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On the Laplacian, the Kirchhoff Index, and the Number of Spanning Trees of the Linear Pentagonal Derivation Chain

Yue Tu, Xiaoling Ma *, Yuqing Zhang and Junyu Ren

College of Mathematics and System Sciences, Xinjiang University, Urumqi 830017, China; ty6@stu.xju.edu.cn (Y.T.); zhangyuqing@stu.xju.edu.cn (Y.Z.); cap_scheddi@stu.xju.edu.cn (J.R.)
* Correspondence: mathmxl115@xju.edu.cn

Abstract: Let P_n be a pentagonal chain with $2n$ pentagons in which two pentagons with two edges in common can be regarded as adding one vertex and two edges to a hexagon. Thus, the linear pentagonal derivation chains QP_n represent the graph obtained by attaching four-membered rings to every two pentagons of P_n. In this article, the Laplacian spectrum of QP_n consisting of the eigenvalues of two symmetric matrices is determined. Next, the formulas for two graph invariants that can be represented by the Laplacian spectrum, namely, the Kirchhoff index and the number of spanning trees, are studied. Surprisingly, the Kirchhoff index is almost one half of the Wiener index of a linear pentagonal derivation chain QP_n.

Keywords: linear pentagonal derived graphs; Laplacian spectrum; Kirchhoff index; number of spanning trees

MSC: 05C99

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1. Introduction

In this work, we will use terminologies and traditional notations from [1]. Let $G = (V(G), E(G))$ be a finite, simple, and undirected connected graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$. The order of G is the number $|V(G)|$ of its vertices and its size is the number $|E(G)|$ of its edges. The adjacency matrix of G, denoted by $A(G)$, is a $0-1$ $n \times n$ matrix whose (i, j)-entry is equal to 1 if v_i and v_j are adjacent in G and 0 otherwise. The degree of v_i in G is denoted by $d_i = d_G(v_i)$.

The Laplacian matrix of G is the matrix $L(G) = D(G) - A(G)$, where $D(G)$ is the diagonal matrix of G whose diagonal entries are the degrees of the vertices of G. The characteristic polynomial of $L(G)$ is defined as

$$\Phi_{L(G)}(\lambda) = \det(\lambda I_n - L(G)),$$

where I_n is the identity matrix of order n. Note that $L(G)$ is positive semi-definite. The Laplacian spectrum of G is denoted by $spec(L(G)) = \{\mu_1, \mu_2, \cdots, \mu_n\}$, and we assume that the eigenvalues are labeled such that $0 = \mu_1 < \mu_2 \leq \cdots \leq \mu_n$.

The distance between vertices v_i and v_j in G, denoted by $d_{ij} = d(v_i, v_j)$, is the length of the shortest path between them in G. The Wiener index, a distance-based topological index, was first presented by Wiener in chemistry back in 1947 [2] and in mathematics about 40 years later [3]. The famous Wiener index $W(G)$ is defined as

$$W(G) = \sum_{i<j} d_{ij},$$

where the sum is taken over all distances between pairs of vertices of G.

At present, the Wiener index has been widely studied, and many research results have been obtained [4–9].

The topological index in a graph distance function can explain the structure and properties of a graph well. In 1993, Klein and Randić [10] introduced a distance function named resistance distance on the basis of electrical network theory. The resistance distance between vertices v_i and v_j, denoted by r_{ij}, is defined to be the effective electrical resistance between them if each edge of G is replaced by a unit resistor. One famous resistance distance-based parameter called the Kirchhoff index, $Kf(G)$ [10], was given by

$$Kf(G) = \sum_{i<j} r_{ij}.$$

Moreover, Klein and Randić [10] proved that $r_{ij} \leq d_{ij}$ and $Kf(G) \leq W(G)$ with equality if and only if G is a tree.

Similar to the Wiener index, the Kirchhoff index is also intrinsic to the graph, not only with some fine, purely mathematical properties, but also with a substantial potential for chemical applications. Unfortunately, it is difficult to compute the resistant distance and Kirchhoff index in a graph due to their computational complexity. Thus, it is necessary to find closed-form formulas for the Kirchhoff index.

It is worth noting that the resistance distance between any two vertices can be obtained in terms of the eigenvalues and eigenvectors of the Laplacian matrix in an electronic network. Therefore, for any connected graph G of order $n \geq 2$, it is shown, independently, by Gutman and Mohar [11] and Zhu et al. [12] that

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

For some graphs with a good structure, such as graphs with good periodicity and good symmetry, researchers can calculate the closed-form formulas of the Kirchhoff index of those graphs. Readers are referred to the references [13–18] and the references therein.

A linear pentagonal chain of length n, denoted by P_n, is a pentagonal chain with $2n$ pentagons in which two pentagons with two edges in common can be regarded as adding one vertex and two edges to a hexagon. Wang and Zhang [19] obtained the explicit closed-form formulas of the Kirchhoff index of linear pentagonal chains. Wei et al. [20] made comparisons between the expected values of the Wiener index and the Kirchhoff index in random pentachains and presented the average values of the Wiener and Kirchhoff indices with respect to the set of all random pentachains with n pentagons. Recently, Sahir and Nayeem [21] derived closed-form formulas for the Kirchhoff index and the Wiener index of the linear pentagonal cylinder graph and the linear pentagonal Möbius chain graph. The study of hexagonal systems have attracted interest because they are natural graph representations of benzenoid hydrocarbon [22], and they have been of great interest and extensively studied; see [5,17,23].

Consider a linear pentagonal chain P_n consisting of $2n$ pentagons. The linear pentagonal derivation chain, denoted by QP_n, is thus the graph obtained by attaching four-membered rings to every two pentagons of P_n, as depicted in Figure 1. It is easy to check that $|V(QP_n)| = 7n + 2$, $|E(QP_n)| = 10n + 1$. Obviously, the linear pentagonal derivation chain QP_n is different from random pentachains, a linear pentagonal cylinder graph, and a linear pentagonal Möbius chain graph.

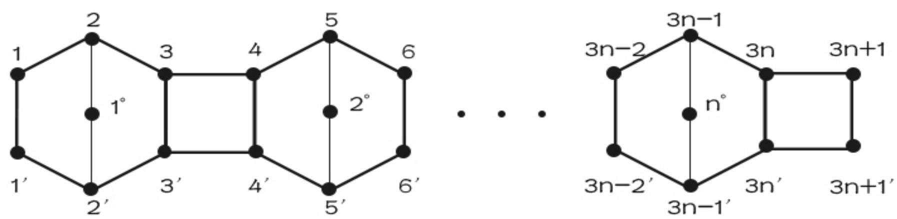

Figure 1. The linear pentagonal derivation chain QP_n.

In this paper, we focus on the linear pentagonal derivation chain QP_n. Firstly, the Laplacian spectrum of QP_n consisting of the eigenvalues of two symmetric matrices, is determined. Next, using the decomposition theorem for the Laplacian characteristic polynomial, the explicit closed-form formulas for the Kirchhoff index and the number of spanning trees of QP_n can be represented. Interestingly, the Kirchhoff index is about half of the Wiener index of a linear pentagonal derivation chain QP_n.

2. Laplacian Polynomial Decomposition and Some Preliminary Results

An automorphism of G is a permutation π of $V(G)$, which has the property that v_iv_j is an edge of G if and only if $\pi(v_i)\pi(v_j)$ is an edge of G. Suppose that G has an automorphism π. It can then be written as the product of disjoint 1-cycles and transpositions.

Assume we label the vertices of QP_n as in Figure 1 and denote

$$V_0 = \{1^\circ, 2^\circ, \ldots, n^\circ\}, V_1 = \{1, 2, \ldots, 3n+1\}, V_2 = \{1', 2', \ldots, (3n+1)'\}.$$

Therefore,

$$\pi = (1^\circ)(2^\circ)\cdots(n^\circ)(1,1')(2,2')\cdots(3n+1,(3n+1)')$$

is an automorphism of QP_n. Hence, the Laplacian matrix $L(G)$ of QP_n can be written as the following block matrix:

$$L(G) = \begin{bmatrix} L_{V_0V_0} & L_{V_0V_1} & L_{V_0V_2} \\ L_{V_1V_0} & L_{V_1V_1} & L_{V_1V_2} \\ L_{V_2V_0} & L_{V_2V_1} & L_{V_2V_2} \end{bmatrix},$$

where $L_{V_iV_j}$ is the submatrix formed by rows corresponding to vertices in V_i and columns corresponding to vertices in V_j for $i, j = 0, 1, 2$.

Let

$$T = \begin{bmatrix} I_n & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & (\frac{1}{\sqrt{2}})I_{3n+1} & (\frac{1}{\sqrt{2}})I_{3n+1} \\ \mathbf{0} & (\frac{1}{\sqrt{2}})I_{3n+1} & -(\frac{1}{\sqrt{2}})I_{3n+1} \end{bmatrix}$$

be the block matrix such that the blocks have the same dimension as the corresponding blocks in $L(G)$. By the unitary transformation $TL(G)T$, we obtain

$$TL(G)T = \begin{bmatrix} L_A & \mathbf{0} \\ \mathbf{0} & L_S \end{bmatrix},$$

where

$$L_A = \begin{bmatrix} L_{V_0V_0} & \sqrt{2}L_{V_0V_1} \\ \sqrt{2}L_{V_1V_0} & L_{V_1V_1} + L_{V_1V_2} \end{bmatrix}, \quad L_S = L_{V_2V_2} - L_{V_1V_2}. \tag{2}$$

Based on the arguments above, Yang and Yu [24] derived the following decomposition theorem for the Laplacian characteristic polynomial of G.

Lemma 1 ([24]). *Suppose $L(G)$, L_A, and L_S are defined as above. We then have*

$$\Phi_{L(G)}(\lambda) = \Phi_{L_A}(\lambda)\Phi_{L_S}(\lambda).$$

Lemma 2 ([25]). *Let G be a connected graph of order n. Therefore,*

$$\tau(G) = \frac{1}{n}\prod_{i=2}^{n}\mu_i, \tag{3}$$

where $\tau(G)$ is the number of spanning trees of G.

Lemma 3 ([26]). *Let M_1, M_2, M_3, and M_4 be, respectively, $p \times p$, $p \times q$, $q \times p$, and $q \times q$ matrices with M_1 and M_4 being invertible. Thus,*

$$\det\begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix} = \det(M_1) \cdot \det(M_4 - M_3 M_1^{-1} M_2) = \det(M_4) \cdot \det(M_1 - M_2 M_4^{-1} M_3),$$

where $M_4 - M_3M_1^{-1}M_2$ and $M_1 - M_2M_4^{-1}M_3$ are called the Schur complements of M_1 and M_4, respectively.

Theorem 1 (Vieta's Formulas [27]). *Let*

$$f(x) = a_n x^n + a_{n-1}x^{n-1} + \cdots + a_1 x + a_0$$

be a polynomial with coefficients in an algebraically closed field K. Here, $a_n \neq 0$. Vieta's formulas relate the roots $x_1, \ldots, x_n$ (counting multiplicities) to the coefficients a_i, $i = 0, \ldots, n$ as follows:

$$\sum_{1 \le j_1 \le \cdots \le j_k \le n} x_{j_1} x_{j_2} \cdots x_{j_k} = (-1)^k \frac{a_{n-k}}{a_k}.$$

3. The Kirchhoff Index and the Number of Spanning Trees of the Linear Pentagonal Derivation Chain QP_n

In this section, on the basis of Lemma 1, we derive the Laplacian eigenvalues of linear pentagonal derivation chains QP_n. Next, we present a complete description of the sum of the Laplacian eigenvalues' reciprocals and the product of the Laplacian eigenvalues, which will be used in obtaining the Kirchhoff index and the number of spanning trees of QP_n, respectively. Finally, we prove that the Kirchhoff index of QP_n is approximately one half of its Wiener index.

Let M be an $n \times n$ square matrix. We will then use $M[i, j, \cdots, k]$ to denote the submatrix obtained by deleting the i-th, j-th, $\cdots$, k-th rows and the corresponding columns of M. According to Figure 1, $L_{V_0V_0}$, $L_{V_0V_1}$, $L_{V_1V_2}$, and $L_{V_1V_1}$ are given as follows:

$$L_{V_0V_0} = \begin{bmatrix} 2 & 0 & \cdots & 0 \\ 0 & 2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 2 \end{bmatrix}_{n\times n} = 2I_n, \quad L_{V_0V_1} = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 0 & 0 \end{bmatrix}_{n\times(3n+1)},$$

$$L_{V_1V_1} = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 3 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 3 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 3 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(3n+1)\times(3n+1)},$$

$$L_{V_1V_2} = \begin{bmatrix} -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 \end{bmatrix}_{(3n+1)\times(3n+1)}.$$

Since $L_{V_1V_0} = L^T_{V_0V_1}, L_{V_2V_2} = L_{V_1V_1}$, and $L_A = \begin{bmatrix} L_{V_0V_0} & \sqrt{2}L_{V_0V_1} \\ \sqrt{2}L_{V_1V_0} & L_{V_1V_1} + L_{V_1V_2} \end{bmatrix}$, $L_S = L_{V_2V_2} - L_{V_1V_2}$ we have

$$L_A = \begin{bmatrix} 2 & 0 & \cdots & 0 & 0 & -\sqrt{2} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 2 & \cdots & 0 & 0 & 0 & 0 & 0 & -\sqrt{2} & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 2 & 0 & 0 & 0 & 0 & 0 & \cdots & -\sqrt{2} & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ -\sqrt{2} & 0 & \cdots & 0 & -1 & 3 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -\sqrt{2} & \cdots & 0 & 0 & 0 & 0 & -1 & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -\sqrt{2} & 0 & 0 & 0 & 0 & 0 & \cdots & 3 & -1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1)\times(4n+1)},$$

and

$$L_S = \begin{bmatrix} 3 & -1 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -1 & 3 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 4 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 3 & -1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 4 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 4 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 3 \end{bmatrix}_{(3n+1)\times(3n+1)}.$$

By Lemma 1, the Laplacian spectrum of QP_n consists of eigenvalues of L_A and L_S. Hence, assume that the eigenvalues of L_A and L_S are, respectively, denoted by $\eta_0 \leq \eta_1 \leq \cdots \leq \eta_{4n}$ and $\zeta_1 \leq \zeta_2 \leq \cdots \leq \zeta_{3n+1}$. Therefore, it is easy to verify that $\eta_0 = 0$, $\eta_i > 0$ $(i = 1, 2, \cdots, 4n)$ and $\zeta_j > 0$ $(j = 1, 2, \cdots, 3n+1)$.

Considering $\eta_0 = 0$, we can assume that

$$\Phi_{L_A}(\lambda) = \det(\lambda I_{4n+1} - L_A) = \lambda^{4n+1} + \alpha_1\lambda^{4n} + \cdots + \alpha_{4n-1}\lambda^2 + \alpha_{4n}\lambda, \tag{4}$$

$$\Phi_{L_S}(\lambda) = \det(\lambda I_{3n+1} - L_S) = \lambda^{3n+1} + \beta_1\lambda^{3n} + \cdots + \beta_{3n-1}\lambda^2 + \beta_{3n}\lambda + \beta_{3n+1}. \tag{5}$$

Theorem 2. *Let α_{4n}, α_{4n-1}, β_{3n}, and β_{3n+1} be defined as above. Suppose QP_n is a linear pentagonal derivation chain with length n. We then have*

$$\begin{aligned} Kf(QP_n) =& (7n+2)\left(-\frac{\alpha_{4n-1}}{\alpha_{4n}} + \frac{(-1)^{3n}\beta_{3n}}{\det L_S}\right) \\ =& \frac{49n^3 + 56n^2 + 7n}{4} \\ &+ \frac{(7n+2)[(5143\sqrt{1365} + 189995)n + 2397\sqrt{1365} + 88559](37+\sqrt{1365})^{n-1}}{65[(79\sqrt{1365} + 2919)(37+\sqrt{1365})^{n-1} + (79\sqrt{1365} - 2919)(37-\sqrt{1365})^{n-1}]} \\ &+ \frac{(7n+2)[(5143\sqrt{1365} - 189995)n + 2397\sqrt{1365} - 88559](37-\sqrt{1365})^{n-1}}{65[(79\sqrt{1365} + 2919)(37+\sqrt{1365})^{n-1} + (79\sqrt{1365} - 2919)(37-\sqrt{1365})^{n-1}]}. \end{aligned} \tag{6}$$

Proof. Since $\Phi_{L_A}(\lambda) = \lambda^{4n+1} + \alpha_1\lambda^{4n} + \cdots + \alpha_{4n-1}\lambda^2 + \alpha_{4n}\lambda$ with $\alpha_{4n} \neq 0$, $\eta_1, \eta_2, \cdots, \eta_{4n}$ are the roots of the above equation. By Vieta's formulas, we obtain

$$\sum_{i=1}^{4n} \frac{1}{\eta_i} = \frac{\sum_{i'=1}^{4n} \prod_{i=1, i\neq i'}^{4n} \eta_i}{\prod_{i=1}^{4n} \eta_i} = -\frac{\alpha_{4n-1}}{\alpha_{4n}}.$$

For $\Phi_{L_S}(\lambda) = \lambda^{3n+1} + \beta_1\lambda^{3n} + \cdots + \beta_{3n-1}\lambda^2 + \beta_{3n}\lambda + \beta_{3n+1}$ with $\beta_{3n+1} \neq 0$, we know $\zeta_1, \zeta_2, \cdots, \zeta_{3n+1}$ are the roots of the above equation. Applying Vieta's Formulas to Equation (5) yields

$$\sum_{j=1}^{3n+1} \frac{1}{\zeta_j} = \frac{\sum_{j'=1}^{3n+1} \prod_{j=1, j\neq j'}^{3n+1} \zeta_j}{\prod_{j=1}^{3n+1} \zeta_j} = \frac{(-1)^{3n}\beta_{3n}}{\det L_S}.$$

Note that $|V(QP_n)| = 7n + 2$. By (1), we obtain

$$\begin{aligned} Kf(QP_n) &= (7n+2)\left(\sum_{i=1}^{4n} \frac{1}{\eta_i} + \sum_{j=1}^{3n+1} \frac{1}{\zeta_j}\right) \\ &= (7n+2)\left(-\frac{\alpha_{4n-1}}{\alpha_{4n}} + \frac{(-1)^{3n}\beta_{3n}}{\det L_S}\right). \end{aligned} \tag{7}$$

In the following, it suffices to determine $-\alpha_{4n-1}$, α_{4n}, $(-1)^{3n}\beta_{3n}$, and $\det L_S$ in Equation (7).

Claim 1. $\alpha_{4n} = 2^{n-1}(7n+2)$.

Proof. It is well known that the number α_{4n} is the sum of the determinants obtained by deleting the i-th row and the corresponding column of L_A for $i = 1, 2, \cdots, 4n+1$ (see also in [28]), that is

$$\alpha_{4n} = \sum_{i=1}^{4n+1} \det L_A[i]. \tag{8}$$

Case 1. $1 \leq i \leq n$. Based on the structure of L_A (see also in (2)), deleting the i-th row and the corresponding column of L_A is equivalent deleting the i-th row and the corresponding column of $2I_n$, the i-th row in $\sqrt{2}L_{V_0V_1}$, and the i-th column in $\sqrt{2}L_{V_1V_0}$. We denote the resulting blocks as $2I_{n-1}$, $B_{(n-1)\times(3n+1)}$, $B^T_{(n-1)\times(3n+1)}$, and $C_{(3n+1)\times(3n+1)}$, respectively. If we then apply Lemma 3 to the resulting matrix, we have

$$\begin{aligned} \det L_A[i] =& \begin{vmatrix} 2I_{n-1} & B_{(n-1)\times(3n+1)} \\ B^T_{(n-1)\times(3n+1)} & C_{(3n+1)\times(3n+1)} \end{vmatrix} \\ =& \begin{vmatrix} 2I_{n-1} & 0 \\ 0 & C_{(3n+1)\times(3n+1)} - \frac{1}{2}B^T_{(n-1)\times(3n+1)}B_{(n-1)\times(3n+1)} \end{vmatrix} \\ =& 2^{n-1}\left|C_{(3n+1)\times(3n+1)} - \frac{1}{2}B^T_{(n-1)\times(3n+1)}B_{(n-1)\times(3n+1)}\right|, \end{aligned}$$

where

$$C-\frac{1}{2}B^TB=\begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(3n+1)\times(3n+1)},$$

and there is only one 3 in the $(3i-1)$-th row of $C-\frac{1}{2}B^TB$ for $1\le i\le n$.

Applying elementary operations of the determinant, we have

$$\det(C-\frac{1}{2}B^TB)=1.$$

Therefore, for $1\le i\le n$, we obtain

$$\det L_A[i]=2^{n-1}. \tag{9}$$

Case 2. $n+1\le i\le 4n+1$. In this case, according to the structure of L_A , deleting the i-th row and the corresponding column of L_A is equal to deleting the $(i-n)$-th row and the corresponding column of $L_{V_1V_1}+L_{V_1V_2}$, the $(i-n)$-th column in $\sqrt{2}L_{V_0V_1}$, and the $(i-n)$-th row in $\sqrt{2}L_{V_1V_0}$. We denote the resulting matrices as $2I_n$, $B_{n\times 3n}$, $B^T_{n\times 3n}$, and $C_{3n\times 3n}$, respectively. Thus, by Lemma 3, we obtain

$$\begin{aligned}\det L_A[i]=&\begin{vmatrix} 2I_n & B_{n\times 3n} \\ B^T_{n\times 3n} & C_{3n\times 3n}\end{vmatrix}=\begin{vmatrix} 2I_n & 0 \\ 0 & C_{3n\times 3n}-\frac{1}{2}B^T_{n\times 3n}B_{n\times 3n}\end{vmatrix}\\ =&2^n\left|C_{3n\times 3n}-\frac{1}{2}B^T_{n\times 3n}B_{n\times 3n}\right|,\end{aligned}$$

where

$$C-\frac{1}{2}B^TB=\begin{bmatrix} E_{(i-n-1)\times(i-n-1)} & 0 \\ 0 & F_{(4n+1-i)\times(4n+1-i)}\end{bmatrix}_{3n\times 3n},$$

and the E,F are as follows:

$$E=\begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(i-n-1)\times(i-n-1)},$$

$$F=\begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1-i)\times(4n+1-i)}.$$

By a direct calculation, one can see that $\det E=\det F=1$, so $\det(C-\frac{1}{2}B^TB)=1$. Hence, for $n+1\le i\le 4n+1$, we obtain

$$\det L_A[i]=2^n. \tag{10}$$

Together with (8)–(10), we have

$$\alpha_{4n} = \sum_{i=1}^{4n+1} \det L_A[i] = \sum_{i=1}^{n} \det L_A[i] + \sum_{i=n+1}^{4n+1} \det L_A[i] = 2^{n-1}(7n+2).$$

This completes the proof. □

Claim 2. $-\alpha_{4n-1} = 2^{n-3}(49n^3 + 56n^2 + 7n)$.

Proof. Note that $-\alpha_{4n-1}$ is the sum of the determinants of the resulting matrix by deleting the i-th row and i-th column as well as the j-th row and j-th column for some $1 \leq i < j \leq 4n+1$ in L_A. That is,

$$-\alpha_{4n-1} = \sum_{1 \leq i < j \leq 4n+1} \det L_A[i,j]. \tag{11}$$

According to the range of i and j, there are three cases in which the number $-\alpha_{4n-1}$ can be calculated as follows.

Case 1. $1 \leq i < j \leq n$. In this case, to delete the i-th and j-th rows and the corresponding columns of L_A is to delete the i-th and j-th rows and the corresponding columns of $2I_n$, the i-th and j-th rows of $\sqrt{2}L_{V_0V_1}$, and the i-th and j-th columns of $\sqrt{2}L_{V_1V_0}$. If we denote the resulting matrices, respectively, as $2I_{n-2}$, $B_{(n-2)\times(3n+1)}$, $B^T_{(n-2)\times(3n+1)}$, and $C_{(3n+1)\times(3n+1)}$ and apply Lemma 3 to the resulting matrix, we have

$$\det L_A[i,j] = \begin{vmatrix} 2I_{n-2} & B_{(n-2)\times(3n+1)} \\ B^T_{(n-2)\times(3n+1)} & C_{(3n+1)\times(3n+1)} \end{vmatrix} = 2^{n-2}|C - \frac{1}{2}B^T B|,$$

where

$$C - \frac{1}{2}B^T B = \begin{bmatrix} 1 & -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 3 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & \cdots & 3 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 1 \end{bmatrix},$$

and there is one 3 in the $(3i-1)$-th and $(3j-1)$-th rows of $C - \frac{1}{2}B^T B$ for $1 \leq i < j \leq n$, respectively.

By straightforward computing, we have

$$|C - \frac{1}{2}B^T B| = 3j - 3i + 2.$$

Therefore, when $1 \leq i < j \leq n$, we obtain

$$\det L_A[i,j] = 2^{n-2}(3j - 3i + 2). \tag{12}$$

Case 2. $n+1 \leq i < j \leq 4n+1$. In this case, to delete the i-th and j-th rows and the corresponding columns of L_A is to delete the $(i-n)$-th and $(j-n)$-th rows and the corresponding columns of $L_{V_1V_1} + L_{V_1V_2}$, the $(i-n)$-th and $(j-n)$-th columns of $\sqrt{2}L_{V_0V_1}$, and the $(i-n)$-th and $(j-n)$-th rows of $\sqrt{2}L_{V_1V_0}$. If we denote the resulting blocks, respectively, as $C_{(3n-1)\times(3n-1)}$, $B_{n\times(3n-1)}$, $B^T_{n\times(3n-1)}$, and $2I_n$ and apply Lemma 3 to the resulting matrix, we have

$$\det L_A[i,j] = \begin{vmatrix} 2I_n & B_{n\times(3n-1)} \\ B^T_{n\times(3n-1)} & C_{(3n-1)\times(3n-1)} \end{vmatrix} = 2^n|C - \frac{1}{2}B^T B|,$$

where

$$C - \frac{1}{2}B^T B = \begin{bmatrix} E_{(i-n-1)\times(i-n-1)} & 0 & 0 \\ 0 & F_{(j-i-1)\times(j-i-1)} & 0 \\ 0 & 0 & G_{(4n+1-j)\times(4n+1-j)} \end{bmatrix}_{(3n-1)\times(3n-1)},$$

and the E, F, G are as follows:

$$E = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(i-n-1)\times(i-n-1)}, F = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(j-i-1)\times(j-i-1)},$$

$$G = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1-j)\times(4n+1-j)}.$$

By direct calculation, one can get

$$\det(C - \frac{1}{2}B^T B) = j - i.$$

Hence, for $n+1 \le i < j \le 4n+1$, we obtain

$$\det L_A[i,j] = 2^n(j-i). \tag{13}$$

Case 3. $1 \le i \le n$, $n+1 \le j \le 4n+1$. Similarly, to delete the i-th and j-th rows and the corresponding columns of L_A is to delete the i-th row and the i-th column of $2I_n$, the $(j-n)$-th row and $(j-n)$-th column of $L_{V_1V_1} + L_{V_1V_2}$, the i-th row and $(j-n)$-th column of $\sqrt{2}L_{V_0V_1}$, and the $(j-n)$-th row and i-th column of $\sqrt{2}L_{V_1V_0}$. If we denote the resulting matrices, respectively, as $2I_{(n-1)}$, $C_{3n\times 3n}$, $B_{(n-1)\times 3n}$, and $B^T_{(n-1)\times 3n}$ and apply Lemma 3 to the resulting matrix, we have

$$\det L_A[i,j] = \begin{vmatrix} 2I_{n-1} & B_{(n-1)\times 3n} \\ B^T_{(n-1)\times 3n} & C_{3n\times 3n} \end{vmatrix} = 2^{n-1}|C - \frac{1}{2}B^T B|.$$

Subcase 3.1. If $1 \le i \le n$, $j = n+1$, then the matrix $C - \frac{1}{2}B^T B$ is

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{3n \times 3n} = M_1,$$

and there is only one 3 in the $(3i-2)$-th row of M_1 for $1 \le i \le n$.

Subcase 3.2. If $1 \le i \le n$, $j = n + 3i - 1$, then the matrix is

$$C - \frac{1}{2}B^T B = \begin{bmatrix} E_{(j-n-1)\times(j-n-1)} & 0 \\ 0 & F_{(4n+1-j)\times(4n+1-j)} \end{bmatrix}_{3n \times 3n} = M_2,$$

where

$$E = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(j-n-1)\times(j-n-1)},$$

$$F = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1-j)\times(4n+1-j)}.$$

Subcase 3.3. If $1 \le i \le n$, $j = n + 3i$ or $1 \le i \le n$, $j = n + 3i + 1$, then the matrix is

$$C - \frac{1}{2}B^T B = \begin{bmatrix} E_{(j-n-1)\times(j-n-1)} & 0 \\ 0 & F_{(4n+1-j)\times(4n+1-j)} \end{bmatrix}_{3n \times 3n} = M_3,$$

where

$$E = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(j-n-1)\times(j-n-1)},$$

$$F = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1-j)\times(4n+1-j)},$$

and there is only one 3 in the $(3i-1)$-th row of E, or

$$E = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 2 \end{bmatrix}_{(j-n-1)\times(j-n-1)},$$

$$F = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ -1 & 2 & -1 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & \cdots & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 3 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 2 & -1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \cdots & -1 & 2 & -1 \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}_{(4n+1-j)\times(4n+1-j)},$$

and there is only one 3 in the $(3i-2)$-th row of F.

By the basic calculation of the determinant, we have $\det M_1 = \det M_2 = \det M_3 = |j-(n+3i-1)|+1$.

Hence, for $1 \le i \le n$, $n+1 \le j \le 4n+1$, we obtain

$$\det L_A[i,j] = 2^{n-1}(|j-(n+3i-1)|+1). \tag{14}$$

Combining this with (11)–(14), we obtain

$$\begin{aligned} -\alpha_{4n-1} &= \sum_{1\le i<j\le 4n+1} \det L_A[i,j] \\ &= \sum_{1\le i<j\le n} \det L_A[i,j] + \sum_{n+1\le i<j\le 4n+1} \det L_A[i,j] + \sum_{1\le i\le n, n+1\le j\le 4n+1} \det L_A[i,j] \\ &= \sum_{1\le i<j\le n} 2^{n-2}(3j-3i+2) + \sum_{n+1\le i<j\le 4n+1} 2^n(j-i) \\ &\quad + \sum_{1\le i\le n, n+1\le j\le 4n+1} 2^{n-1}(|j-(n+3i-1)|+1) \\ &=2^{n-3}(n^3+2n^2-3n) + 2^{n-1}(9n^3+9n^2+2n) + 2^{n-1}\left[\frac{6n^3+9n^2+n}{2}\right] \\ &=2^{n-3}(49n^3+56n^2+7n). \end{aligned}$$

This completes the proof. □

In order to determine $(-1)^{3n}\beta_{3n}$ and $\det L_S$ in (7), we consider the k order principal submatrix, W_k, formed by the first k rows and the first k columns of L_S, $k=1,2,\cdots,3n+1$. Put $w_k := \det W_k$. We proceed by proving the following fact.

Fact 1. For $6 \le k \le 3n$, the integers w_k satisfy the recurrence

$$w_k = 37w_{k-3} - w_{k-6},$$

with the initial conditions $w_0 = 1, w_1 = 3, w_2 = 8, w_3 = 29, w_4 = 108$, and $w_5 = 295$.

Proof. It is easy to verify that $w_0 = 1, w_1 = 3, w_2 = 8, w_3 = 29, w_4 = 108$, and $w_5 = 295$. For $2 \le k \le 3n$, expanding $\det W_k$ with regard to its last row, we have

$$\begin{cases} w_{3i+2} = 3w_{3i+1} - w_{3i}, & i = 0,1,\dots.,n-1; \\ w_{3i} = 4w_{3i-1} - w_{3i-2}, & i = 1,2,\dots.,n; \\ w_{3i+1} = 4w_{3i} - w_{3i-1}, & i = 1,2,\dots.,n-1. \end{cases}$$

For $0 \le i \le n-1$, let $a_i = w_{3i+2}$; for $1 \le i \le n$, let $b_i = w_{3i}$; for $1 \le i \le n-1$, let $d_i = w_{3i+1}$. Therefore,

$$\begin{cases} a_i = 3d_i - b_i \\ b_i = 4a_{i-1} - d_{i-1} \\ d_i = 4b_i - a_{i-1} \end{cases}.$$

Hence, $a_i = 37a_{i-1} - a_{i-2}$, $b_i = 37b_{i-1} - b_{i-2}$ and $d_i = 37d_{i-1} - d_{i-2}$. Therefore, for $6 \le k \le 3n$, w_k satisfies the recurrence

$$w_k = 37w_{k-3} - w_{k-6},$$

where $w_0 = 1, w_1 = 3, w_2 = 8, w_3 = 29, w_4 = 108$ and $w_5 = 295$. $\square$

Claim 3. $\det L_S = \left(\frac{79}{2} + \frac{2919}{2\sqrt{1365}}\right)\left(\frac{37+\sqrt{1365}}{2}\right)^{n-1} + \left(\frac{79}{2} - \frac{2919}{2\sqrt{1365}}\right)\left(\frac{37-\sqrt{1365}}{2}\right)^{n-1}$.

Proof. By Fact 1, the characteristic equation of a_i is $x^2 = 37x - 1$, whose roots are $x_1 = \frac{37+\sqrt{1365}}{2}$ and $x_2 = \frac{37-\sqrt{1365}}{2}$. Assume that $a_i = y_1(\frac{37+\sqrt{1365}}{2})^i + y_2(\frac{37-\sqrt{1365}}{2})^i$. Considering the initial conditions $a_0 = w_2 = 8$ and $a_1 = w_5 = 295$, we obtain the systems of the following equations:

$$\begin{cases} y_1 + y_2 = 8 \\ y_1\dfrac{37+\sqrt{1365}}{2} + y_2\dfrac{37-\sqrt{1365}}{2} = 295 \end{cases}.$$

A direct computation shows that $y_1 = 4 + \frac{147}{\sqrt{1365}}, y_2 = 4 - \frac{147}{\sqrt{1365}}$, so

$$a_i = (4 + \frac{147}{\sqrt{1365}})(\frac{37+\sqrt{1365}}{2})^i + (4 - \frac{147}{\sqrt{1365}})(\frac{37+\sqrt{1365}}{2})^i.$$

In the same way, we can obtain b_i and d_i as follows:

$$\begin{cases} b_i = (\dfrac{1}{2} + \dfrac{\sqrt{1365}}{130})(\dfrac{37+\sqrt{1365}}{2})^i + (\dfrac{1}{2} - \dfrac{\sqrt{1365}}{130})(\dfrac{37-\sqrt{1365}}{2})^i \\ d_i = (\dfrac{3}{2} + \dfrac{105}{2\sqrt{1365}})(\dfrac{37+\sqrt{1365}}{2})^i + (\dfrac{3}{2} - \dfrac{105}{2\sqrt{1365}})(\dfrac{37-\sqrt{1365}}{2})^i \end{cases}.$$

Since $w_{3i} = b_i, w_{3i+1} = d_i$ and $w_{3i+2} = a_i$, we obtain

$$w_i = \begin{cases} (\dfrac{1}{2} + \dfrac{\sqrt{1365}}{130})(\dfrac{37+\sqrt{1365}}{2})^{\frac{i}{3}} + (\dfrac{1}{2} - \dfrac{\sqrt{1365}}{130})(\dfrac{37-\sqrt{1365}}{2})^{\frac{i}{3}}, \ if\ i \equiv 0 \pmod 3 \\ (\dfrac{3}{2} + \dfrac{105}{2\sqrt{1365}})(\dfrac{37+\sqrt{1365}}{2})^{\frac{i-1}{3}} + (\dfrac{3}{2} - \dfrac{105}{2\sqrt{1365}})(\dfrac{37-\sqrt{1365}}{2})^{\frac{i-1}{3}}, \ if\ i \equiv 1 \pmod 3 \\ (4 + \dfrac{147}{\sqrt{1365}})(\dfrac{37+\sqrt{1365}}{2})^{\frac{i-2}{3}} + (4 - \dfrac{147}{\sqrt{1365}})(\dfrac{37-\sqrt{1365}}{2})^{\frac{i-2}{3}}, \ if\ i \equiv 2 \pmod 3 \end{cases}. \tag{15}$$

By an expansion formula, we can obtain $\det L_S$ with respect to its last row as

$$\begin{aligned}\det L_S =&3\det W_{3n}-\det W_{3n-1}\\ =&3w_{3n}-w_{3n-1}\\ =&3\Big[\big(\frac{1}{2}+\frac{\sqrt{1365}}{130}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{n}+\big(\frac{1}{2}-\frac{\sqrt{1365}}{130}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{n}\Big]\\ &-\Big[\big(4+\frac{147}{\sqrt{1365}}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{n-1}+\big(4-\frac{147}{\sqrt{1365}}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{n-1}\Big]\\ =&\big(\frac{79}{2}+\frac{2919}{2\sqrt{1365}}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{n-1}+\big(\frac{79}{2}-\frac{2919}{2\sqrt{1365}}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{n-1}.\end{aligned}$$

This completes the proof. □

Claim 4.

$$\begin{aligned}(-1)^{3n}\beta_{3n}=&\Big[\frac{(5143\sqrt{1365}+189995)n}{130\sqrt{1365}}+\frac{2397\sqrt{1365}+88559}{130\sqrt{1365}}\Big]\big(\frac{37+\sqrt{1365}}{2}\big)^{n-1}\\ &+\Big[\frac{(5143\sqrt{1365}-189995)n}{130\sqrt{1365}}+\frac{2397\sqrt{1365}-88559}{130\sqrt{1365}}\Big]\big(\frac{37-\sqrt{1365}}{2}\big)^{n-1}.\end{aligned}$$

Proof. Since $(-1)^{3n}\beta_{3n}$ is the sum of all those principal minors of L_S, each of which is of size $3n\times 3n$, we have

$$(-1)^{3n}\beta_{3n}=\sum_{i=1}^{3n+1}\det L_S[i]=\sum_{i=1}^{3n+1}\begin{vmatrix}W_{i-1} & 0\\ 0 & H\end{vmatrix}=\sum_{i=1}^{3n+1}\det W_{i-1}\det H. \tag{16}$$

Note that H is a $(3n+1-i)\times(3n+1-i)$ matrix obtained from L_S by deleting the first i rows and the corresponding columns. Let $q_{3n+1-i}=\det H$. Whence, we get $q_i=37q_{i-3}-q_{i-6}$, where $q_0=1$, $q_1=3$, $q_2=11$, $q_3=30$, $q_4=109$, $q_5=406$. Thus,

$$q_l=\begin{cases}\big(\frac{1}{2}+\frac{23}{2\sqrt{1365}}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{\frac{l}{3}}+\big(\frac{1}{2}-\frac{23}{2\sqrt{1365}}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{\frac{l}{3}}, & if\ l\equiv 0(\mod 3)\\ \big(\frac{3}{2}+\frac{107}{2\sqrt{1365}}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{\frac{l-1}{3}}+\big(\frac{3}{2}-\frac{107}{2\sqrt{1365}}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{\frac{l-1}{3}}, & if\ l\equiv 1(\mod 3)\\ \big(\frac{11}{2}+\frac{405}{2\sqrt{1365}}\big)\big(\frac{37+\sqrt{1365}}{2}\big)^{\frac{l-2}{3}}+\big(\frac{11}{2}-\frac{405}{2\sqrt{1365}}\big)\big(\frac{37-\sqrt{1365}}{2}\big)^{\frac{l-2}{3}}, & if\ l\equiv 2(\mod 3)\end{cases}. \tag{17}$$

Therefore, by (16),

$$\begin{aligned}(-1)^{3n}\beta_{3n}&=\sum_{i=1}^{3n+1}w_{i-1}q_{3n+1-i}=\sum_{i=0}^{3n}w_iq_{3n-i}\\ &=\sum_{l=0}^{n}w_{3l}q_{3n-3l}+\sum_{l=0}^{n-1}w_{3l+1}q_{3n-(3l+1)}+\sum_{l=0}^{n-1}w_{3l+2}q_{3n-(3l+2)}.\end{aligned} \tag{18}$$

Combining (15) with (17), we know that

$$
\begin{aligned}
\sum_{l=0}^{n} w_{3l}q_{3n-3l} =& \sum_{l=0}^{n}\Big[\Big(\frac{1}{2}+\frac{\sqrt{1365}}{130}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{l}+\Big(\frac{1}{2}-\frac{\sqrt{1365}}{130}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{l}\Big]\\
&\cdot\Big[\Big(\frac{1}{2}+\frac{23}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-l}+\Big(\frac{1}{2}-\frac{23}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-l}\Big]\\
=&\frac{(44\sqrt{1365}+1430)(n+1)+777+21\sqrt{1365}}{130\sqrt{1365}}\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n}\\
&+\frac{(44\sqrt{1365}-1430)(n+1)-777+21\sqrt{1365}}{130\sqrt{1365}}\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n},
\end{aligned}
\tag{19}
$$

$$
\begin{aligned}
\sum_{l=0}^{n-1} w_{3l+1}q_{3n-(3l+1)} =& \sum_{l=0}^{n-1}\Big[\Big(\frac{3}{2}+\frac{105}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{l}+\Big(\frac{3}{2}-\frac{105}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{l}\Big]\\
&\cdot\Big[\Big(\frac{11}{2}+\frac{405}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-l-1}+\Big(\frac{11}{2}-\frac{405}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-l-1}\Big]\\
=&\Big[\frac{(2919+79\sqrt{1365})n+84}{182}+\frac{1554}{91\sqrt{1365}}\Big]\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-1}\\
&+\Big[\frac{(2919-79\sqrt{1365})n+84}{182}-\frac{1554}{91\sqrt{1365}}\Big]\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-1},
\end{aligned}
\tag{20}
$$

and

$$
\begin{aligned}
\sum_{l=0}^{n-1} w_{3l+2}q_{3n-(3l+2)} =& \sum_{l=0}^{n-1}\Big[\Big(4+\frac{147}{\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{l}+\Big(4-\frac{147}{\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{l}\Big]\\
&\cdot\Big[\Big(\frac{3}{2}+\frac{107}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-l-1}+\Big(\frac{3}{2}-\frac{107}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-l-1}\Big]\\
=&\Big[\frac{(32109+869\sqrt{1365})n}{2730}+\frac{1147}{130\sqrt{1365}}+\frac{31}{130}\Big]\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-1}\\
&+\Big[\frac{(32109-869\sqrt{1365})n}{2730}-\frac{1147}{130\sqrt{1365}}+\frac{31}{130}\Big]\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-1}.
\end{aligned}
\tag{21}
$$

Hence, if (19)–(21) is placed into (18), Claim 4 follows directly. □

Finally, substituting Claims 1–4 into (1), Theorem 2 follows immediately. □

Theorem 3. *Let QP_n be a linear pentagonal derivation chain with length n. Therefore,*

$$
\tau(QP_n)=2^{n-1}\Big[\Big(\frac{79}{2}+\frac{2919}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-1}+\Big(\frac{79}{2}-\frac{2919}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-1}\Big].
$$

Proof. According to Lemma 3, we know that $\tau(G)=\frac{1}{n}\prod_{i=2}^{n}\mu_i$, where μ_i represents the Laplacian eigenvalues of G for $i=1,2,\cdots,n$. Note that the eigenvalues of L_A and L_S are η_i $(i=0,1,2,\ldots,4n)$ and ζ_j $(j=1,2,\ldots,3n+1)$, respectively. Therefore, by Claims 2 and 3,

$$
\begin{aligned}
\tau(QP_n)&=\frac{1}{7n+2}\prod_{i=1}^{4n}\eta_i\prod_{j=1}^{3n+1}\zeta_j\\
&=\frac{1}{7n+2}\alpha_{4n}\det L_S\\
&=2^{n-1}\Big[\Big(\frac{79}{2}+\frac{2919}{2\sqrt{1365}}\Big)\Big(\frac{37+\sqrt{1365}}{2}\Big)^{n-1}+\Big(\frac{79}{2}-\frac{2919}{2\sqrt{1365}}\Big)\Big(\frac{37-\sqrt{1365}}{2}\Big)^{n-1}\Big].
\end{aligned}
$$

This completes the proof. □

Based on Theorem 2, we can easily obtain the Kirchhoff indices of linear pentagonal derivation chains from QP_1 to QP_{40}, which are listed in Table 1.

By Theorem 3, it is not difficult to obtain the numbers of spanning trees of linear pentagonal derivation chains from QP_1 to QP_9, which are shown in Table 2.

Table 1. The Kirchhoff indices of linear pentagonal derivation chains from QP_1 to QP_{40}.

n	$Kf(QP_n)$	n	$Kf(QP_n)$	n	$Kf(QP_n)$	n	$Kf(QP_n)$
1	41.22	11	18,925.15	21	122,861.13	31	385,349.16
2	197.02	12	24,278.65	22	140,762.34	32	423,148.08
3	541.84	13	30,556.18	23	160,322.57	33	463,341.02
4	1149.18	14	37,831.23	24	181,615.33	34	506,001.47
5	2092.54	15	46,171.29	25	204,714.10	35	551,202.95
6	3445.42	16	55,667.88	26	229,692.39	36	599,018.95
7	5281.33	17	66,376.49	27	256,623.70	37	649,522.97
8	7673.75	18	78,376.62	28	285,581.53	38	702,788.51
9	10,696.20	19	91,741.77	29	316,639.39	39	758,889.07
10	14,422.16	20	106,545.44	30	349,870.77	40	817,898.15

Table 2. The number of spanning trees of linear pentagonal derivation chains from QP_1 to QP_9.

n	$\tau(QP_n)$	n	$\tau(QP_n)$	n	$\tau(QP_n)$
1	79	4	31944040	7	12916125352384
2	5842	5	2362130992	8	955094596407424
3	431992	6	174669917248	9	70625335632739900

At the end of this section, we characterize the relation between the Kirchhoff index and the Wiener index of QP_n.

Theorem 4. *Let QP_n be a linear pentagonal derivation chain with length n. Therefore,*

$$\lim_{n\to\infty} \frac{Kf(QP_n)}{W(QP_n)} = \frac{1}{2}.$$

Proof. Firstly, we determine $W(QP_n)$, we evaluate d_{ij} for all vertices (fixed i and for all j), and we then add them all together and divide them by two in the end. The expression of each type of vertex is

$$\bullet\ f(3i,n) = \frac{(3n-3i+2)(3n-3i+1)}{2} + \frac{3i(3i-1)}{2} + \frac{(3n-3i+3)(3n-3i+2)}{2} + \sum_{k=2}^{3i} k + \sum_{k=0}^{i-1}(2+3k) + \sum_{k=0}^{n-i} 3k$$
$$= 21i^2 - 21ni - 13i + \frac{21n^2+27n}{2} + 3.$$

$$\bullet\ f(3i+1,n) = \frac{(3n-3i+1)(3n-3i)}{2} + \frac{3i(3i+1)}{2} + \frac{(3n-3i+2)(3n-3i+1)}{2} + \frac{(3i+2)(3i+1)}{2} - 1 + \sum_{k=0}^{n-i-1}(2+3k) + \sum_{k=0}^{i} 3k$$
$$= 21i^2 - 21ni + i + \frac{21n^2+13n}{2} + 1.$$

$$\bullet\ f(3i+2,n) = \frac{(3n-3i)(3n-3i-1)}{2} + \frac{(3i+2)(3i+1)}{2} + \frac{(3n-3i)(3n-3i+1)}{2} + \frac{(3i+2)(3i+3)}{2} + 1 + \sum_{k=0}^{n-i-2}(4+3k) + \sum_{k=0}^{i-1}(4+3k)$$
$$= 21i^2 - 21ni + 15i + \frac{21n^2-n}{2} + 4.$$

$$\bullet\ f(2,n) = \frac{21n^2-n+8}{2}.$$

$$\bullet\ f(3n+1,n) = \frac{21n^2+15n+2}{2}.$$

$$\bullet\ f(3n-1,n) = \frac{21n^2-13n+20}{2}.$$

$$\bullet\ f(i^\circ,n) = 2\Big[\frac{(3n-3i+4)(3n-3i+3)}{2} + \frac{3i(3i-1)}{2} - 1\Big] + \sum_{k=0}^{n-i^\circ-1}(5+3k) + \sum_{k=0}^{i^\circ-2}(5+3k)$$
$$= 21i^2 - 21ni - 27i + \frac{21n^2+49n}{2} + 8.$$

$$\bullet\ f(1^\circ,n) = \frac{23n^2+n+8}{2}.$$

$$\bullet\ f(n^\circ,n) = \frac{23n^2-11n+20}{2}.$$

Hence,

$$W(QP_n) = \Big[\sum_{i=1}^{n} f(3i,n) + \sum_{i=0}^{n-1} f(3i+1,n) + \sum_{i=1}^{n-2} f(3i+2,n) + f(2,n) + f(3n+1,n) + f(3n-1,n)\Big] + \frac{\sum_{i^\circ=2}^{n-1} f(i^\circ,n) + f(1^\circ,n) + f(n^\circ,n)}{2}$$
$$= \frac{49n^3+76n^2+15n+6}{2}.$$

Together with Theorem 2, our result follows immediately. □

4. Conclusions

In this paper, according to the Laplacian spectrum, we obtain the Kirchhoff index and the number of spanning trees of a linear pentagonal derivation chain. At the same time, we also compute the Wiener index of the linear pentagonal derivation chain. Surprisingly, the Kirchhoff index of the linear pentagonal derivation chain is approximately one half of its Wiener index. Motivated from related works, we believe that the normalized Laplacian spectrum and the degree-Kirchhoff index of the linear pentagonal derivation chain, respectively, should be investigated. We reserve the above problems for further research.

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