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On Normalized Laplacians, Degree-Kirchhoff Index and Spanning Tree of Generalized Phenylene

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Abstract: The normalized Laplacian is extremely important for analyzing the structural properties of non-regular graphs. The molecular graph of generalized phenylene consists of n hexagons and $2n$ squares, denoted by $L_n^{6,4,4}$. In this paper, by using the normalized Laplacian polynomial decomposition theorem, we have investigated the normalized Laplacian spectrum of $L_n^{6,4,4}$ consisting of the eigenvalues of symmetric tri-diagonal matrices $\mathcal{L}_A$ and $\mathcal{L}_S$ of order $4n + 1$. As an application, the significant formula is obtained to calculate the multiplicative degree-Kirchhoff index and the number of spanning trees of generalized phenylene network based on the relationships between the coefficients and roots.

Keywords: generalized phenylene; normalized Laplacian; degree-Kirchhoff index; spanning tree

MSC: 05C69; 05C90

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1. Introduction and Preliminaries

In this paper, only simple, undirected, and finite graphs are considered. Assume that $G = (V_G, E_G)$ is a graph with vertex set V_G and edge set E_G . The order of G is denoted by $n = |V_G|$ and the size of G is denoted by $m = |E_G|$. The fundamental expressions and methodologies of graph theory have been used (see [1]). Assume that G is a graph of n vertices, adjacency matrix $A_G = [a_{ij}]_{n \times n}$ is a matrix, such that a_{ij} equals 1 if vertices v_i and v_j are adjacent and zero for otherwise. Assume that $D_G = \text{diag}(d_{v_1}, \dots, d_{v_n})$ is the vertex degree diagonal matrix of order n , where d_{v_i} is the degree of v_i , $1 \leq i \leq n$. Then $L_G = D_G - A_G$ is called the (combinational) Laplacian matrix of G .

The traditional concept of distance between vertices v_i and v_j , is the length of the shortest path obtained by joining these vertices of graph G and that is denoted by $d_{ij} = d_G(v_i, v_j)$. In graph theory, distance is also an essential invariant from which distance based parameters are obtained. In [2], a well-known distance based parameter named as *Wiener index* and denoted by W_G is introduced for the first time. This parameter is obtained by adding the distances between every pair of vertices in G , that is, $W_G = \sum_{\{v_i, v_j\} \subseteq V_G} d_{ij}$. Eventually, Gutman [3] also developed the Gutman index, which is a weighted variant of the Wiener index and defined as $\text{Gut}(G) = \sum_{\{v_i, v_j\} \subseteq V_G} d_i d_j d_{ij}$.

In [4], Klein and Randić suggested a novel distance function r_{ij} for a graph depending upon the electrical network theory, which is called the resistance distance. The Kirchhoff index was generated by Klein and Ivanciuc [5] and Klein and Randić [4] based on the resistance distance parameter and is denoted by $Kf(G) = \sum_{\{v_i, v_j\} \subseteq V_G} r_{ij}$.

Gutman and Mohar [6] established a result separately for the Kirchhoff index that is represented as,

$$Kf(G) = \sum_{i < j} r_{ij} = n \sum_{i=2}^n \frac{1}{\mu_i} \quad (1)$$

where $\mu_1 < \mu_2 \leq \dots \leq \mu_n$ with $\mu_1 = 0$ and $n \geq 2$ are the eigenvalues of L_G .

In [7], Chung proposed the *normalized Laplacian*, denoted by $\mathcal{L}_G$, that is, $\mathcal{L}_G = I - D_G^{-\frac{1}{2}}(D_G^{-1}A)D_G^{-\frac{1}{2}} = D_G^{-\frac{1}{2}}L_GD_G^{-\frac{1}{2}}$. As a result, it is easy to understand that

$$(\mathcal{L}_G)_{ij} = \begin{cases} 1, & \text{if } i = j; \\ -\frac{1}{\sqrt{d_i d_j}}, & \text{if } i \neq j, v_i \sim v_j; \\ 0, & \text{otherwise,} \end{cases} \quad (2)$$

where d_i (d_j) be the degree of the vertex v_i (v_j) and $(\mathcal{L}_G)_{ij}$ show the (i, j) -th values of $\mathcal{L}_G$. In 2007, Chen and Zhang [8] presented a new index based on normalized Laplacian, which is called the *multiplicative degree-Kirchhoff index* and defined it as, $Kf^*(G) = 2|E_G| \sum_{i=2}^n \frac{1}{\lambda_i}$. Moreover, the Kirchhoff index has gained much attention due to its widespread use in chemistry, physics, mathematics, and theoretical computer science. Many scientists have previously proposed new closed formulae of Kirchhoff and multiplicative degree-Kirchhoff indices, along with linear polyomino chains [9], circulant graphs [10], quadrilateral graphs [11], cycles [12], composite graphs [13], and so on. There are several results on the degree-Kirchhoff index and normalized Laplacian (see [14–25]).

Due to the widely applications, the molecular graphs phenylenes, pentagonal, hexagonal, and octagonal networks have attracted strong interests of chemists, mathematicians, and engineering. Phenylenes are two connected graphs with structure-property that each of their cells (or interior faces) has become a hexagon or square with the same edge length. Phenylene systems are essential in theoretical chemistry because they can reflect a hydrocarbon in nature. In [26,27], Gutman et al. addressed the phenylene enumeration problem using the Kekulé structure. Later, Pavlović and Gutman [28] have solved the problem of evaluating the Wiener index of phenylenes. Chen and Zhang [29] calculated the expected value of Wiener index (or the number of perfect matches) of the unique phenylene chain using a specific analytical expression. Recently, Geng and Lei [30] explicitly calculated the Kirchhoff index and spanning tree of phenylene chain.

In this article, by using the decomposition theorem for the normalized Laplacian characteristic polynomial, the multiplicative degree-Kirchhoff index, as well as spanning trees of $L_n^{6,4,4}$ are given explicit closed-form formulas.

2. Preliminaries

In the following section, we present some preliminary findings. In this context, the *characteristic polynomial* of the square matrix A is abbreviated as $\Psi(A) = \det(xI_n - A)$. We use abbreviations for simplicity $L_n^{6,4,4}$ to $\mathbb{L}_n$. It is not hard to find that $\pi = [(1, 1') \dots (4n + 1, (4n + 1)')] is an automorphism. The vertices of $\mathbb{L}_n$ as represented in Figure 1, then $V_1 = \{1, 2, \dots, 4n + 1\}$, $V_2 = \{1', 2', \dots, (4n + 1)'\}$, $|V(\mathbb{L}_n)| = 8n + 2$ and $|E(\mathbb{L}_n)| = 11n + 1$. The normalized Laplacian $\mathcal{L}(\mathbb{L}_n)$, the block matrix could be represented as follows.$

$$\mathcal{L}(\mathbb{L}_n) = \begin{pmatrix} \mathcal{L}_{V_{11}} & \mathcal{L}_{V_{12}} \\ \mathcal{L}_{V_{21}} & \mathcal{L}_{V_{22}} \end{pmatrix}.$$

Note that $\mathcal{L}_{V_{12}}(\mathbb{L}_n) = \mathcal{L}_{V_{21}}(\mathbb{L}_n)$ and $\mathcal{L}_{V_{11}}(\mathbb{L}_n) = \mathcal{L}_{V_{22}}(\mathbb{L}_n)$.

Figure 1. The graph $L_n^{6,4,4}$.

Let

$$T = \begin{pmatrix} \frac{1}{\sqrt{2}}I_{4n+1} & \frac{1}{\sqrt{2}}I_{4n+1} \\ \frac{1}{\sqrt{2}}I_{4n+1} & -\frac{1}{\sqrt{2}}I_{4n+1} \end{pmatrix}.$$

Then

$$T\mathcal{L}(\mathbb{L}_n)T' = \begin{pmatrix} \mathcal{L}_A & 0 \\ 0 & \mathcal{L}_S \end{pmatrix}.$$

$$\mathcal{L}_A(\mathbb{L}_n) = \mathcal{L}_{V_{11}} + \mathcal{L}_{V_{12}} \text{ and } \mathcal{L}_S(\mathbb{L}_n) = \mathcal{L}_{V_{11}} - \mathcal{L}_{V_{12}}. \quad (3)$$

The following lemmas are required to proceed in the future.

Lemma 1 (see [9]). Assume that G is a graph and let $\mathcal{L}_A, \mathcal{L}_S$ be described above. Then we have, $\Psi(\mathcal{L}(G)) = \Psi(\mathcal{L}_A(G)) \cdot \Psi(\mathcal{L}_S(G))$.

Lemma 2 (see [8]). Assume that G is an n vertex graph having size m , then $Kf^*(G) = 2m \sum_{i=2}^n \frac{1}{\mu_i}$.

Lemma 3 (see [7]). Assume that G is a connected graph having size m , then $\tau(G) = \frac{1}{2m} \prod_{i=1}^n d_i \prod_{k=2}^n \mu_k$, where $\tau(G)$ is spanning tree.

3. Main Results

In this section, the normalized Laplacian eigenvalues of $\mathbb{L}_n$ are first obtained. Next, we resolve to discover the calculation for multiplicative degree-Kirchhoff index (or spanning tree) of $\mathbb{L}_n$. Given a square matrix A with order n , we will write to $A[\{i_1, i_2, \dots, i_k\}]$ as the submatrix generated by eliminating the i_1 th, i_2 th, $\dots$, i_k th columns and rows of A . According to Equation (3), the block matrices could be represented as follows.

$$\mathcal{L}_{V_{11}}(\mathbb{L}_n) = \begin{pmatrix} 1 & -\frac{1}{2} & 0 & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & 1 & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & 1 \end{pmatrix}_{(4n+1) \times (4n+1)}$$

and

$$\mathcal{L}_S(\mathbb{L}_n) = \text{diag}\left(-\frac{1}{2}, 0, -\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}, \dots, -\frac{1}{3}, -\frac{1}{2}\right), \text{ a diagonal matrix of order } 4n+1.$$

Hence,

$$\mathcal{L}_A(\mathbb{L}_n) = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & 0 & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{1}{2} \end{pmatrix}_{(4n+1) \times (4n+1)}$$

and

$$\mathcal{L}_S(\mathbb{I}_n) = \begin{pmatrix} \frac{3}{2} & -\frac{1}{2} & 0 & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{4}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{4}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{3} & \frac{4}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & \frac{4}{3} & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{3}{2} \end{pmatrix}_{(4n+1) \times (4n+1)}.$$

Assume that the eigenvalues of $\mathcal{L}_A(\mathbb{I}_n)$ and $\mathcal{L}_S(\mathbb{I}_n)$, are respectively, represented as α_i ($i = 1, 2, \dots, 4n+1$) and β_j ($j = 1, 2, \dots, 4n+1$). According to Lemma 1 the spectrum of $\mathbb{I}_n$ is $\{\alpha_1, \alpha_2, \dots, \alpha_{4n+1}, \beta_1, \beta_2, \dots, \beta_{4n+1}\}$ and it is simple to see that $\alpha_1 = 0$, $\alpha_i > 2$, ($i = 2, 3, \dots, 4n+1$) and $\beta_j > 0$ ($j = 1, 2, \dots, 4n+1$). Hence, we have the lemma below.

Lemma 4. Suppose that $L_n^{6,4,4}$ be the generalized phenylenes $2n$ squares and n hexagons. Then

$$Kf^*(L_n^{6,4,4}) = 2(11n+1) \left[\sum_{i=2}^{4n+1} \frac{1}{\alpha_i} + \sum_{j=1}^{4n+1} \frac{1}{\beta_j} \right], \quad (4)$$

where α_i , ($i = 2, 3, \dots, 4n+1$) ($\alpha_i > 2$) and β_i , ($i = 1, 2, \dots, 4n+1$) are eigenvalues of $\mathcal{L}_A$ and $\mathcal{L}_S$, respectively.

According to the relationship between the coefficients and roots of $\Psi(\mathcal{L}_A)$ (respectively. $\Psi(\mathcal{L}_S)$), standard formulae of $\sum_{i=2}^{4n+1} \frac{1}{\alpha_i}$ (respectively. $\sum_{j=1}^{4n+1} \frac{1}{\beta_j}$) are given in the next lemmas.

Lemma 5. Suppose that $0 = \alpha_1 < \alpha_2 \leq \dots \leq \alpha_{4n+1}$ to be described as above. Then

$$\sum_{i=2}^{4n+1} \frac{1}{\alpha_i} = \frac{242n^3 + 66n^2 + 13n}{33n+3}.$$

Proof. Suppose that $\Psi(\mathcal{L}_A) = x^{4n+1} + a_1x^{4n} + \dots + a_{4n-1}x^2 + a_{4n}x$. Then $\alpha_2, \alpha_3, \dots, \alpha_{4n+1}$ are roots satisfies the equation below:

$$x^{4n} + a_1x^{4n-1} + \dots + a_{4n-1}x + a_{4n} = 0.$$

and so $\frac{1}{\alpha_2}, \frac{1}{\alpha_3}, \dots, \frac{1}{\alpha_{4n+1}}$ are roots satisfies the equation below:

$$a_{4n}x^{4n} + a_{4n-1}x^{4n-1} + \dots + a_1x + 1 = 0.$$

Hence, by Vieta's theorem (see [31], p. 81), we obtain

$$\sum_{i=2}^{4n+1} \frac{1}{\alpha_i} = \frac{(-1)^{4n-1}a_{4n-1}}{(-1)^{4n}a_{4n}}. \quad (5)$$

For the sake of convenience, we take S_i to the i -th order principal sub-matrix of $\mathcal{L}_A$, yield by the first i th columns and rows, $i = 1, 2, \dots, 4n$. Let $s_i = \det S_i$. Then

$$s_1 = \frac{1}{2}, s_2 = \frac{1}{4}, s_3 = \frac{1}{12}, s_4 = \frac{1}{36}, s_5 = \frac{1}{108}, s_6 = \frac{1}{216}, s_7 = \frac{1}{648}, s_8 = \frac{1}{1944}$$

and

$$\begin{cases} s_{4i} = \frac{2}{3}s_{4i-1} - \frac{1}{9}s_{4i-2}, & \text{for } 1 \leq i \leq n; \\ s_{4i+1} = \frac{2}{3}s_{4i} - \frac{1}{9}s_{4i-1}, & \text{for } 0 \leq i \leq n-1; \\ s_{4i+2} = s_{4i+1} - \frac{1}{6}s_{4i}, & \text{for } 0 \leq i \leq n-1; \\ s_{4i+3} = \frac{2}{3}s_{4i+2} - \frac{1}{6}s_{4i+1}, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

These formulas in general form could be derived by a straightforward calculation as shown below.

Case 1. Suppose s_{4i} , s_{4i+1} , s_{4i+2} and s_{4i+3} are defined as above. We have

$$\begin{cases} s_{4i} = \frac{3}{2}\left(\frac{1}{54}\right)^i, & \text{for } 1 \leq i \leq n; \\ s_{4i+1} = \frac{1}{2}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1; \\ s_{4i+2} = \frac{1}{4}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1; \\ s_{4i+3} = \frac{1}{12}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

In contrast, we take T_i to the i -th order principal sub-matrix of $\mathcal{L}_A$, built into the last i th columns and rows, $i = 1, 2, \dots, 4n$. Let $t_i = \det T_i$. Then

$$t_1 = \frac{1}{2}, t_2 = \frac{1}{6}, t_3 = \frac{1}{18}, t_4 = \frac{1}{36}, t_5 = \frac{1}{108}, t_6 = \frac{1}{324}, t_7 = \frac{1}{972}, t_8 = \frac{1}{1944}$$

and

$$\begin{cases} t_{4i} = t_{4i-1} - \frac{1}{6}t_{4i-2}, & \text{for } 1 \leq i \leq n; \\ t_{4i+1} = \frac{2}{3}t_{4i} - \frac{1}{6}t_{4i-1}, & \text{for } 0 \leq i \leq n-1; \\ t_{4i+2} = \frac{2}{3}t_{4i+1} - \frac{1}{9}t_{4i}, & \text{for } 0 \leq i \leq n-1; \\ t_{4i+3} = \frac{2}{3}t_{4i+2} - \frac{1}{9}t_{4i+1}, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

These formulas in general form could be derived by a straightforward calculation as shown below.

Case 2. Suppose t_{4i} , t_{4i+1} , t_{4i+2} and t_{4i+3} are defined as above. We have

$$\begin{cases} t_{4i} = \frac{3}{2}\left(\frac{1}{54}\right)^i, & \text{for } 1 \leq i \leq n; \\ t_{4i+1} = \frac{1}{2}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1; \\ t_{4i+2} = \frac{1}{6}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1; \\ t_{4i+3} = \frac{1}{18}\left(\frac{1}{54}\right)^i, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

When case 1 and case 2 are combined, the following fact can be deduced.

Fact 1. $(-1)^{4n}a_{4n} = \frac{11n+1}{72}\left(\frac{1}{54}\right)^{n-1}$.

Proof of Fact 1. The diagonal entries of $\mathcal{L}_A$ are denoted by l_{ii} . Due to the $(-1)^{4n}a_{4n}$ is a total of all principal minors of $\mathcal{L}_A$ with $4n$ rows and columns, we have

$$(-1)^{4n}a_{4n} = \sum_{i=1}^{4n+1} \det \mathcal{L}_A[i] = \sum_{i=1}^{4n+1} \det \begin{pmatrix} S_{i-1} & 0 \\ 0 & T \end{pmatrix} = \sum_{i=1}^{4n+1} \det S_{i-1} \det T, \quad (6)$$

where

$$T = \begin{pmatrix} k_{i+1,i+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & k_{4n,4n} & -\frac{1}{\sqrt{6}} \\ 0 & \cdots & -\frac{1}{\sqrt{6}} & k_{4n+1,4n+1} \end{pmatrix}.$$

Combining Case 1, Case 2 and Equation (6), we find

$$\begin{aligned}
 (-1)^{4n} a_{4n} &= \sum_{i=1}^{4n+1} \det \mathcal{L}_A[i] = \sum_{k=1}^n \det \mathcal{L}_A[4k] + \sum_{k=1}^{n-1} \det \mathcal{L}_A[4k+1] \\
 &\quad + \sum_{k=0}^{n-1} \det \mathcal{L}_A[4k+2] + \sum_{k=0}^{n-1} \det \mathcal{L}_A[4k+3] + s_{4k} + t_{4k} \\
 &= \sum_{k=1}^n s_{4(k-1)+3} t_{4(n-k)+1} + \sum_{k=1}^{n-1} s_{4k} t_{4(n-k)} + \sum_{k=0}^{n-1} s_{4k+1} t_{4(n-k-1)+3} \\
 &\quad + \sum_{k=0}^{n-1} s_{4k+2} t_{4(n-k-1)+2} + s_{4n} + t_{4n} \\
 &= \frac{11n+1}{72} \left(\frac{1}{54} \right)^{n-1}.
 \end{aligned}$$

as desired.

Fact 2. $(-1)^{4n-1} a_{4n-1} = \frac{242n^3+66n^2+13n}{216} \left(\frac{1}{54} \right)^{n-1}$.

Proof of Fact 2. Due to the $(-1)^{4n-1} a_{4n-1}$ is total of all principal minors of $\mathcal{L}_A$ with $3n-1$ rows and columns, we have

$$(-1)^{4n-1} a_{4n-1} = \begin{vmatrix} S_{i-1} & 0 & 0 \\ 0 & X & 0 \\ 0 & 0 & T \end{vmatrix}, \quad 1 \leq i < j \leq 4n+1, \quad (7)$$

where

$$X = \begin{pmatrix} k_{i+1,i+1} & -\frac{1}{\sqrt{6}} & \cdots & 0 \\ -\frac{1}{\sqrt{6}} & k_{i+2,i+2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & k_{j-1,j-1} \end{pmatrix} \text{ and } T = \begin{pmatrix} k_{j+1,j+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & k_{4n,4n} & -\frac{1}{\sqrt{6}} \\ 0 & \cdots & -\frac{1}{\sqrt{6}} & k_{4n+1,4n+1} \end{pmatrix}.$$

Notice that

$$(-1)^{4n-1} a_{4n-1} = \sum_{1 \leq i < j} \mathcal{L}_A[i, j] = \sum_{1 \leq i < j} S_{i-1} \det X \det T = \sum_{1 \leq i < j} s_{i-1} t_{4n+1-j} \det X. \quad (8)$$

In view of Equation (8), we know that $\det X$ will change as a result of the various i and j options. Hence, we will discuss by separating the cases below.

Case 1. Let $i = 4k$ and $j = 4l$, for $1 \leq i < j \leq 4n+1$. Therefore, $1 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 1)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = 12(l-k) \left(\frac{1}{54} \right)^{l-k}.$$

Case 2. Let $i = 4k$ and $j = 4l + 1$, for $1 \leq i < i + 1 < j \leq 4n + 1$. Therefore, $1 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = (4l - 4k + 1) \left(\frac{1}{54} \right)^{l-k}.$$

Case 3. Let $i = 4k$ and $j = 4l + 2$, for $1 \leq i < j \leq 4n + 1$. Therefore, $1 \leq k \leq l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k + 1)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{4}{3}l - \frac{4}{3}k + \frac{2}{3} \right) \left(\frac{1}{54} \right)^{l-k}.$$

Case 4. Let $i = 4k$ and $j = 4l + 3$, for $1 \leq i < j \leq 4n + 1$. Therefore, $1 \leq k \leq l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k + 2)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{2}{3}l - \frac{2}{3}k + \frac{1}{2} \right) \left(\frac{1}{54} \right)^{l-k}.$$

Case 5. Let $i = 4k + 1$ and $j = 4l$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 2)$.

$$\det X = \begin{vmatrix} 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{2}{3}l - \frac{2}{3}k - \frac{1}{6} \right) \left(\frac{1}{54} \right)^{l-k-1}.$$

Case 6. Let $i = 4k + 1$ and $j = 4l + 1$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 1)$.

$$\det X = \begin{vmatrix} 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{2}{9}l - \frac{2}{9}k\right) \left(\frac{1}{54}\right)^{l-k-1}.$$

Case 7. Let $i = 4k + 1$ and $j = 4l + 2$, for $1 \leq i < i + 1 < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k)$.

$$\det X = \begin{vmatrix} 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = (4l - 4k + 1) \left(\frac{1}{54}\right)^{l-k}.$$

Case 8. Let $i = 4k + 1$ and $j = 4l + 3$, for $1 \leq i < i + 1 < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k + 1)$.

$$\det X = \begin{vmatrix} 1 & -\frac{1}{\sqrt{6}} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{6}} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{3} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = (2l - 2k + 1) \left(\frac{1}{54}\right)^{l-k}.$$

Case 9. Let $i = 4k + 2$ and $j = 4l$, for $1 \leq i < i + 1 < j \leq 4n + 1$. Therefore, $0 \leq k < k + 1 < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 3)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{4}{3}l - \frac{4}{3}k - \frac{2}{3}\right) \left(\frac{1}{54}\right)^{l-k-1}.$$

Case 10. Let $i = 4k + 2$ and $j = 4l + 1$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 2)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{4}{9}l - \frac{4}{9}k - \frac{1}{9} \right) \left(\frac{1}{54} \right)^{l-k-1}.$$

Case 11. Let $i = 4k + 2$ and $j = 4l + 2$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k - 1)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = 8(l - k) \left(\frac{1}{54} \right)^{l-k}.$$

Case 12. Let $i = 4k + 2$ and $j = 4l + 3$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = (4l - 4k + 1) \left(\frac{1}{54} \right)^{l-k}.$$

Case 13. Let $i = 4k + 3$ and $j = 4l$, for $1 \leq i < i + 1 < j \leq 4n + 1$. Therefore, $0 \leq k < k + 1 < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 4)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = (4l - 4k - 3) \left(\frac{1}{54} \right)^{l-k-1}.$$

Case 14. Let $i = 4k + 3$ and $j = 4l + 1$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n$. In this case, X is the square matrix of order $(4l - 4k - 3)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{6}} & \frac{2}{3} \end{vmatrix} = \left(\frac{4}{3}l - \frac{4}{3}k - \frac{2}{3}\right) \left(\frac{1}{54}\right)^{l-k-1}.$$

Case 15. Let $i = 4k + 3$ and $j = 4l + 2$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k - 2)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = \left(\frac{4}{9}l - \frac{4}{9}k - \frac{1}{9}\right) \left(\frac{1}{54}\right)^{l-k-1}.$$

Case 16. Let $i = 4k + 3$ and $j = 4l + 3$, for $1 \leq i < j \leq 4n + 1$. Therefore, $0 \leq k < l \leq n - 1$. In this case, X is the square matrix of order $(4l - 4k - 1)$.

$$\det X = \begin{vmatrix} \frac{2}{3} & -\frac{1}{3} & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{\sqrt{6}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{6}} & 1 & -\frac{1}{\sqrt{6}} & \cdots & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{6}} & \frac{2}{3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & \frac{2}{3} & -\frac{1}{3} \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{3} & \frac{2}{3} \end{vmatrix} = \left(\frac{2}{9}l - \frac{2}{9}k\right) \left(\frac{1}{54}\right)^{l-k-1}.$$

If Equation (8) and Cases 1–16 are combined, we have

$$\begin{aligned} (-1)^{4n-1} a_{4n-1} &= \sum_{1 \leq i < j \leq 4n+1} s_{i-1} t_{4n+1-j} \cdot \det X_{j-1-i} \\ &= \zeta_1 + \zeta_2 + \zeta_3 + \zeta_4, \end{aligned} \quad (9)$$

where

$$\begin{aligned} \zeta_1 &= \sum_{1 \leq k < l \leq n} \det \mathcal{L}_A[4k, 4l] + \sum_{1 \leq k \leq l \leq n-1} \det \mathcal{L}_A[4k, 4l + 1] + \sum_{1 \leq k \leq l \leq n-1} \det \mathcal{L}_A[4k, 4l + 2] \\ &\quad + \sum_{1 \leq k \leq l \leq n-1} \det \mathcal{L}_A[4k, 4l + 3] + \sum_{1 \leq k \leq n} \det \mathcal{L}_A[4k, 4n + 1] \\ &= \frac{n(n^2 - 1)}{12} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(4n-5)}{48} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(2n-1)}{36} \left(\frac{1}{54}\right)^{n-1} \\ &\quad + \frac{n(n-1)(4n+1)}{48} \left(\frac{1}{54}\right)^{n-1} + \frac{n(2n-1)}{12} \left(\frac{1}{54}\right)^{n-1} \\ &= \frac{11n^3 - 6n^2 - 2n}{36} \left(\frac{1}{54}\right)^{n-1}, \end{aligned}$$

$$\begin{aligned}
\xi_2 &= \sum_{1 \leq k < l \leq n} \det \mathcal{L}_A[4k+1, 4l] + \sum_{1 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+1, 4l+1] + \sum_{1 \leq k \leq l \leq n-1} \det \mathcal{L}_A[4k+1, 4l+2] \\
&+ \sum_{1 \leq k \leq l \leq n-1} \det \mathcal{L}_A[4k+1, 4l+3] + \sum_{1 \leq k \leq n-1} \det \mathcal{L}_A[4k+1, 4n+1] + \sum_{1 \leq l \leq n} \det \mathcal{L}_A[1, 4l] \\
&+ \sum_{1 \leq l \leq n-1} \det \mathcal{L}_A[1, 4l+1] + \sum_{0 \leq l \leq n-1} \det \mathcal{L}_A[1, 4l+2] + \sum_{0 \leq l \leq n-1} \det \mathcal{L}_A[1, 4l+3] + X_{4n-1} \\
&= \frac{n(n-1)(4n+1)}{48} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(n-2)}{12} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(4n-5)}{72} \left(\frac{1}{54}\right)^{n-1} \\
&+ \frac{n(n-1)(2n-1)}{24} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)}{6} \left(\frac{1}{54}\right)^{n-1} + \frac{n(2n+1)}{12} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)}{6} \left(\frac{1}{54}\right)^{n-1} \\
&+ \frac{n(2n-1)}{18} \left(\frac{1}{54}\right)^{n-1} + \frac{n^2}{6} \left(\frac{1}{54}\right)^{n-1} + \frac{2n}{9} \left(\frac{1}{54}\right)^{n-1} \\
&= \frac{44n^3 + 31n^2 + 25n}{144} \left(\frac{1}{54}\right)^{n-1},
\end{aligned}$$

$$\begin{aligned}
\xi_3 &= \sum_{0 \leq k < l \leq n} \det \mathcal{L}_A[4k+2, 4l] + \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+2, 4l+1] + \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+2, 4l+2] \\
&+ \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+2, 4l+3] + \sum_{0 \leq k \leq n-1} \det \mathcal{L}_A[4k+2, 4n+1] \\
&= \frac{n(n+1)(2n+1)}{36} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(4n+1)}{72} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n^2-1)}{27} \left(\frac{1}{54}\right)^{n-1} \\
&+ \frac{n(n+1)(4n-1)}{72} \left(\frac{1}{54}\right)^{n-1} + \frac{n(2n+1)}{18} \left(\frac{1}{54}\right)^{n-1} \\
&= \frac{22n^3 + 21n^2 + 2n}{108} \left(\frac{1}{54}\right)^{n-1}
\end{aligned}$$

and

$$\begin{aligned}
\xi_4 &= \sum_{0 \leq k < l \leq n} \det \mathcal{L}_A[4k+3, 4l] + \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+3, 4l+1] + \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+3, 4l+2] \\
&+ \sum_{0 \leq k < l \leq n-1} \det \mathcal{L}_A[4k+3, 4l+3] + \sum_{0 \leq k \leq n-1} \det \mathcal{L}_A[4k+3, 4n+1] \\
&= \frac{n(n+1)(4n-1)}{48} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(2n-1)}{24} \left(\frac{1}{54}\right)^{n-1} + \frac{n(n-1)(4n+1)}{72} \left(\frac{1}{54}\right)^{n-1} \\
&+ \frac{n(n^2-1)}{12} \left(\frac{1}{54}\right)^{n-1} + \frac{n^2}{6} \left(\frac{1}{54}\right)^{n-1} \\
&= \frac{44n^3 + 9n^2 - 11}{144} \left(\frac{1}{54}\right)^{n-1}.
\end{aligned}$$

By substituting ξ_1 , ξ_2 , ξ_3 and ξ_4 into Equation (9), the Fact 3 is completed. The required results of Lemma 5 can be obtained by combining Fact 1 and Fact 3. $\square$

Lemma 6. Let $0 = \beta_1 < \beta_2 \leq \dots \leq \beta_{4n+1}$ be the eigenvalues of $\mathcal{L}_S$ as above. Then

$$\sum_{j=1}^{4n+1} \frac{1}{\beta_j} = \frac{v_1 + v_2}{840[(2408 + 235\sqrt{105})(41 + 4\sqrt{105})^{n-1} + (2408 - 235\sqrt{105})(41 - 4\sqrt{105})^{n-1}]},$$

where $v_1 = (1, 394, 820 + 136, 133\sqrt{105} + 2380n(3525 + 344\sqrt{105}))(41 + 4\sqrt{105})^{n-1}$ and $v_2 = (1, 394, 820 - 136, 133\sqrt{105} + 2380n(3525 - 344\sqrt{105}))(41 - 4\sqrt{105})^{n-1}$.

Proof. Suppose that $\Psi(\mathcal{L}_S) = x^{4n+1} + b_1x^{4n} + \dots + b_{4n}x + b_{4n+1}$.
So $\frac{1}{\beta_1}, \frac{1}{\beta_2}, \dots, \frac{1}{\beta_{4n+1}}$ are roots satisfies the equation below:

$$b_{4n+1}x^{4n+1} + b_{4n}x^{4n} + \dots + b_1x + 1 = 0.$$

By Vieta's theorem (see [31], p. 81), we find

$$\sum_{i=1}^{4n+1} \frac{1}{\beta_i} = \frac{(-1)^{4n}b_{4n}}{(-1)^{4n+1}b_{4n+1}} = \frac{(-1)^{4n}b_{4n}}{\det \mathcal{L}_S}. \quad (10)$$

In order to find $\det \mathcal{L}_S$ and $(-1)^{4n}b_{4n}$, consider D_i to be the i -th order principal sub-matrix of $\mathcal{L}_S$, created by the first i rows and columns, $1 \leq i \leq 4n$. Let $d_i = \det D_i$. Then $d_1 = \frac{3}{2}, d_2 = \frac{5}{4}, d_3 = \frac{17}{12}, d_4 = \frac{7}{4}, d_5 = \frac{235}{108}, d_6 = \frac{407}{216}, d_7 = \frac{1393}{648}, d_8 = \frac{5164}{1944}$ and

$$\begin{cases} d_{4i} = \frac{4}{3}d_{4i-1} - \frac{1}{9}d_{4i-2}, & \text{for } 1 \leq i \leq n; \\ d_{4i+1} = \frac{4}{3}d_{4i} - \frac{1}{9}d_{4i-1}, & \text{for } 0 \leq i \leq n-1; \\ d_{4i+2} = d_{4i+1} - \frac{1}{6}d_{4i}, & \text{for } 0 \leq i \leq n-1; \\ d_{4i+3} = \frac{4}{3}d_{4i+2} - \frac{1}{6}d_{4i+1}, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

We have adopted similar computation as described above.

$$\begin{cases} d_{4i} = \frac{210+11\sqrt{105}}{280} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{210-11\sqrt{105}}{280} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 1 \leq i \leq n; \\ d_{4i+1} = \frac{45+4\sqrt{105}}{60} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{45-4\sqrt{105}}{60} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1; \\ d_{4i+2} = \frac{1050+101\sqrt{105}}{1680} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{1050-101\sqrt{105}}{1680} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1; \\ d_{4i+3} = \frac{595+58\sqrt{105}}{840} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{595-58\sqrt{105}}{840} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

Fact 3. $\det \mathcal{L}_S = \frac{2408+235\sqrt{105}}{2016} \left(\frac{41+4\sqrt{105}}{54} \right)^{n-1} + \frac{2408-235\sqrt{105}}{2016} \left(\frac{41-4\sqrt{105}}{54} \right)^{n-1}$.

Proof of Fact 3. We can achieve $\det \mathcal{L}_S$ in relation to its last row as

$$\begin{aligned} \det \mathcal{L}_S &= \frac{3}{2} \det d_{4n} - \frac{1}{6} \det d_{4n-1} = \frac{3}{2} \left[\frac{210+11\sqrt{105}}{280} \left(\frac{41+4\sqrt{105}}{54} \right)^n + \frac{210-11\sqrt{105}}{280} \left(\frac{41-4\sqrt{105}}{54} \right)^n \right] \\ &\quad - \frac{1}{6} \left[\frac{595+58\sqrt{105}}{840} \left(\frac{41+4\sqrt{105}}{54} \right)^{n-1} + \frac{595-58\sqrt{105}}{840} \left(\frac{41-4\sqrt{105}}{54} \right)^{n-1} \right] \\ &= \frac{2408+235\sqrt{105}}{2016} \left(\frac{41+4\sqrt{105}}{54} \right)^{n-1} + \frac{2408-235\sqrt{105}}{2016} \left(\frac{41-4\sqrt{105}}{54} \right)^{n-1}. \end{aligned}$$

On the other hand, consider H_i to be the i -th order principal sub-matrix of $\mathcal{L}_S$, created by the last i rows and columns, $1 \leq i \leq 4n$. Let $h_i = \det H_i$. Then $h_1 = \frac{3}{2}, h_2 = \frac{11}{6}, h_3 = \frac{41}{18}, h_4 = \frac{71}{36}, h_5 = \frac{9}{4}, h_6 = \frac{901}{324}, h_7 = \frac{3361}{972}, h_8 = \frac{5821}{1944}$ and

$$\begin{cases} h_{4i} = h_{4i-1} - \frac{1}{6}h_{4i-2}, & \text{for } 1 \leq i \leq n; \\ h_{4i+1} = \frac{4}{3}h_{4i} - \frac{1}{6}h_{4i-1}, & \text{for } 0 \leq i \leq n-1; \\ h_{4i+2} = \frac{4}{3}h_{4i+1} - \frac{1}{9}h_{4i}, & \text{for } 0 \leq i \leq n-1; \\ h_{4i+3} = \frac{4}{3}h_{4i+2} - \frac{1}{9}h_{4i+1}, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

We have adopted similar computation as described above.

$$\begin{cases} h_{4i} = \frac{42+3\sqrt{105}}{56} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{42-3\sqrt{105}}{56} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 1 \leq i \leq n; \\ h_{4i+1} = \frac{21+2\sqrt{105}}{28} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{21-2\sqrt{105}}{28} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1; \\ h_{4i+2} = \frac{154+15\sqrt{105}}{168} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{154-15\sqrt{105}}{168} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1; \\ h_{4i+3} = \frac{41+4\sqrt{105}}{36} \left(\frac{41+4\sqrt{105}}{54} \right)^i + \frac{41-4\sqrt{105}}{36} \left(\frac{41-4\sqrt{105}}{54} \right)^i, & \text{for } 0 \leq i \leq n-1. \end{cases}$$

Fact 4.

$$\begin{aligned} (-1)^{4n} b_{4n} = & \frac{1,394,820 + 136,133\sqrt{105} + 2380n(3525 + 344\sqrt{105})}{1,693,440} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} \\ & + \frac{1,394,820 - 136,133\sqrt{105} + 2380n(3525 - 344\sqrt{105})}{1,693,440} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1}. \end{aligned}$$

Proof of Fact 4. We noticed that $(-1)^{4n} b_{4n}$ is a total of all principal minors of $\mathcal{L}_S$ which have $4n$ rows and columns, then

$$(-1)^{4n} b_{4n} = \sum_{i=1}^{4n+1} \det \mathcal{L}_S[i] = \sum_{i=1}^{4n+1} \det \begin{pmatrix} D_{i-1} & 0 \\ 0 & H_{4n+1-i} \end{pmatrix} = \sum_{i=1}^{4n+1} \det d_{i-1} \det h_{4n+1-i}, \quad (11)$$

where

$$H_{4n+1-i} = \begin{pmatrix} l_{i+1,i+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{4n,4n} & -\frac{1}{\sqrt{6}} \\ 0 & \cdots & -\frac{1}{\sqrt{6}} & l_{4n+1,4n+1} \end{pmatrix}.$$

In line with the above Equation (10), we find

$$\begin{aligned} (-1)^{4n} b_{4n} = & \sum_{i=1}^{4n+1} \det \mathcal{L}_S[i] = \sum_{k=1}^n \det \mathcal{L}_S[4k] + \sum_{k=0}^{n-1} \det \mathcal{L}_S[4k+1] \\ & + \sum_{k=0}^{n-1} \det \mathcal{L}_S[4k+2] + \sum_{k=0}^{n-1} \det \mathcal{L}_S[4k+3] + d_{4n} \\ = & \sum_{k=1}^n d_{4(k-1)+3} h_{4(n-k)+1} + \sum_{k=1}^{n-1} d_{4k} h_{4(n-k)} + \sum_{k=0}^{n-1} d_{4k+1} h_{4(n-k-1)+3} \\ & + \sum_{k=0}^{n-1} d_{4k+2} h_{4(n-k-1)+2} + d_{4n} + h_{4n}. \end{aligned} \quad (12)$$

The following forms could be derived using the above equations.

$$\begin{aligned} \sum_{k=1}^n d_{4(k-1)+3} h_{4(n-k)+1} = & n \left[\frac{3525 + 344\sqrt{105}}{3360} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{3525 - 344\sqrt{105}}{3360} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1} \right] \\ & + \frac{27\sqrt{105}}{15,680} \left(\frac{41 + 4\sqrt{105}}{54} \right)^n - \frac{27\sqrt{105}}{15,680} \left(\frac{41 - 4\sqrt{105}}{54} \right)^n, \end{aligned} \quad (13)$$

$$\begin{aligned} \sum_{k=1}^{n-1} d_{4k} h_{4(n-k)} = & (n-1) \left[\frac{1755 + 156\sqrt{105}}{2240} \left(\frac{41 + 4\sqrt{105}}{54} \right)^n + \frac{1755 - 156\sqrt{105}}{2240} \left(\frac{41 - 4\sqrt{105}}{54} \right)^n \right] \\ & + \frac{17}{1,128,960} \sqrt{105} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} - \frac{17}{1,128,960} \sqrt{105} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1}, \end{aligned} \quad (14)$$

$$\sum_{k=0}^{n-1} d_{4k+1} h_{3(n-k-1)+3} = n \left[\frac{3525 + 344\sqrt{105}}{2160} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{3525 - 344\sqrt{105}}{2160} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1} \right] \\ + \frac{11}{1120} \sqrt{105} \left(\frac{41 + 4\sqrt{105}}{54} \right)^n - \frac{11}{1120} \sqrt{105} \left(\frac{41 - 4\sqrt{105}}{54} \right)^n, \quad (15)$$

$$\sum_{k=0}^{n-1} d_{4k+2} h_{4(n-k-1)+2} = n \left[\frac{45,825 + 4472\sqrt{105}}{40,320} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{45,825 - 4472\sqrt{105}}{40,320} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1} \right] \\ + \frac{15}{12,544} \sqrt{105} \left(\frac{41 + 4\sqrt{105}}{54} \right)^n - \frac{15}{12,544} \sqrt{105} \left(\frac{41 - 4\sqrt{105}}{54} \right)^n \quad (16)$$

and

$$d_{4n} + h_{4n} = \frac{210 + 13\sqrt{105}}{140} \left(\frac{41 + 4\sqrt{105}}{54} \right)^n + \frac{210 - 13\sqrt{105}}{140} \left(\frac{41 - 4\sqrt{105}}{54} \right)^n. \quad (17)$$

Fact 3 is derived by substituting Equations (13)–(17) into (12).

Lemma 3 follows directly from Equation (10) and Facts 3 and 4. $\square$

We can easily obtain the following theorems by combining Lemmas 4–6.

Theorem 1. Let $L_n^{6,4,4}$ be a generalized phenylenes with n hexagons and $2n$ squares. Then

$$Kf^*(L_n(6,4,4)) = 2(11n + 1) \left[\frac{242n^3 + 66n^2 + 13n}{33n + 3} + \frac{(-1)^{4n} b_{4n}}{\det \mathcal{L}_S} \right],$$

where

$$(-1)^{4n} b_{4n} = \frac{1,394,820 + 136,133\sqrt{105} + 2380n(3525 + 344\sqrt{105})}{1,693,440} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} \\ + \frac{1,394,820 - 136,133\sqrt{105} + 2380n(3525 - 344\sqrt{105})}{1,693,440} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1},$$

$$\det \mathcal{L}_S = \frac{2408 + 235\sqrt{105}}{2016} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{2408 - 235\sqrt{105}}{2016} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1}.$$

Theorem 2. Let $L_n^{6,4,4}$ be a generalized phenylenes with n hexagons and $2n$ squares. Then

$$\tau(L_n^{6,4,4}) = 2^{n+1} \cdot 3^{3n-1} \left[\frac{2408 + 235\sqrt{105}}{2016} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{2408 - 235\sqrt{105}}{2016} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1} \right].$$

Proof. By Lemma 3, then we have $\prod_{i=2}^{4n+1} \alpha_i \prod_{i=1}^{4n+1} \beta_i \prod_{v \in V_{L_n^{6,4,4}}} d_{L_n^{6,4,4}} = 2|E_{L_n^{6,4,4}}| \tau(L_n^{6,4,4})$.

Noted that

$$\prod_{v \in V_{L_n^{6,4,4}}} d_{L_n^{6,4,4}} = 2^{2n+4} \cdot 3^{6n-2}, \quad |E_{L_n^{6,4,4}}| = 11n + 1,$$

$$\prod_{i=2}^{4n+1} \alpha_i = \frac{11n + 1}{72} \left(\frac{1}{54} \right)^{n-1},$$

$$\prod_{i=1}^{4n+1} \beta_i = \frac{2408 + 235\sqrt{105}}{2016} \left(\frac{41 + 4\sqrt{105}}{54} \right)^{n-1} + \frac{2408 - 235\sqrt{105}}{2016} \left(\frac{41 - 4\sqrt{105}}{54} \right)^{n-1}.$$

Hence, Theorem 2 immediately follows, along with Lemma 3. $\square$

4. Conclusions

In this article, the molecular graph $L_n^{6,4,4}$ of generalized phenylene containing $2n$ squares and n hexagons is considered. According to the decomposition theorem of normalized Laplacian polynomial, we achieve expressive formulas for the degree-Kirchhoff index and spanning tree of $L_n^{6,4,4}$.

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