The normalized Laplacian, degree-Kirchhoff index and spanning trees of graphs derived from the strong prism of linear hexagonal chain

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Abstract: Let L_n be a linear hexagonal chain with n hexagons. Let L_n^2 be the graph obtained by the strong prism of a linear hexagonal chain with n hexagons, i.e. the strong product of L_n and K_2. In this paper, explicit expressions for degree-Kirchhoff index and number of spanning trees of L_n^2 are determined, respectively. Furthermore, it is interesting to find that the degree-Kirchhoff index of L_n^2 is almost one eighth of its Gutman index.

Keywords: Linear hexagonal chain; Normalized Laplacian; Degree-Kirchhoff index; Spanning tree

AMS subject classification: 05C50

1. Introduction

In this paper, we only consider simple and undirected graphs. Let $G = (V(G), E(G))$ be a graph with the vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(G)$. The *adjacency matrix* of G is a square matrix $A(G) = (a_{ij})_{n\times n}$ with entries $a_{ij} = 1$ or 0 according as the corresponding vertices v_i and v_j are adjacent or not. Let $D(G) = \mathrm{diag}(d_{v_1}, d_{v_2}, \ldots, d_{v_n})$ be the diagonal matrix of vertex degrees, where d_{v_i} is the degree of v_i in G for $1 \leqslant i \leqslant n$. The (*combinatorial*) *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$.

The classical distance between vertices v_i and v_j in a graph G, denoted by $d(v_i, v_j)$, is the length of a shortest path in G connecting them. A well-known topological descriptor called *Wiener index*, $W(G)$, was given by $W(G) = \sum_{i<j} d(v_i, v_j)$ in [37]. Later, Gutman [10] introduced the weighted version of Wiener index, namely *Gutman index* of G, which was defined as $Gut(G) = \sum_{i<j} d_{v_i} d_{v_j} d(v_i, v_j)$. In [10], it was shown that when G is a tree on n vertices, then the Wiener index and Gutman index are closely related by $Gut(G) = 4W(G) - (2n-1)(n-1)$.

On the basis of electrical network theory, Klein and Randić [19] proposed a novel distance function, namely the *resistance distance*, on a graph. The term resistance distance was used because of the physical interpretation: place unit resistors on each edge of a graph G and take the resistance distance, $r(v_i, v_j)$, between vertices v_i and v_j of G to be the effective resistance between them. This novel parameter is in fact intrinsic to the graph and has some nice interpretations and applications in chemistry (see [16, 17] for details). It is well known that the resistance distance between two arbitrary vertices in an electronic network can be obtained in terms of the eigenvalues and eigenvectors of the Laplacian matrix associated with the network. One famous resistance distance-based parameter called the *Kirchhoff index*, $Kf(G)$, was given by $Kf(G) = \sum_{i<j} r(v_i, v_j)$; see [19]. Later it is shown [17, 23] that

$$Kf(G) = \sum_{i<j} r(v_i, v_j) = n \sum_{i=2}^{n} \frac{1}{\mu_i},$$

where $0 = \mu_1 \leqslant \mu_2 \leqslant \cdots \leqslant \mu_n$ $(n \geqslant 2)$ are the eigenvalues of $L(G)$.

In recent years, the *normalized Laplacian*, $\mathcal{L}(G)$, which is consistent with the matrix in spectral geometry and random walks [7], has attracted more and more researchers' attention. One of the original motivations for

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defining the normalized Laplacian was to deal more naturally with nonregular graphs. The normalized Laplacian is defined to be

$$\mathcal{L} = I - D^{\frac{1}{2}}(D^{-1}A)D^{-\frac{1}{2}} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}$$

(with the convention that if the degree of vertex v_i in G is 0, then $(d_{v_i})^{-\frac{1}{2}} = 0$; see [7]). Thus it is easy to obtain that

$$(\mathcal{L}(G))_{ij} = \begin{cases} 1, & \text{if } i = j; \\ -\frac{1}{\sqrt{d_{v_i}d_{v_j}}}, & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j; \\ 0, & \text{otherwise,} \end{cases} \tag{1.1}$$

where $(\mathcal{L}(G))_{ij}$ denotes the (i,j)-entry of $\mathcal{L}(G)$. In 2007, Chen and Zhang [6] showed that the resistance distance can be expressed naturally in terms of the eigenvalues and eigenvectors of the normalized Laplacian and proposed another graph invariant, defined by $Kf^*(G) = \sum_{i<j} d_{v_i}d_{v_j}r(v_i, v_j)$, which is called the *degree-Kirchhoff index* (see [9, 12]). It is closely related to the corresponding spectrum of the normalized Laplacian (see Lemma 2.3 in the next section). The spectrum of $\mathcal{L}(G)$ is denoted by $S(G) = \{\lambda_1, \lambda_2, \ldots, \lambda_n\}$ with $0 = \lambda_1 \leqslant \lambda_2 \leqslant \ldots \leqslant \lambda_n$. It is well known that G is connected if and only if $\lambda_2 > 0$.

It is well-known [19] that $r(v_i, v_j) \leq d(v_i, v_j)$ with equality if and only if there is a unique path connecting vertices v_i and v_j in G. As an immediate consequence, for a tree G, $Kf(G) = W(G)$ and $Kf^*(G) = Gut(G)$. Thus in the research on the Kirchhoff index and the degree Kirchhoff index of graphs, it is primarily of interest in the case of cycle-containing graphs. Up to now, closed-form formula for Kirchhoff index and degree Kirchhoff index have been given for some classes of graphs, such as cycles [18], circulant graphs [44], composite graphs [45], linear polynomial chains [13, 14, 41], linear crossed chains [30, 48] and some other topics on Kirchhoff index and degree-Kirchhoff index of graphs may be referred to [1, 2, 5, 14, 21, 22, 24, 30, 31, 34, 42, 47, 20, 26, 27, 28, 36, 49] and references therein.

A hexagonal system (benzenoid hydrocarbon) is a finite 2-connected plan graph such that each interior face (or say a cell) is surrounded by a regular hexagon of length one. Hexagonal systems are very important in theoretical chemistry because they are natural graph representations of benzenoid hydrocarbon. Hence, hexagonal systems have been of great interest and extensively studied. In 1991, Kennedy and Quintas [15] considered the prefect matchings in random hexagonal chain graphs. Later, the Wiener index and the Edge-Szeged index of a hexagonal chain are, respectively, determined in [8] and [33]. Lou and Huang [25] provided a complete description of the characteristic polynomial of a hexagonal system. Yang and Zhang [41] computed the Kirchhoff index of a linear hexagonal chain. Recently, Huang and Li [11] obtained explicit formulae for the resistance distance between any two vertices of a hexagonal chain. Xiao et al.[39] determined the first three maximal values of the Mostar index among all hexagonal chains with given number of hexagons, and characterize the corresponding extremal graphs. For more results on hexagonal system one may be referred to [40, 41, 46] and the references therein.

Let L_n denote a linear hexagonal chain with n hexagons as depicted in Fig. 1. Then it is routine to check that $|V(L_n)| = 4n + 2$ and $|E(L_n)| = 5n + 1$.

Given two graphs G and H, the strong product of G and H, denoted by $G \boxtimes H$, is the graph with vertex set $V(G) \times V(H)$, where two distinct vertices (u_1, v_1) and (u_2, v_2) are adjacent whenever u_1 and u_2 are equal or adjacent in G, and v_1 and v_2 are equal or adjacent in H. Specially, the strong product of G and K_2 is called the strong prism of G. Very recently, Pan et al. [31] determined some resistance distance-based invariants and number of spanning trees of graphs derived from the strong prism of some special graphs, such as the path P_n and the cycle C_n. Li et al. [24] determined the expressions for Kirchhoff index, degree Kirchhoff index and number of spanning trees of graphs derived from the strong prism of the star S_n. Along this line, we consider the

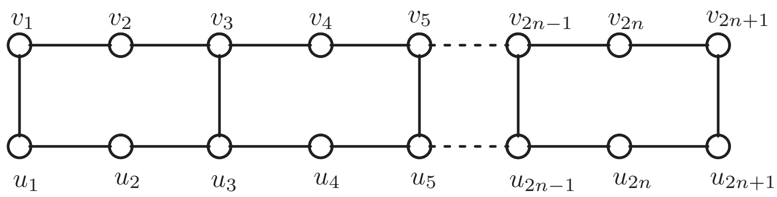

Figure 1: Graph L_n and its labeled vertices.

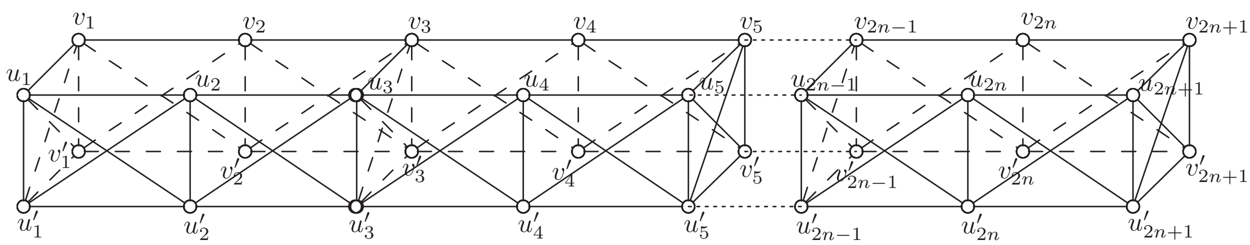

Figure 2: Graph L_n^2 and its labeled vertices.

strong prism of a linear hexagonal chain L_n. Let L_n^2 be the strong prism of L_n as depicted in Fig. 2. Obviously, $|V(L_n^2)| = 8n+4$ and $|E(L_n^2)| = 24n+6$.

In this paper, motivated by [3, 6, 11, 12, 13, 14, 24, 30, 31, 35, 38, 41], explicit expressions for degree-Kirchhoff index and number of spanning trees of L_n^2 are determined, respectively. Furthermore, we are surprised to see that the degree-Kirchhoff index of L_n^2 is approximately one eighth of its Gutman index.

2. Preliminaries

Throughout this paper, we shall denote by $\Phi(B) = \det(xI - B)$ the *characteristic polynomial* of the square matrix B. In particular, if $B = \mathcal{L}(G)$, we write $\Phi(\mathcal{L}(G))$ by $\Psi(G;x)$ and call $\Psi(G;x)$ the *normalized Laplacian characteristic polynomial* of G.

Let $V_1 = \{u_1, u_2, \ldots, u_{2n+1}, v_1, v_2, \ldots, v_{2n+1}\}, V_2 = \{u'_1, u'_2, \ldots, u'_{2n+1}, v'_1, v'_2, \ldots, v'_{2n+1}\}$. Then by a suitable arrangement of vertices in L_n^2, $\mathcal{L}(L_n^2)$ can be written as the following block matrix

$$\mathcal{L}(L_n^2) = \left(\begin{array}{c|c} \mathcal{L}_{V_{11}} & \mathcal{L}_{V_{12}} \\ \hline \mathcal{L}_{V_{21}} & \mathcal{L}_{V_{22}} \end{array}\right),$$

where $\mathcal{L}_{V_{ij}}$ is the submatrix formed by rows corresponding to vertices in V_i and columns corresponding to vertices in V_j for $i, j = 1, 2$. Owing to the symmetry construction of the graph L_n^2, it is obvious that $\mathcal{L}_{V_{11}} = \mathcal{L}_{V_{22}}$ and $\mathcal{L}_{V_{12}} = \mathcal{L}_{V_{21}}$. Let

$$T = \left(\begin{array}{c|c} \frac{1}{\sqrt{2}} I_{4n+2} & \frac{1}{\sqrt{2}} I_{4n+2} \\ \hline \frac{1}{\sqrt{2}} I_{4n+2} & -\frac{1}{\sqrt{2}} I_{4n+2} \end{array}\right) \tag{2.1}$$

be the block matrix such that the blocks have the same dimension as the corresponding blocks in $\mathcal{L}(L_n^2)$. By a simple calculation, one can see that

$$T\mathcal{L}(L_n^2)T = \left(\begin{array}{c|c} \mathcal{L}_A(L_n^2) & \mathbf{0} \\ \hline \mathbf{0} & \mathcal{L}_S(L_n^2) \end{array}\right), \tag{2.2}$$

where $\mathcal{L}_A(L_n^2) = \mathcal{L}_{V_{11}} + \mathcal{L}_{V_{12}}$ and $\mathcal{L}_S(L_n^2) = \mathcal{L}_{V_{11}} - \mathcal{L}_{V_{12}}$.

Thus similar to the decomposition theorem obtained in [13, 14, 24, 41], we can obtain the following decomposition theorem of the normalized Laplacian polynomial.

Lemma 2.1. *Let $\mathcal{L}(L_n^2), \mathcal{L}_A(L_n^2), \mathcal{L}_S(L_n^2)$ be defined as above. Then*

$$\Psi(L_n^2; x) = \Phi(\mathcal{L}_A(L_n^2)) \cdot \Phi(\mathcal{L}_S(L_n^2)).$$

Lemma 2.2 ([7])**.** *Let G be an n-vertex connected graph with m edges, then $\prod_{i=1}^{n} d_{v_i} \prod_{k=2}^{n} \lambda_k = 2m\tau(G)$, where $\tau(G)$ is the number of spanning trees of G.*

Lemma 2.3 ([6])**.** *Let G be an n-vertex connected graph with m edges, then $Kf^*(G) = 2m \sum_{i=2}^{n} \frac{1}{\lambda_i}$.*

3. Degree-Kirchhoff index and number of spanning trees of L_n^2

In this section, we first determine the normalized Laplacian eigenvalues of L_n^2 according to Lemma 2.1. Then we provide a complete description of the sum of the normalized Laplacian eigenvalues' reciprocals and the product of the normalized Laplacian eigenvalues which will be used in computing the degree-Kirchhoff index and the number of spanning trees of L_n^2. Finally, we show that the degree-Kirchhoff index of L_n^2 is approximately one eighth of its Gutman index.

For convenience, we abbreviate $\mathcal{L}_A(L_n^2)$ and $\mathcal{L}_S(L_n^2)$ to $\mathcal{L}_A$ and $\mathcal{L}_S$, respectively. We label the vertices of L_n^2 as depicted in Fig. 2. Obviously,

$$\mathcal{L}_{V_{11}} = \begin{pmatrix}
1 & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 \\
-\frac{1}{5} & 1 & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & -\frac{1}{\sqrt{35}} & 1 & \cdots & 0 & 0 & 0 & 0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{35}} & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 \\
0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & 1 & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & 1 & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} \\
-\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 & 1 & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & 1 & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{35}} & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{\sqrt{35}} & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & 1 & -\frac{1}{5} \\
0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & 1
\end{pmatrix}_{(4n+2)\times(4n+2)}$$

and

$$
\mathcal{L}_{V_{12}}
$$

$$
=\begin{pmatrix}
-\frac{1}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 \\
-\frac{1}{5} & -\frac{1}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & -\frac{1}{\sqrt{35}} & -\frac{1}{7} & \cdots & 0 & 0 & 0 & 0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{7} & -\frac{1}{\sqrt{35}} & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 \\
0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & -\frac{1}{5} & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} \\
-\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & -\frac{1}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{35}} & -\frac{1}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{7} & -\frac{1}{\sqrt{35}} & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & -\frac{1}{5} & -\frac{1}{5} \\
0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & -\frac{1}{5}
\end{pmatrix}_{(4n+2)\times(4n+2)}.
$$

Since $\mathcal{L}_A = \mathcal{L}_{V_{11}} + \mathcal{L}_{V_{12}}$ and $\mathcal{L}_S = \mathcal{L}_{V_{11}} - \mathcal{L}_{V_{12}}$, thus

$$
\mathcal{L}_A
$$

$$
=2\begin{pmatrix}
\frac{2}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 \\
-\frac{1}{5} & \frac{2}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & -\frac{1}{\sqrt{35}} & \frac{3}{7} & \cdots & 0 & 0 & 0 & 0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \frac{3}{7} & -\frac{1}{\sqrt{35}} & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 \\
0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{5} & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & \frac{2}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} \\
-\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{2}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & -\frac{1}{5} & \frac{2}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 & 0 & -\frac{1}{\sqrt{35}} & \frac{3}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 & 0 & 0 & 0 & \cdots & \frac{3}{7} & -\frac{1}{\sqrt{35}} & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{5} & -\frac{1}{5} \\
0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & \frac{2}{5}
\end{pmatrix}_{(4n+2)\times(4n+2)}
$$

and

$$\mathcal{L}_S = \begin{pmatrix}
\frac{6}{5} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & \frac{6}{5} & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & \frac{8}{7} & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \\
0 & 0 & 0 & \cdots & \frac{8}{7} & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & \frac{6}{5} & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & \frac{6}{5} & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \frac{6}{5} & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \frac{6}{5} & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & \frac{8}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & \frac{8}{7} & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & \frac{6}{5} & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 & 0 & \frac{6}{5}
\end{pmatrix}_{(4n+2)\times(4n+2)}.$$

Therefore, by Lemma 2.1, we have the normalized Laplacian eigenvalues of L_n^2 consists of the eigenvalues of $\mathcal{L}_A$ and $\mathcal{L}_S$. Since $\mathcal{L}_S$ is a diagonal matrix, one can easily see that $\frac{6}{5}$ with multiplicity $2n+4$ and $\frac{8}{7}$ with multiplicity $2n-2$ are all the eigenvalues of $\mathcal{L}_S$. Next, we provide a complete description of the sum of the reciprocals of the eigenvalues of $\mathcal{L}_A$ and the product of the eigenvalues of $\mathcal{L}_A$ which will be used in computing the degree-Kirchhoff index and the number of spanning trees of L_n^2.

Let

$$C = \begin{pmatrix}
\frac{2}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 \\
-\frac{1}{5} & \frac{2}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & 0 \\
0 & -\frac{1}{\sqrt{35}} & \frac{3}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & \frac{3}{7} & -\frac{1}{\sqrt{35}} & 0 \\
0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{5} & -\frac{1}{5} \\
0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & \frac{2}{5}
\end{pmatrix}_{(2n+1)\times(2n+1)},$$

where $C_{11} = C_{2n+1,2n+1} = C_{ii} = \frac{2}{5}$ for even $i \in \{2, 4, \ldots, 2n\}$; $C_{ii} = \frac{3}{7}$ for odd $i \in \{3, 5, \ldots, 2n-1\}$; $C_{12} = C_{21} = C_{2n,2n+1} = C_{2n+1,2n} = -\frac{1}{5}$; $C_{i,i+1} = C_{i+1,i} = -\frac{1}{\sqrt{35}}$ for $2 \le i \le 2n-1$ and $C_{ij} = 0$ if $|i-j| > 1$. Let

$$D = \begin{pmatrix}
-\frac{1}{5} & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & -\frac{1}{7} & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -\frac{1}{7} & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{5}
\end{pmatrix}_{(2n+1)\times(2n+1)},$$

where $D_{11} = D_{2n+1,2n+1} = -\frac{1}{5}$; $D_{ii} = -\frac{1}{7}$ for odd $i \in \{3, 5, \ldots, 2n-1\}$ and $D_{ij} = 0$ otherwise. Then $\frac{1}{2}\mathcal{L}_A$ can be written as the following block matrix

$$\frac{1}{2}\mathcal{L}_A = \left(\begin{array}{c|c} C & D \\ \hline D & C \end{array}\right).$$

Let

$$T = \left(\begin{array}{c|c} \frac{1}{\sqrt{2}} I_{2n+1} & \frac{1}{\sqrt{2}} I_{2n+1} \\ \hline \frac{1}{\sqrt{2}} I_{2n+1} & -\frac{1}{\sqrt{2}} I_{2n+1} \end{array}\right)$$

be the block matrix such that the blocks have the same dimension as the corresponding blocks in $\frac{1}{2}\mathcal{L}_A$. Then

$$T(\frac{1}{2}\mathcal{L}_A)T = \left(\begin{array}{c|c} C+D & \mathbf{0} \\ \hline \mathbf{0} & C-D \end{array}\right).$$

Let $M = C + D$ and $N = C - D$. It is easy to check that the eigenvalues of $\frac{1}{2}\mathcal{L}_A$ consists of the eigenvalues of M and N. Suppose that the eigenvalues of M and N are respectively, denoted by α_i and β_j $(i, j = 1, 2, \ldots, 2n+1)$ with $\alpha_1 \leqslant \alpha_2 \leqslant \ldots \leqslant \alpha_{2n+1}, \beta_1 \leqslant \beta_2 \leqslant \ldots \leqslant \beta_{2n+1}$. Then the eigenvalues of $\mathcal{L}_A$ are $2\alpha_1, 2\alpha_2, \ldots, 2\alpha_{2n+1}, 2\beta_1, 2\beta_2, \ldots, 2\beta_{2n+1}$. Since all the eigenvalues of $\mathcal{L}_A$ are the normalized Laplacian eigenvalues of L_n^2, we get $\alpha_1, \beta_1 \geqslant 0$.

In the following, we will prove $\alpha_1 = 0$, and $\alpha_i > 0, \beta_j > 0$ for $2 \leqslant i \leqslant 2n+1, 1 \leqslant j \leqslant 2n+1$. For $1 \leqslant i \leqslant 2n$, let M_i be the ith order principal submatrix formed by the first i rows and columns of M and $b_i := \det M_i$. We first derive the formula of b_i, which will be used in calculating $\det M$.

Lemma 3.1. *For $1 \leqslant i \leqslant 2n, b_i = \frac{7+\sqrt{35}}{10}\left(\frac{1}{\sqrt{35}}\right)^i + \frac{7-\sqrt{35}}{10}\left(-\frac{1}{\sqrt{35}}\right)^i$.*

Proof. It is straightforward to calculate that $b_1 = \frac{1}{5}, b_2 = \frac{1}{25}, b_3 = \frac{1}{175}$ and $b_4 = \frac{1}{875}$. For $3 \leqslant i \leqslant 2n$, expanding $\det M_i$ with regard to its last row, we have

$$b_i = \begin{cases} \dfrac{2}{5}b_{i-1} - \dfrac{1}{35}b_{i-2}, & \text{if } i \text{ is even;} \\ \dfrac{2}{7}b_{i-1} - \dfrac{1}{35}b_{i-2}, & \text{if } i \text{ is odd..} \end{cases}$$

For $1 \le i \le n$, let $c_i = b_{2i}$ and for $1 \le i \le n-1$, let $d_i = b_{2i+1}$. Then $c_1 = \frac{1}{25}, d_1 = \frac{1}{175}$ and, for $i \ge 2$, we have

$$\begin{cases} c_i = \dfrac{2}{5}d_{i-1} - \dfrac{1}{35}c_{i-1}, \\ d_i = \dfrac{2}{7}c_i - \dfrac{1}{35}d_{i-1}. \end{cases} \tag{3.1}$$

From the first equation in (3.1), one has $d_{i-1} = \frac{5}{2}c_i + \frac{1}{14}c_{i-1}$. Hence, $d_i = \frac{5}{2}c_{i+1} + \frac{1}{14}c_i$. Substituting d_{i-1} and d_i into the second equation in (3.1) yields $c_{i+1} = \frac{2}{35}c_i - \frac{1}{1225}c_{i-1}$, $i \ge 2$. In a similar way, we can obtain $d_i = \frac{2}{35}d_{i-1} - \frac{1}{1225}d_{i-2}$, $i \ge 3$. Therefore, b_i satisfies the recurrence relation

$$b_i = \frac{2}{35}b_{i-2} - \frac{1}{1225}b_{i-4}, \quad (i \ge 5), \quad b_1 = \frac{1}{5}, \quad b_2 = \frac{1}{25}, \quad b_3 = \frac{1}{175}, \quad b_4 = \frac{1}{875}. \tag{3.2}$$

Then the characteristic equation of $\{b_i\}_{i \geqslant 1}$ is $x^4 = \frac{2}{35}x^2 - \frac{1}{1225}$, whose roots are $x_1 = x_2 = \frac{1}{\sqrt{35}}, x_3 = x_4 = -\frac{1}{\sqrt{35}}$. Then the general solution of (3.2) is

$$b_i = (y_1 i + y_2)\left(\frac{1}{\sqrt{35}}\right)^i + (y_3 i + y_4)\left(-\frac{1}{\sqrt{35}}\right)^i. \tag{3.3}$$

Combining with the initial conditions in (3.2) yields the system of equations

$$\begin{cases} \dfrac{1}{\sqrt{35}}(y_1 + y_2) - \dfrac{1}{\sqrt{35}}(y_3 + y_4) = \dfrac{1}{5}, \\ \left(\dfrac{1}{\sqrt{35}}\right)^2(2y_1 + y_2) + \left(\dfrac{1}{\sqrt{35}}\right)^2(2y_3 + y_4) = \dfrac{1}{25}, \\ \left(\dfrac{1}{\sqrt{35}}\right)^3(3y_1 + y_2) - \left(\dfrac{1}{\sqrt{35}}\right)^3(3y_3 + y_4) = \dfrac{1}{175}, \\ \left(\dfrac{1}{\sqrt{35}}\right)^4(4y_1 + y_2) + \left(\dfrac{1}{\sqrt{35}}\right)^4(4y_3 + y_4) = \dfrac{1}{875}. \end{cases}$$

The unique solution of this system of equations is $y_1 = 0, y_2 = \frac{7+\sqrt{35}}{10}, y_3 = 0, y_4 = \frac{7-\sqrt{35}}{10}$. Thus the result follows by substituting y_1, y_2, y_3, and y_4 back into (3.3), as desired. $\square$

Corollary 3.2. *$\alpha_1 = 0$, $\alpha_i > 0$ $(i = 2, 3, \dots, 2n+1)$.*

Proof. Expanding $\det M$ with respect to its last row yields

$$\begin{aligned}\det M &= \frac{1}{5}b_{2n} - \frac{1}{25}b_{2n-1}\\ &= \frac{1}{5}\cdot\frac{7}{5}\cdot\left(\frac{1}{\sqrt{35}}\right)^{2n} - \frac{1}{25}\cdot\frac{\sqrt{35}}{5}\cdot\left(\frac{1}{\sqrt{35}}\right)^{2n-1}\\ &= \frac{1}{25}\cdot\left(\frac{1}{\sqrt{35}}\right)^{2n-1}\cdot\left(\frac{7}{\sqrt{35}} - \frac{\sqrt{35}}{5}\right)\\ &= 0.\end{aligned}$$

On the other hand, by algebraic theory, we have $\det M = \prod_{i=1}^{2n+1}\alpha_i$. Combining with $0 \leq 2\alpha_1 \leq 2\alpha_2 \leq \dots \leq 2\alpha_{2n+1}$ are the normalized Laplacian eigenvalues of L_n^2, we obtain $\alpha_1 = 0$, $\alpha_i > 0$ $(i = 2, 3, \dots, 2n+1)$, as desired. $\square$

Note that $|E(L_n^2)| = 24n + 6$, the following lemma is an immediate consequence of Lemma 2.3 and Corollary 3.2.

Lemma 3.3. *Let L_n^2 be the strong prism of a linear hexagonal chain with n hexagons. Then*

$$Kf^*(L_n^2) = 2(24n+6)\left[(2n+4)\times\frac{5}{6} + (2n-2)\times\frac{7}{8} + \frac{1}{2}\sum_{i=2}^{2n+1}\frac{1}{\alpha_i} + \frac{1}{2}\sum_{j=1}^{2n+1}\frac{1}{\beta_j}\right],$$

where $0 = \alpha_1 < \alpha_2 \leqslant \dots \leqslant \alpha_{2n+1}, 0 < \beta_1 \leqslant \beta_2 \leqslant \dots \leqslant \beta_{2n+1}$ are the eigenvalues of M and N, respectively.

Based on the relationship between the roots and coefficients of $\Phi(M)$ (resp. $\Phi(N)$), the formula of $\sum_{i=2}^{2n+1}\frac{1}{\alpha_i}$ (resp. $\sum_{j=1}^{2n+1}\frac{1}{\beta_j}$) is derived in the next two lemmas.

Lemma 3.4. *Let α_i $(i = 1, 2, \dots, 2n+1)$ be defined as above. Then*

$$\sum_{i=2}^{2n+1}\frac{1}{\alpha_i} = \frac{4n(12n^2+9n+4)}{12n+3}.$$

Proof. Suppose that $\Phi(M) = x^{2n+1} + a_1x^{2n} + \cdots + a_{2n-1}x^2 + a_{2n}x = x(x^{2n} + a_1x^{2n-1} + \cdots + a_{2n-1}x + a_{2n})$. Then α_i $(i = 2, 3, \dots, 2n+1)$ satisfies the following equation

$$x^{2n} + a_1x^{2n-1} + \cdots + a_{2n-1}x + a_{2n} = 0.$$

and so $\frac{1}{\alpha_i}$ $(i = 2, 3, \dots, 2n+1)$ satisfies the following equation

$$a_{2n}x^{2n} + a_{2n-1}x^{2n-1} + \cdots + a_1x + 1 = 0.$$

By Vieta's Theorem, we have

$$\sum_{i=2}^{2n+1}\frac{1}{\alpha_i} = \frac{-a_{2n-1}}{a_{2n}}. \tag{3.4}$$

Then based on Lemma 3.1, we give the expressions of a_{2n} and $-a_{2n-1}$ by the following two claims, respectively. For the sake of convenience, we let the diagonal entries of M be k_{ii} and b_0 be 1.

Claim 1. $a_{2n} = \frac{84n+21}{25}\cdot\left(\frac{1}{35}\right)^n$.

Proof of Claim 1. Since the number $a_{2n}(=(-1)^{2n}a_{2n})$ is the sum of those principal minors of M which have $2n$ rows and columns, we have

$$\begin{aligned}
a_{2n} &= \sum_{i=1}^{2n+1} \begin{vmatrix}
k_{11} & -\frac{1}{5} & \cdots & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{5} & k_{22} & \cdots & 0 & 0 & 0 & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 0 & \cdots & k_{i-1,i-1} & 0 & 0 & \cdots & 0 \\
0 & 0 & \cdots & 0 & k_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\
\vdots & \vdots & \cdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & \cdots & k_{2n,2n} & -\frac{1}{5} \\
0 & 0 & \cdots & 0 & 0 & \cdots & -\frac{1}{5} & k_{2n+1,2n+1}
\end{vmatrix} \\
&= \sum_{i=1}^{2n+1} \left(\begin{vmatrix}
k_{11} & -\frac{1}{5} & \cdots & 0 \\
-\frac{1}{5} & k_{22} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & k_{i-1,i-1}
\end{vmatrix} \begin{vmatrix}
k_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\
\vdots & \ddots & \vdots & \vdots \\
0 & \cdots & k_{2n,2n} & -\frac{1}{5} \\
0 & \cdots & -\frac{1}{5} & k_{2n+1,2n+1}
\end{vmatrix} \right). \qquad (3.5)
\end{aligned}$$

Note that a permutation similarity transformation of a square matrix preserves its determinant. Together with the property of M, the right hand side of (3.5) is equal to b_{2n+1-i}. By Lemma 3.1, we have

$$\begin{aligned}
a_{2n} = &\sum_{i=1}^{2n+1} b_{i-1}b_{2n+1-i} = \sum_{i=2}^{2n} b_{i-1}b_{2n+1-i} + 2b_{2n} \\
= &\sum_{i=2}^{2n} \Big[\frac{7+\sqrt{35}}{10}\left(\frac{1}{\sqrt{35}}\right)^{i-1} + \frac{7-\sqrt{35}}{10}\left(-\frac{1}{\sqrt{35}}\right)^{i-1}\Big] \\
&\times \Big[\frac{7+\sqrt{35}}{10}\left(\frac{1}{\sqrt{35}}\right)^{2n+1-i} + \frac{7-\sqrt{35}}{10}\left(-\frac{1}{\sqrt{35}}\right)^{2n+1-i}\Big] + 2\cdot\frac{7}{5}\left(\frac{1}{35}\right)^{n} \\
= &\frac{84n+21}{25}\cdot\left(\frac{1}{35}\right)^{n}.
\end{aligned}$$

This completes the proof of Claim 1.

Claim 2. $-a_{2n-1} = \frac{28n(12n^2+9n+4)}{25}\cdot\left(\frac{1}{35}\right)^{n}$.

Proof of Claim 2. Note that the number $-a_{2n-1}(=(-1)^{2n-1}a_{2n-1})$ is the sum of those principal minors of M

which have $(2n-1)$ rows and columns, hence $-a_{2n-1}$ equals

$$\sum_{1\leqslant i<j\leqslant 2n+1}\begin{vmatrix} k_{11} & -\frac{1}{5} & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ -\frac{1}{5} & k_{22} & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & k_{i-1,i-1} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & k_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & -\frac{1}{\sqrt{35}} & k_{i+2,i+2} & \cdots & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & k_{j-1,j-1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & k_{j+1,j+1} & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & k_{2n,2n} & -\frac{1}{5} \\ 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & -\frac{1}{5} & k_{2n+1,2n+1} \end{vmatrix}$$

$$= \sum_{1\leqslant i<j\leqslant 2n+1}\left(\begin{vmatrix} k_{11} & -\frac{1}{5} & \cdots & 0 \\ -\frac{1}{5} & k_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & k_{i-1,i-1}\end{vmatrix}\begin{vmatrix} k_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\ -\frac{1}{\sqrt{35}} & k_{i+2,i+2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & k_{j-1,j-1}\end{vmatrix}\right.$$
$$\left.\times\begin{vmatrix} k_{j+1,j+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & k_{2n,2n} & -\frac{1}{5} \\ 0 & \cdots & -\frac{1}{5} & k_{2n+1,2n+1}\end{vmatrix}\right). \tag{3.6}$$

Note that a permutation similarity transformation of a square matrix preserves its determinant. Hence, together with the property of M, the right hand side of (3.6) is equal to b_{2n+1-j}. Thus,

$$-a_{2n-1} = \sum_{1\leqslant i<j\leqslant 2n+1} b_{i-1}b_{2n+1-j}\cdot\det P, \tag{3.7}$$

where

$$P = \begin{pmatrix} k_{i+1,i+1} & -\frac{1}{\sqrt{35}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{35}} & k_{i+2,i+2} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{35}} & k_{i+3,i+3} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & k_{j-2,j-2} & -\frac{1}{\sqrt{35}} \\ 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & k_{j-1,j-1}\end{pmatrix}_{(j-i-1)\times(j-i-1)}.$$

By the expression of M, we know that $\det P$ will change according to the different choice of i and j. Hence, we proceed by distinguishing the following four cases.

Case 1. *Both i and j are even. Without loss of generality, let $i = 2k$ and $j = 2l$. Since $1 \leq i < j \leq 2n+1$, we* *have $1 \leq k < l \leq n$. In this case, P is a $(2l-2k-1)\times(2l-2k-1)$ matrix. Hence,*

$$\det P = \begin{vmatrix} \frac{2}{7} & -\frac{1}{\sqrt{35}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{35}} & \frac{2}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{35}} & \frac{2}{7} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{2}{5} & -\frac{1}{\sqrt{35}} \\ 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{7} \end{vmatrix} = 10(l-k)\left(\frac{1}{35}\right)^{l-k}.$$

Case 2. *Both i and j are odd. Without loss of generality, let $i = 2k+1$ and $j = 2l+1$. As $1 \leq i < j \leq 2n+1$, we have $0 \leq k < l \leq n$. In this case, P is a $(2l-2k-1)\times(2l-2k-1)$ matrix. So*

$$\det P = \begin{vmatrix} \frac{2}{5} & -\frac{1}{\sqrt{35}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{35}} & \frac{2}{7} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{35}} & \frac{2}{5} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{2}{7} & -\frac{1}{\sqrt{35}} \\ 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{5} \end{vmatrix} = 14(l-k)\left(\frac{1}{35}\right)^{l-k}.$$

Case 3. *i is even and j is odd. Without loss of generality, let $i = 2k$ and $j = 2l+1$. As $1 \leq i < j \leq 2n+1$, we have $1 \leq k \leq l \leq n$. In this case, P is a $(2l-2k)\times(2l-2k)$ matrix. Thus,*

$$\det P = \begin{vmatrix} \frac{2}{7} & -\frac{1}{\sqrt{35}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{35}} & \frac{2}{5} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{35}} & \frac{2}{7} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{2}{7} & -\frac{1}{\sqrt{35}} \\ 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{5} \end{vmatrix} = (2l-2k+1)\left(\frac{1}{35}\right)^{l-k}.$$

Case 4. *i is odd and j is even. Without loss of generality, let $i = 2k-1$ and $j = 2l$. As $1 \leq i < j \leq 2n+1$, we have $1 \leq k \leq l \leq n$. In this case, P is a $(2l-2k)\times(2l-2k)$ matrix. Thus,*

$$\det P = \begin{vmatrix} \frac{2}{5} & -\frac{1}{\sqrt{35}} & 0 & \cdots & 0 & 0 \\ -\frac{1}{\sqrt{35}} & \frac{2}{7} & -\frac{1}{\sqrt{35}} & \cdots & 0 & 0 \\ 0 & -\frac{1}{\sqrt{35}} & \frac{2}{5} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{2}{5} & -\frac{1}{\sqrt{35}} \\ 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{35}} & \frac{2}{7} \end{vmatrix} = (2l-2k+1)\left(\frac{1}{35}\right)^{l-k}.$$

Combining with Lemma 3.1 and Cases 1-4 we have

$$\begin{aligned}\sum_{1\leqslant i<j\leqslant 2n+1} b_{i-1}b_{2n+1-j}\cdot\det P =& 10\sum_{1\leqslant k<l\leqslant n}\frac{(l-k)b_{2k-1}b_{2n+1-2l}}{35^{l-k}} + 14\sum_{0\leqslant k<l\leqslant n}\frac{(l-k)b_{2k}b_{2n-2l}}{35^{l-k}} \\ &+ \sum_{1\leqslant k\leqslant l\leqslant n}\frac{(2l-2k+1)(b_{2k-2}b_{2n-2l+1}+b_{2k-1}b_{2n-2l})}{35^{l-k}} \\ =& \frac{28n(12n^2+9n+4)}{25}\left(\frac{1}{35}\right)^{n}.\end{aligned}$$

Thus, Claim 2 holds.

Substituting Claims 1-2 into (3.4) yields $\sum_{i=2}^{2n+1}\frac{1}{\alpha_i} = \frac{4n(12n^2+9n+4)}{12n+3}$, as desired. □

Lemma 3.5. *Let β_j $(1 \leqslant j \leqslant 2n+1)$ denote the eigenvalues of N as above. Then*

$$\sum_{j=1}^{2n+1} \frac{1}{\beta_j} = \frac{\left[48+55\sqrt{2}+68(3+2\sqrt{2})n\right](\sqrt{2}+1)^{2n} + \left[48-55\sqrt{2}+68(3-2\sqrt{2})n\right](\sqrt{2}-1)^{2n}}{8\sqrt{2}\left[\left(\sqrt{2}+1\right)^{2n+2} - \left(\sqrt{2}-1\right)^{2n+2}\right]}.$$

Proof. Suppose that $\Phi(N) = x^{2n+1} + h_1 x^{2n} + \cdots + h_{2n}x + h_{2n+1}$. Then β_j $(j = 1, 2, \ldots, 2n+1)$ satisfies the following equation

$$x^{2n+1} + h_1 x^{2n} + \cdots + h_{2n}x + h_{2n+1} = 0$$

and so $\frac{1}{\beta_j}$ $(j = 1, 2, \ldots, 2n+1)$ satisfies the following equation

$$h_{2n+1}x^{2n+1} + h_{2n}x^{2n} + \cdots + h_1 x + 1 = 0.$$

By Vieta's Theorem, we have

$$\sum_{j=1}^{2n+1} \frac{1}{\beta_j} = -\frac{h_{2n}}{h_{2n+1}} = \frac{h_{2n}}{\det N}. \tag{3.8}$$

For $1 \leqslant i \leqslant 2n$, let W_i be the ith order principal submatrix formed by the first i rows and columns of N and $w_i = \det W_i$. The following fact gives the formula of w_i, which will be used to calculate h_{2n} and $\det N$.

Fact 1. *For $1 \leqslant i \leqslant 2n$,*

$$w_i = \begin{cases} \dfrac{\sqrt{70}+\sqrt{35}}{10}\left(\dfrac{\sqrt{2}+1}{\sqrt{35}}\right)^i + \dfrac{\sqrt{70}-\sqrt{35}}{10}\left(\dfrac{\sqrt{2}-1}{\sqrt{35}}\right)^i, & \textit{if } i \textit{ is odd;} \\ \dfrac{14+7\sqrt{2}}{20}\left(\dfrac{\sqrt{2}+1}{\sqrt{35}}\right)^i + \dfrac{14-7\sqrt{2}}{20}\left(\dfrac{\sqrt{2}-1}{\sqrt{35}}\right)^i, & \textit{if } i \textit{ is even.} \end{cases}$$

Proof of Fact 1. It is easy to see that $w_1 = \frac{3}{5}, w_2 = \frac{1}{5}, w_3 = \frac{17}{175}$ and $w_4 = \frac{29}{875}$. For $3 \leqslant i \leqslant 2n$, expanding $\det W_i$ with respect to its last row, we obtain

$$w_i = \begin{cases} \dfrac{4}{7}w_{i-1} - \dfrac{1}{35}w_{i-2}, & \text{if } i \text{ is odd;} \\ \dfrac{2}{5}w_{i-1} - \dfrac{1}{35}w_{i-2}, & \text{if } i \text{ is even.} \end{cases}$$

For $1 \leq i \leq n$, let $e_i = w_{2i}$ and for $1 \leq i \leq n-1$, let $f_i = w_{2i+1}$. Then $e_1 = \frac{1}{5}$, $f_1 = \frac{17}{175}$ and for $i \geq 2$, we have

$$\begin{cases} e_i = \dfrac{2}{5}f_{i-1} - \dfrac{1}{35}e_{i-1}, \\ f_i = \dfrac{4}{7}e_i - \dfrac{1}{35}f_{i-1}. \end{cases} \tag{3.9}$$

From the first equation in (3.9), one has $f_{i-1} = \frac{5}{2}e_i + \frac{1}{14}e_{i-1}$. Hence, $f_i = \frac{5}{2}e_{i+1} + \frac{1}{14}e_i$. Substituting f_{i-1} and f_i into the second equation in (3.9) yields $e_{i+1} = \frac{6}{35}e_i - \frac{1}{1225}e_{i-1}$, $i \geq 2$. Similarly, we can obtain $f_i = \frac{6}{35}f_{i-1} - \frac{1}{1225}f_{i-2}$, $i \geq 3$. Therefore, w_i satisfies the recurrence relation

$$w_i = \frac{6}{35}w_{i-2} - \frac{1}{1225}w_{i-4}, \quad (i \geq 5), \quad w_1 = \frac{3}{5}, \quad w_2 = \frac{1}{5}, \quad w_3 = \frac{17}{175}, \quad w_4 = \frac{29}{875}. \tag{3.10}$$

Then the characteristic equations of $\{w_i\}_{i \geqslant 1}$ is $x^4 = \frac{6}{35}x^2 - \frac{1}{1225}$, whose roots are $x_1 = \frac{3+2\sqrt{2}}{35}$, $x_2 = -\frac{3+2\sqrt{2}}{35}$, $x_3 = \frac{3-2\sqrt{2}}{35}$ and $x_4 = -\frac{3-2\sqrt{2}}{35}$. The general solution of (3.10) is

$$w_i = \left(\frac{3+2\sqrt{2}}{35}\right)^i y_1 + \left(-\frac{3+2\sqrt{2}}{35}\right)^i y_2 + \left(\frac{3-2\sqrt{2}}{35}\right)^i y_3 + \left(-\frac{3-2\sqrt{2}}{35}\right)^i y_4. \tag{3.11}$$

Together with the initial conditions in (3.10), we have the system of equations

$$\begin{cases} \dfrac{3+2\sqrt{2}}{35}(y_1-y_2)+\dfrac{3-2\sqrt{2}}{35}(y_3-y_4)=\dfrac{3}{5}, \\ \left(\dfrac{3+2\sqrt{2}}{35}\right)^2(y_1+y_2)+\left(\dfrac{3-2\sqrt{2}}{35}\right)^2(y_3+y_4)=\dfrac{1}{5}, \\ \left(\dfrac{3+2\sqrt{2}}{35}\right)^3(y_1-y_2)+\left(\dfrac{3-2\sqrt{2}}{35}\right)^3(y_3-y_4)=\dfrac{17}{175}, \\ \left(\dfrac{3+2\sqrt{2}}{35}\right)^4(y_1+y_2)+\left(\dfrac{3-2\sqrt{2}}{35}\right)^4(y_3+y_4)=\dfrac{29}{875}. \end{cases}$$

Solving it, we get the unique solution of this system of equations is $y_1=\frac{7\sqrt{2}+14+2\sqrt{70}+2\sqrt{35}}{40}$, $y_2=\frac{7\sqrt{2}+14-2\sqrt{70}-2\sqrt{35}}{40}$, $y_3=\frac{7\sqrt{2}-14+2\sqrt{70}-2\sqrt{35}}{40}$ and $y_4=\frac{7\sqrt{2}-14-2\sqrt{70}+2\sqrt{35}}{40}$. Thus Fact 1 follows by substituting y_1, y_2, y_3 and y_4 back into (3.11).

By expanding $\det N$ with regards to its last row, we have

$$\det N=\frac{3}{5}\det W_{2n}-\frac{1}{25}\det W_{2n-1}=\frac{3}{5}w_{2n}-\frac{1}{25}w_{2n-1}.$$

Together with Fact 1, we immediately have the following fact.

Fact 2. $\det N=\frac{7\sqrt{2}\left[(\sqrt{2}+1)^{2n+2}-(\sqrt{2}-1)^{2n+2}\right]}{100\cdot 35^n}$.

The formula of h_{2n} is presented by the following fact. For the sake of convenience, let the diagonal entries of N be l_{ii} and w_0 be 1.

Fact 3. $h_{2n}=\frac{7\left[48+55\sqrt{2}+68(3+2\sqrt{2})n\right](\sqrt{2}+1)^{2n}+7\left[48-55\sqrt{2}+68(3-2\sqrt{2})n\right](\sqrt{2}-1)^{2n}}{800\cdot 35^n}$.

Proof of Fact 3. Since $h_{2n}(=(-1)^{2n}h_{2n})$ is the sum of those principal minors of N which have $2n$ rows and columns, we have

$$\begin{aligned} h_{2n} &= \sum_{i=1}^{2n+1}\begin{vmatrix} l_{11} & -\frac{1}{5} & \cdots & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{5} & l_{22} & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & l_{i-1,i-1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & l_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & l_{2n,2n} & -\frac{1}{5} \\ 0 & 0 & \cdots & 0 & 0 & \cdots & -\frac{1}{5} & l_{2n+1,2n+1} \end{vmatrix} \\ &= \sum_{i=1}^{n+1}\left(\begin{vmatrix} l_{11} & -\frac{1}{5} & \cdots & 0 \\ -\frac{1}{5} & l_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{i-1,i-1} \end{vmatrix}\begin{vmatrix} l_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{2n,2n} & -\frac{1}{5} \\ 0 & \cdots & -\frac{1}{5} & l_{2n+1,2n+1} \end{vmatrix}\right). \end{aligned}$$

Note that a permutation similarity transformation of a square matrix preserves its determinant. Together with the property of N, we have

$$\det W_{2n+1-i}=\begin{vmatrix} l_{i+1,i+1} & -\frac{1}{\sqrt{35}} & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{2n,2n} & -\frac{1}{5} \\ 0 & \cdots & -\frac{1}{5} & l_{2n+1,2n+1} \end{vmatrix}.$$

Whence

$$h_{2n} = \sum_{i=1}^{2n+1} w_{i-1}w_{2n+1-i} = 2w_{2n} + \sum_{k=1}^{n-1} w_{2k}w_{2n-2k} + \sum_{l=1}^{n} w_{2l-1}w_{2n-2l+1}.$$

By Fact 1, we have

$$2w_{2n} = \frac{14+7\sqrt{2}}{10}\left(\frac{\sqrt{2}+1}{\sqrt{35}}\right)^{2n} + \frac{14-7\sqrt{2}}{10}\left(\frac{\sqrt{2}-1}{\sqrt{35}}\right)^{2n},$$

$$\begin{aligned}\sum_{k=1}^{n-1} w_{2k}w_{2n-2k} =& \sum_{k=1}^{n-1}\left[\frac{14+7\sqrt{2}}{20}\left(\frac{\sqrt{2}+1}{\sqrt{35}}\right)^{2k} + \frac{14-7\sqrt{2}}{20}\left(\frac{\sqrt{2}-1}{\sqrt{35}}\right)^{2k}\right] \\ &\times\left[\frac{14+7\sqrt{2}}{20}\left(\frac{\sqrt{2}+1}{\sqrt{35}}\right)^{2n-2k} + \frac{14-7\sqrt{2}}{20}\left(\frac{\sqrt{2}-1}{\sqrt{35}}\right)^{2n-2k}\right] \\ =& \frac{\left[196(3+2\sqrt{2})n - 49(16+5\sqrt{2})\right](\sqrt{2}+1)^{2n} + \left[196(3-2\sqrt{2})n - 49(16-5\sqrt{2})\right](\sqrt{2}-1)^{2n}}{800\cdot 35^n},\end{aligned}$$

and

$$\begin{aligned}\sum_{l=1}^{n} w_{2l+1-1}w_{2n-2l+1+1} =& \sum_{l=1}^{n}\left[\frac{\sqrt{70}+\sqrt{35}}{10}\left(\frac{\sqrt{2}+1}{\sqrt{35}}\right)^{2l-1} + \frac{\sqrt{70}-\sqrt{35}}{10}\left(\frac{\sqrt{2}-1}{\sqrt{35}}\right)^{2l-1}\right] \\ &\times\left[\frac{\sqrt{70}+\sqrt{35}}{10}\left(\frac{\sqrt{2}+1}{\sqrt{35}}\right)^{2n-2l+1} + \frac{\sqrt{70}-\sqrt{35}}{10}\left(\frac{\sqrt{2}-1}{\sqrt{35}}\right)^{2n-2l+1}\right] \\ =& \frac{\left[140(3+2\sqrt{2})n + 35\sqrt{2}\right](\sqrt{2}+1)^{2n} + \left[140(3-2\sqrt{2})n - 35\sqrt{2}\right](\sqrt{2}-1)^{2n}}{400\cdot 35^n},\end{aligned}$$

Thus, Fact 3 follows immediately.

In view of (3.8), Facts 2 and 3, Lemma 3.5 follows directly. □

By Lemmas 3.3 – 3.5, the following result follows immediately.

Theorem 3.6. *Let L_n^2 be the strong prism of a linear hexagonal chain with n hexagons. Then*

$$Kf^*(L_n^2) = (96n^3 + 236n^2 + 149n + 19) + (12n+3)\varphi(n),$$

where

$$\varphi(n) = \frac{\left[48 + 55\sqrt{2} + 68(3+2\sqrt{2})n\right](\sqrt{2}+1)^{2n} + \left[48 - 55\sqrt{2} + 68(3-2\sqrt{2})n\right](\sqrt{2}-1)^{2n}}{4\sqrt{2}\left[\left(\sqrt{2}+1\right)^{2n+2} - \left(\sqrt{2}-1\right)^{2n+2}\right]}.$$

The explicit closed formula of the number of spanning trees of L_n^2 is in the following.

Theorem 3.7. *Let L_n^2 be the strong prism of a linear hexagonal chain with n hexagons. Then*

$$\tau(L_n^2) = \sqrt{2}\cdot 2^{12n-5}\cdot 3^{2n+4}\left[\left(\sqrt{2}+1\right)^{2n+2} - \left(\sqrt{2}-1\right)^{2n+2}\right].$$

Proof. From the proof of Lemma 3.4, we know that $\alpha_i\,(i = 2, 3, \ldots, 2n+1)$ is the root of the equation $x^{2n} + a_1x^{2n-1} + \cdots + a_{2n-1}x + a_{2n} = 0$. Then we have

$$\prod_{i=2}^{2n+1} \alpha_i = a_{2n}.$$

By Claim 1, we have

$$\prod_{i=2}^{2n+1} 2\alpha_i = \frac{84n+21}{25}\left(\frac{1}{35}\right)^n \cdot 2^{2n}.$$

Similarly,

$$\prod_{j=1}^{2n+1} 2\beta_j = \frac{2^{2n+1}\cdot 7\sqrt{2}\left[\left(\sqrt{2}+1\right)^{2n+2}-\left(\sqrt{2}-1\right)^{2n+2}\right]}{100\cdot 35^n}.$$

Note that

$$\prod_{x\in V(L_n^2)} d_{v_i}(L_n^2) = 5^{4n+8}\cdot 7^{4n-4}, \quad |E(L_n^2)| = 24n+6.$$

Together with Lemma 2.2, we have

$$\begin{aligned}\tau(L_n^2) &= \frac{1}{2|E(L_n^2)|}\Big[\big(\prod_{i=1}^{8n+4} d_i(L_n^2)\big)\cdot\big(\frac{6}{5}\big)^{2n+4}\cdot\big(\frac{8}{7}\big)^{2n-2}\cdot\big(\prod_{i=2}^{2n+1}2\alpha_i\big)\cdot\big(\prod_{j=1}^{2n+1}2\beta_j\big)\Big]\\ &= \sqrt{2}\cdot 2^{12n-5}\cdot 3^{2n+4}\left[\left(\sqrt{2}+1\right)^{2n+2}-\left(\sqrt{2}-1\right)^{2n+2}\right].\end{aligned}$$

□

At the end of this section, we show that the degree-Kirchhoff index of L_n^2 is approximately one eighth of its Gutman index.

Theorem 3.8. *Let L_n^2 be the strong prism of a linear hexagonal chain with n hexagons. Then*

$$Gut(L_n^2) = 768n^3 + 1152n^2 + 892n + 38.$$

Proof. We compute $d_x d_y d(x,y)$ for all vertices (fixed x and for all y) (there are three types of vertices) and then add all together and finally divided by two. The expressions of each type of vertices are:

Corner vertex of L_n^2:

$$f_1(n) = 2\left[\sum_{k=1}^{2n} 5\cdot 5\cdot k + \sum_{k=2}^{2n-1} 5\cdot 7\cdot k + 5\cdot 5(4n+2)\right] + 5\cdot 5\cdot 1 = 240n^2+180n+55.$$

Vertex in $\{u_{2i}, v_{2i}, u'_{2i}, v'_{2i}\}$, where $1\le i\le n$:

$$\begin{aligned}f_2(i,n) &= 2\left[\sum_{k=2}^{2i-1} 5\cdot 5\cdot k + \sum_{k=2}^{2n-2i+1} 5\cdot 5\cdot k + 5\cdot 5\cdot 3 + \sum_{k=1}^{2i-2} 5\cdot 7\cdot k + \sum_{k=1}^{2n-2i} 5\cdot 7\cdot k + 5\cdot 5(4n+2)\right] + 5\cdot 5\cdot 1\\ &= 480i^2 - 480i + 170 + 240n^2 - 480ni + 420n + 125.\end{aligned}$$

Vertex in $\{u_{2i+1}, v_{2i+1}, u'_{2i+1}, v'_{2i+1}\}$, where $1\le i\le n-1$:

$$\begin{aligned}f_3(i,n) &= 2\left[\sum_{k=1}^{2i} 7\cdot 5\cdot k + \sum_{k=1}^{2n-2i} 7\cdot 5\cdot k + \sum_{k=2}^{2i-1} 7\cdot 7\cdot k + \sum_{k=2}^{2n-2i-1} 7\cdot 7\cdot k + 7\cdot 7\cdot 1 + 5\cdot 7(4n+2)\right] + 7\cdot 7\cdot 1\\ &= 672i^2 + 336n^2 - 672ni + 252n + 91.\end{aligned}$$

Hence,

$$\begin{aligned}Gut(L_n^2) &= \frac{8f_1(n) + 4\sum_{i=1}^{n} f_2(i,n) + 4\sum_{i=1}^{n-1} f_3(i,n)}{2}\\ &= 768n^3 + 1152n^2 + 892n + 38.\end{aligned}$$

This completes the proof. □

Based on Theorems 3.6 and 3.8, we obtain

Theorem 3.9. *Let L_n^2 denote a linear hexagonal chain with n hexagons. Then*

$$\lim_{n\to\infty}\frac{Kf^*(L_n^2)}{Gut(L_n^2)} = \frac{1}{8}.$$

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