{n-1}^2 - b_1)\\
&+ \Psi(D_{n-1}^2 - a_1 - b_1) + \Psi(D_{n-1}^2 - d_1)\\
&+ \Psi(D_{n-1}^2 - a_1 - d_1)\\
=& (0,1,1,0,1,0,0,0,0) \times \Psi^*_{b_1d_1}(D_{n-1}^2)\\
&+ (0,1,1,0,1,0,0,0,0) \times \Psi^*_{b_1d_1}(D_{n-1}^2 - a_1). \qquad (46)
\end{aligned}
$$

By Eqs. (38-46), we obtain $\Psi^*_{db}(D_n^2|w) = (B_{51}, B_{52}, B_{53}, 0, 0) \times \Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2)$. In summary, we show that $\Psi_{abcdw}(D_n^2) = B \cdot \Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2)$ if $\theta_1 = \alpha$.

For the case $\theta_1 = \beta$, by Definition 2 and the symmetry of D_n^2, we have $\Psi_{abcdw}(D_n^2) = Q \cdot \Psi_{wdcba}(D_n^2) = Q \cdot B \cdot \Psi_{w_1d_1c_1b_1a_1}(D_{n-1}^2) = Q \cdot B \cdot Q \cdot \Psi_{a_1b_1c_1d_1w_1}(D_{n-1}^2)$. ■

Theorem 9. *Let $D_n^2 := \theta_1\theta_2\theta_3 \cdots \theta_{n-1}$ be a double hexagonal chain with $n \geq 2$ naphthalene units. Then*

$$\Psi(D_n^2) = \zeta \cdot Y_1 \cdot Y_2 \cdot \cdots \cdot Y_{n-1} \cdot \eta,$$

where $Y_i = B$ if $\theta_i = \alpha$, and $Y_i = Q \cdot B \cdot Q$ if $\theta_i = \beta$ $(i = 1, 2, \ldots, n-1)$, ζ is the first row of I_{45} and $\eta = \Psi_{abcdw}(D_1^2)$.

Proof. Applying Theorem 8 repeatedly, and by Proposition 7, we get

$$\Psi_{abcdw}(D_n^2) = Y_1 \cdot Y_2 \cdot \cdots \cdot Y_{n-1} \cdot \eta,$$

where $Y_i = B$ if $\theta_i = \alpha$, otherwise $Y_i = Q \cdot B \cdot Q$. Since $\Psi(D_n^2)$ is the first component of vector $\Psi_{abcdw}(D_n^2)$, the conclusion holds. ■

Example 3. For the $2 \times n$ benzenoid parallelogram in Example 1, by Theorem 9, we have

$$\Psi(D_n^2) = \zeta \cdot B^{n-1} \cdot \eta.$$

Table 2. The number of maximal matchings of $2 \times n$ benzenoid parallelograms.

n	1	2	3	4	5	6	7	$\cdots$
$\Psi(D_n^2)$	20	175	1630	15234	143254	1349460	12710345	$\cdots$

The Table 2 gives the first several values of the number of maximal matchings of $2 \times n$ benzenoid parallelograms as the n entries, this novel sequence is not on OEIS [15].

Example 4. For the $2 \times n$ double zigzag chain in Example 2, by Theorem 9, we get

$$\Psi(D_n^2) = \begin{cases} \zeta \cdot (BQ)^{n-1} \cdot \eta, & n \textit{ is odd}; \\ \zeta \cdot (BQ)^{n-2} \cdot B \cdot \eta, & n \textit{ is even}. \end{cases}$$

Table 3. The number of maximal matchings of double zigzag chains.

n	1	2	3	4	5	6	7	$\cdots$
$\Psi(D_n^2)$	20	175	1476	12698	109355	939709	8075439	$\cdots$

The Table 3 gives some initial values of the number of maximal matchings of $2 \times n$ double zigzag chains as the n entries, the new sequence is not on OEIS [15].

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Appendix

$$Q_1 = \begin{pmatrix} 1&0&0&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&0&0&0\\ 0&0&0&0&0&1&0&0&0\\ 0&0&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&1&0&0\\ 0&0&0&0&0&0&0&0&1\\ 0&0&0&0&0&0&0&1&0 \end{pmatrix} \quad B_{11} = \begin{pmatrix} 1&1&2&1&0&1&0&0&0\\ 0&1&1&1&1&1&0&0&0\\ 0&1&1&1&0&1&0&0&0\\ 0&0&0&1&0&0&1&1&1\\ 1&1&1&0&0&0&0&0&0\\ 1&1&1&0&0&1&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&1&0&0&1&0&0&0 \end{pmatrix}$$

$$B_{12} = \begin{pmatrix} 1&1&2&1&1&1&0&0&0\\ 0&1&1&1&1&1&0&0&0\\ 0&0&1&1&0&1&1&1&1\\ 0&0&0&1&0&0&1&1&1\\ 1&1&2&1&1&1&0&0&0\\ 1&1&1&0&1&1&0&0&0\\ 1&1&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&1&1&0&1&1&1&1 \end{pmatrix} \quad B_{13} = \begin{pmatrix} 0&1&1&1&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&1&0&1&0&0&1&0&1\\ 0&0&0&0&0&0&0&0&0\\ 1&0&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&1&1&1 \end{pmatrix}$$

$$B_{21} = \begin{pmatrix} 0&1&0&0&0&0&0&0&0\\ 0&1&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0 \end{pmatrix} \quad B_{22} = \begin{pmatrix} 1&1&2&1&0&1&0&0&0\\ 0&1&1&1&1&1&0&0&0\\ 0&0&1&1&0&1&0&1&0\\ 0&0&0&1&0&0&1&1&1\\ 1&0&1&0&0&0&0&0&0\\ 1&1&1&0&0&1&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&1&0&0&1&0&0&0 \end{pmatrix}$$

$$B_{23} = \begin{pmatrix} 1&1&2&1&0&1&0&0&0\\ 1&0&1&0&1&1&0&0&0\\ 0&0&1&1&0&0&1&1&0\\ 0&0&0&1&0&0&1&1&1\\ 1&0&1&0&0&0&0&0&0\\ 1&1&1&0&0&1&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&1&0&0&1&0&0&0 \end{pmatrix} \quad B_{31} = \begin{pmatrix} 1&2&2&0&0&1&0&1&0\\ 0&1&1&1&1&1&0&0&0\\ 0&0&1&1&0&1&0&1&0\\ 0&0&0&1&0&0&1&1&1\\ 1&1&1&0&0&0&0&0&0\\ 1&1&1&0&0&1&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&1&0&0&1&0&0&0 \end{pmatrix}$$

$$B_{32} = \begin{pmatrix} 0&1&1&1&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&1&1&1\\ 0&0&0&0&0&0&0&0&0\\ 0&1&1&1&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&1&1&1 \end{pmatrix} \quad B_{33} = \begin{pmatrix} 1&0&1&0&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&1&1&1\\ 0&0&0&0&0&0&0&0&0\\ 1&0&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&1&1&0&1&1&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&1&0&0&1&1&1 \end{pmatrix}$$

$$B_{41} = \begin{pmatrix} 2&1&0&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0&0\\ 0&1&0&0&1&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0 \end{pmatrix} \quad B_{42} = \begin{pmatrix} 2&1&0&0&0&0&0&0&0\\ 1&1&0&0&1&0&0&0&0\\ 1&1&0&0&0&0&0&0&0\\ 0&1&0&0&1&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 2&1&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 1&1&0&0&1&0&0&0&0\\ 1&0&0&0&0&0&0&0&0 \end{pmatrix}$$

$$B_{43} = \begin{pmatrix} 1&1&0&0&0&0&0&0&0\\ 0&1&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&1&0&0&1&0&0&0&0\\ 0&0&0&0&0&0&0&0&0 \end{pmatrix} \quad B_{51} = \begin{pmatrix} 1&1&2&1&0&0&0&0&0\\ 0&0&1&1&0&0&0&0&0\\ 0&1&1&1&1&0&0&0&0\\ 0&0&0&1&0&0&0&0&1\\ 1&1&1&0&0&0&0&0&0\\ 1&0&1&0&0&0&0&0&0\\ 1&0&0&0&0&0&0&0&0\\ 0&0&1&0&0&0&0&0&0\\ 0&1&1&0&1&0&0&0&0 \end{pmatrix}$$

$$B_{52} = \begin{pmatrix} 1&1&2&1&1&0&0&0&0\\ 0&0&1&1&0&0&0&0&1\\ 0&1&1&1&1&0&0&0&0\\ 0&0&0&1&0&0&0&0&1\\ 1&1&1&0&1&0&0&0&0\\ 1&1&2&1&1&0&0&0&0\\ 1&1&1&0&1&0&0&0&0\\ 0&0&1&1&0&0&0&0&1\\ 0&1&1&0&1&0&0&0&0 \end{pmatrix} \quad B_{53} = \begin{pmatrix} 0&1&1&1&1&0&0&0&0\\ 0&0&0&1&0&0&0&0&1\\ 0&0&0&0&0&0&0&0&0\\ 0&0&0&0&0&0&0&0&0\\ 0&1&1&0&1&0&0&0&0\\ 0&1&1&1&1&0&0&0&0\\ 0&1&1&0&1&0&0&0&0\\ 0&0&0&1&0&0&0&0&1\\ 0&0&0&0&0&0&0&0&0 \end{pmatrix}$$