The Laplacians and Normalized Laplacians of the linear chain networks and applications

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Abstract

In recent years, spectrum analysis and computation have developed rapidly in order to explore and characterize the properties of network sciences. Let $L_n$ be obtained from the transformation of the graph $L_{6,4,4}^n$, which obtained by attaching crossed two four-membered rings to the terminal of crossed phenylene. Firstly, we study the (normalized) Laplacian spectrum of $L_n$ based on the decomposition theorem for the corresponding matrices. Secondly, we obtain the closed-term formulas for the (multiplicative degree) Kirchhoff index and the number of spanning trees from the relationship between roots and coefficients in linear chain networks. Finally, we are surprised to find that the (multiplicative degree) Kirchhoff index of $L_n$ is nearly to one quarter of its (Gutman) Wiener index when $n$ tends to infinity.
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Abstract. In recent years, spectrum analysis and computation have developed rapidly in order to explore and characterize the properties of network sciences. Let $L_n$ be obtained from the transformation of the graph $L_n^{6,4,4}$, which obtained by attaching crossed two four-membered rings to the terminal of crossed phenylenes. Firstly, we study the (nomalized) Laplacian spectrum of $L_n$ based on the decomposition theorem for the corresponding matrices. Secondly, we obtain the closed-term formulas for the (multiplicative degree) Kirchhoff index and the number of spanning trees from the relationship between roots and coefficients in linear chain networks. Finally, we are surprised to find that the (multiplicative degree) Kirchhoff index of $L_n$ is nearly to one quarter of its (Gutman) Wiener index when $n$ tends to infinity.

Keywords: (Multiplicative degree) Kirchhoff index; Wiener index; Gutman index; Spanning trees.

1. Introduction

Throughout this article, we only consider simple, undirected and finite graphs and assume that all graphs are connected. Suppose $\mathcal{G}$ be a graph with the vertex set $V(\mathcal{G}) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(\mathcal{G}) = \{e_1, e_2, \ldots, e_m\}$. The adjacency matrix $A(\mathcal{G})$ is a $0-1$ matrix indexed by the vertices of $\mathcal{G}$ and defined by $a_{ij} = 1$ if and only if $v_s v_t \in E(\mathcal{G})$. For more notation, one can be referred to [1].

The Laplacian matrix of graph $\mathcal{G}$ is defined as $L(\mathcal{G}) = D(\mathcal{G}) - A(\mathcal{G})$, and assume that the eigenvalues of $L(\mathcal{G})$ are labeled $0 = \mu_1 < \mu_2 \leq \cdots \leq \mu_n$.

$$
(L(\mathcal{G}))_{st} = \begin{cases} 
 d_s, & s = t; \\
 -1, & s \neq t \text{ and } v_s \sim v_t; \\
 0, & \text{otherwise.}
\end{cases}
$$

The normalized Laplacian matrix is given by

$$
(L(\mathcal{G}))_{st} = \begin{cases} 
 1, & s = t; \\
 -\frac{1}{\sqrt{d_s d_t}}, & s \neq t \text{ and } v_s \sim v_t; \\
 0, & \text{otherwise.}
\end{cases}
$$

The distance, $d_{ij} = d_{\mathcal{G}}(u_s, u_t)$, between vertices $u_s$ and $u_t$ of $\mathcal{G}$ is the length of a shortest $u_s, u_t$-path in $\mathcal{G}$. The Wiener index [2,3] is the sum of the distances of any two vertices in the graph $\mathcal{G}$, that is

$$
W(\mathcal{G}) = \sum_{s < t} d_{st}.
$$

In 1947, the distance-based invariant first appeared in chemistry [3, 4] and began to apply it to mathematics 30 years later [5]. Nowadays, the Wiener index is widely used in mathematics [6–8] and chemistry [9–11].

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In a simple graph $G$, the degree, $d_i = d_G(v_i)$, of a vertex $v_i$ is the number of edges at $v_i$. The Gutman index [12] of the simple graph $G$ is expressed by

$$\text{Gut}(G) = \sum_{s < t} d_s d_t.$$  

(1.3)

Klein and Randić initially outlined the concepts associated with the resistance distance [13] of the graph. Assume that each edge is replaced by a unit resistor, and we use $r_{st}$ to denote the resistance distance between two vertices $s$ and $t$. Similar to Wiener index, the Kirchhoff index [14, 15] of graph $G$ is expressed as the sum of the resistance distances between each two vertices, that is

$$\text{Kf}(G) = \sum_{s < t} r_{st}.$$ 

In 2007, Chen and Zhang [16] defined the multiplicative degree-Kirchhoff index [17,18], that is

$$\text{Kf}^*(G) = \sum_{s < t} d_s d_t r_{st}.$$ 

Phenyl is a conjugated hydrocarbon, and $L_n^{6,4,4}$ denote a linear chain, containing $n$ hexagons and $2n - 1$ squares, please see it in Figure 1.

With the rapid changes of the times, organic chemistry has also developed rapidly, which has led to a growing interest in polycyclic aromatic compounds. The benzene molecular graph has attracted the attention of elites in various industries such as biology [19, 20], mathematics [21, 22], chemistry [23, 24], computers [25, 26], and materials [27] because of its increasing application in daily life.

In 1985, the computational method and procedure of the matrix decomposition theorem were proposed by Yang [28]. This led to the solution of some problems in graph networks and allowed the unprecedented development of self-homogeneous linear hydrocarbon chains. For example, in 2021, X.L. Ma [30] got the normalized Laplacian spectrum of linear phenylene, and the linear phenylene containing has $n$ hexagons and $n - 1$ squares. L. Lan [31] explored the linear phenylene with $n$ hexagons and $n$ squares. Umar Ali [32] analyzed the strong prism of a graph $G$ is the strong product of the complete graph of order 2 and G. X.Y. Geng [33] obtained the Laplacian spectrum of $L_n^{6,4,4}$, which containing $n$ hexagons and $2n - 1$ squares. J.B. Liu [34] derived the Kirchhoff index and complexity of $O_n$, which denoting linear octagonal-quadrilateral networks. C. Liu [35] got the Laplacian spectrum and Kirchhoff index of $L_n$, and the $L_n$ has $t$ hexagons and $3t + 1$ quadrangles. J.B. Liu [36] explored the multiplicative degree-Kirchhoff index and complexity based on the graph $L_{2n}$. For more results, refer to [37–47].

Inspired by these recent works, we try to investigate the Laplacians and the normalized Laplaceians for graph transformations on phenyl dicyclobutadieno derivatives.

The various sections of this article are as follows: In Section 2, we proposed some concepts and lemmas and use them in subsequent articles. In Section 3 and Section 4, we acquired the Laplacian matrix and the normalized Laplacian matrix, then we make sure the Kirchoff index, the multiplicative degree-Kirchoff index and the complexity of $L_n$. In Section 5, we obtained conclusions based on the calculations in this paper.

2. Preliminary Works

In this article, graph $L_n$ and graph $L_n^{6,4,4}$ are portrayed in Figure 1. Define the characteristic polynomial of matrix $U$ of order $n$ is $P_U(x) = \det(xI - U)$.

It is easy to understand that $\pi = (1, \bar{1})(2, \bar{2}) \cdots (4n, \bar{4n})$ is an automorphism. Set $V_1 = \{1, 2, \cdots, 4n\}$, $V_2 = \{\bar{1}, \bar{2}, \cdots, \bar{4n}\}$, $|V(L_n)| = 8n$, $|E(L_n)| = 19n - 4$. Thus the (normalized) Laplacians matrix can be
expressed in the form of block matrix, that is

\[
L(L_n) = \begin{pmatrix} L_{V_0 V_0} & L_{V_0 V_1} & L_{V_0 V_2} \\ L_{V_1 V_0} & L_{V_1 V_1} & L_{V_1 V_2} \\ L_{V_2 V_0} & L_{V_2 V_1} & L_{V_2 V_2} \end{pmatrix}, \quad \mathcal{L}(L_n) = \begin{pmatrix} \mathcal{L}_{V_0 V_0} & \mathcal{L}_{V_0 V_1} & \mathcal{L}_{V_0 V_2} \\ \mathcal{L}_{V_1 V_0} & \mathcal{L}_{V_1 V_1} & \mathcal{L}_{V_1 V_2} \\ \mathcal{L}_{V_2 V_0} & \mathcal{L}_{V_2 V_1} & \mathcal{L}_{V_2 V_2} \end{pmatrix},
\]

where \(L_{V,s}\) and \(\mathcal{L}_{V,s}\) is a submatrix consisting of rows corresponding to the vertices in \(V_s\) and columns corresponding to the vertices in \(V_t\), \(s,t = 0,1,2\).

Let

\[
Q = \begin{pmatrix} I_t & 0 \\ 0 & \frac{1}{\sqrt{2}} I_{4n} \\ 0 & \frac{1}{\sqrt{2}} I_{4n} \end{pmatrix},
\]

then

\[
QL(L_G)Q' = \begin{pmatrix} L_A(G) & 0 \\ 0 & L_S(G) \end{pmatrix}, \quad QL(L_G)Q' = \begin{pmatrix} \mathcal{L}_A(G) & 0 \\ 0 & \mathcal{L}_S(G) \end{pmatrix},
\]

and \(Q'\) is the transposition of \(Q\).

\[
L_A = L_{V_1 V_1} + L_{V_1 V_2}, \quad L_S = L_{V_2 V_1} - L_{V_1 V_2}, \quad \mathcal{L}_A = \mathcal{L}_{V_1 V_1} + \mathcal{L}_{V_1 V_2}, \quad \mathcal{L}_S = \mathcal{L}_{V_2 V_1} - \mathcal{L}_{V_1 V_2}.
\]

**Theorem 2.1.** [30] Set \(G\) is a graph and think that \(L_A(G), L_S(G), \mathcal{L}_A(G), \mathcal{L}_S(G)\) are determined as above, then

\[
\varrho_{L(L_n)}(y) = \theta_{L_A(G)}(y)\theta_{L_S(G)}(y), \quad \varrho_{L(L_n)}(y) = \theta_{\mathcal{L}_A(G)}(y)\theta_{\mathcal{L}_S(G)}(y).
\]

**Lemma 2.2.** [48] With the extensive study of Kirchhoff index, Gutman and Mohar proposed a algorithm based on the relation between Kirchhoff index and the Laplacian eigenvalues, namely

\[
Kf(G) = n \sum_{i=2}^{n} \frac{1}{\xi_i},
\]
and the eigenvalues of $L(G)$ are $0 = \xi_1 < \xi_2 \leq \cdots \leq \xi_n (n \geq 2)$.

**Lemma 2.3.** [15] Let’s say that the eigenvalues of $L(G)$ are $\varepsilon_1 \leq \varepsilon_2 \leq \cdots \leq \varepsilon_n$, then its multiplicative degree-Kirchhoff index can be denoted by

$$K_f^*(G) = 2m \sum_{t=2}^{n} \frac{1}{\varepsilon_t}.$$  

**Lemma 2.4.** [1] The number of spanning trees of the $G$ can also be called the complexity of $G$. If $G$ is a graph with $|V_G| = n$ and $|E_G| = m$. Let $\lambda_i (i = 2, 3, \ldots, n)$ be the eigenvalues of $L(G)$. Then the complexity of $G$ is

$$2m\tau(G) = \prod_{i=1}^{n} d_i \cdot \prod_{i=2}^{n} \lambda_i.$$  

### 3. Kirchhoff index of $L_n$

In this section, the main objective is to find out the Kirchhoff index of $L_n$. Then, combining the definition of the Laplacian matrix and Eq.(1.1), we can write these block matrices as follows.

\[
L_{V_1V_1} = \begin{pmatrix}
3 & -1 & & & \\
-1 & 4 & -1 & & \\
& -1 & 5 & -1 & \\
& & -1 & 5 & -1 \\
& & & -1 & 4 & -1 \\
& & & & -1 & 5 & -1 \\
& & & & & -1 & 4 & -1 \\
& & & & & & -1 & 5 & -1 \\
& & & & & & & -1 & 3 \\
\end{pmatrix}_{(4n) \times (4n)}
\]

\[
L_{V_1V_2} = \begin{pmatrix}
-1 & -1 & & & \\
-1 & 0 & -1 & & \\
& -1 & -1 & -1 & \\
& & -1 & -1 & -1 \\
& & & -1 & -1 & -1 \\
& & & & -1 & 0 & -1 \\
& & & & & -1 & -1 & -1 \\
& & & & & & -1 & 0 & -1 \\
& & & & & & & -1 & -1 \\
& & & & & & & & -1 \\
\end{pmatrix}_{(4n) \times (4n)}
\]
Hence,

\[
L_A = \begin{pmatrix}
2 & -2 & & & \\
-2 & 4 & -2 & & \\
& -2 & 4 & -2 & \\
& & -2 & 4 & -2 \\
& & & -2 & 4 \\
& & & & -2 \end{pmatrix}
\]

and

\[
L_S = \text{diag}(4,4,6,6,4,\ldots,6,4,6,4)_{(4n)}.
\]

Assume that \(0 = \alpha_1 < \alpha_2 \leq \alpha_3 \leq \cdots \leq \alpha_{4n}\) are the roots of \(P_{L_A}(x) = 0\), and \(0 < \beta_1 \leq \beta_2 \leq \beta_3 \leq \cdots \leq \beta_{4n}\) are the roots of \(P_{L_S}(x) = 0\). By Lemma 2.2, we immediately have

\[
Kf(L_n) = 2(4n)^2 \left( \sum_{i=2}^{4n} \frac{1}{\alpha_i} + \sum_{j=1}^{4n} \frac{1}{\beta_j} \right).
\]

(3.4)

Obviously, \(\sum_{j=1}^{4n} \frac{1}{\beta_j}\) can be obtained according to \(L_S\).

\[
\sum_{j=1}^{4n} \frac{1}{\beta_j} = \frac{1}{6} \times (3n - 2) + \frac{1}{4} \times (n + 2) = \frac{9n + 2}{12}.
\]

(3.5)

Next, we focus on computing \(\sum_{i=2}^{4n} \frac{1}{\alpha_i}\). Let

\[
P_{L_A}(x) = \det(xI - L_A) = x(x^{4n-1} + a_1 x^{4n-2} + \cdots + a_{4n-2} x + a_{4n-1}), \ a_{4n-1} \neq 0.
\]

Based on the Vieta’s theorem of \(P_{L_A}(x)\), we can exactly get the following equation,

\[
\sum_{i=2}^{4n} \frac{1}{\alpha_i} = \frac{(-1)^{4n-2} a_{4n-2}}{(-1)^{4n-1} a_{4n-1}}.
\]

For the sake of convenience, let \(M_s\) is used to express the \(s-th\) order principal minors of matrix \(A\), and \(m_s = \det M_s\) is recorded. We can get \(m_1 = 2, \ m_2 = 4, \ m_3 = 8\).

And

\[
m_s = 4m_{s-1} - 4m_{s-2}, \ 4 \leq s \leq 4n,
\]

by further induction, we have

\[
m_s = 2^s.
\]

In this way, we can get two theorems.

**Theorem 3.1.** \((-1)^{4n-1} a_{4n-1} = (4n)2^{4n-1}\).
Proof. Due to the sum of all the principal minors of order \(4n - 1\) of \(L_A\) is \((-1)^{4n-1} a_{4n-1}\), then

\[
(-1)^{4n-1} a_{4n-1} = \sum_{s=1}^{4n} det L_A[s] = \sum_{s=1}^{4n} det \begin{pmatrix} M_{s-1} & 0 \\ 0 & U_{4n-s} \end{pmatrix} = \sum_{s=1}^{4n} det M_{s-1} \cdot det U_{4n-s},
\]

where

\[
M_{s-1} = \begin{pmatrix} l_{11} & -2 & \cdots & 0 \\ -2 & l_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{s-1,s-1} \end{pmatrix}_{(s-1) \times (s-1)},
\]

\[
U_{4n-s} = \begin{pmatrix} l_{s+1,s+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{4n-1,4n-1} & -2 \\ 0 & \cdots & -2 & l_{4n,4n} \end{pmatrix}_{(4n-s) \times (4n-s)}.
\]

Let \(m_0 = 1, det U_0 = 1\), because of the symmetry of matrix \(L_A\), then \(det U_{4n-s} = det M_{4n-s}\). Hence

\[
(-1)^{4n-1} a_{4n-1} = \sum_{s=1}^{4n} det m_{s-1} \cdot det m_{4n-s} = (4n)2^{4n-1},
\]

as desired.

Theorem 3.2. \((-1)^{4n-2} a_{4n-2} = \frac{(4n-1)(4n)(4n+1)2^{4n-3}}{3}\)

Proof. Since the \((-1)^{4n-2} a_{4n-2}\) is the total of all the principal minors of order \(4n - 2\) of \(L_A\), we have

\[
(-1)^{4n-2} a_{4n-2} = \sum_{1 \leq s < t \leq 4n} det L_A[s, t],
\]

where

\[
L_A[s, t] = \begin{pmatrix} M_{p-1} & 0 & 0 \\ 0 & N_{t-s-1} & 0 \\ 0 & 0 & U_{4n-t} \end{pmatrix}, 1 \leq s < t \leq 4n,
\]

and

\[
N_{t-s-1} = \begin{pmatrix} 4 & -2 & \cdots & \cdots & 4 & -2 \\ -2 & 4 & -2 & \cdots & -2 & 4 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots \\ \vdots & \vdots & \cdots & \cdots & \cdots & \cdots \\ -2 & 4 & -2 & \cdots & \cdots & \cdots \\ -2 & 4 & -2 & \cdots & \cdots & \cdots \end{pmatrix}_{(t-s-1) \times (t-s-1)} = (t-s)2^{t-s-1}.
\]
Therefore, we can have

\[
(-1)^{4n-2}a_{4n-2} = \sum_{1 \leq s < t \leq 4n} \det M_{s-1} \cdot \det N_{t-s-1} \cdot \det U_{4n-t}
\]

\[
= \sum_{1 \leq s < t \leq 4n} (t - s)^{2t-s-1} \cdot \det m_{s-1} \cdot m_{4n-t}
\]

\[
= \frac{(4n - 1)(4n)(4n + 1)2^{4n-3}}{3}.
\]

The proof is over.

From the results of Theorem 3.1 and Theorem 3.2, we can get

\[
\sum_{i=2}^{4n} \frac{1}{\alpha_i} = (-1)^{4n-2}a_{4n-2} - \frac{16n^2 - 1}{12},
\]

(3.6)

where the eigenvalues of \( L_\alpha \) are \( 0 = \alpha_1 < \alpha_2 \leq \alpha_3 \leq \cdots \leq \alpha_{4n} \).

**Theorem 3.3.** Suppose \( L_n^{6,4,4} \) be the dicyclobutadieno derivative of phenylenes and the graph \( L_n \) be obtained from the transformation of the graph \( L_n^{6,4,4} \).

\[
Kf(L_n) = \frac{32n^3 + 18n^2 + 2n}{3}.
\]

**Proof.** Substituting Eqs. (3.5) and (3.6) into (3.4), the Kirchhoff index of \( L_n \) can be expressed

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

\[
= (8n) \left( \frac{9n + 2}{12} + \frac{(4n + 1)(4n - 1)}{12} \right)
\]

\[
= \frac{32n^3 + 18n^2 + 2n}{3}.
\]

The result as desired

The Kirchhoff index of \( L_n \) from \( L_1 \) to \( L_{15} \), see Table 1.

<table>
<thead>
<tr>
<th>( G )</th>
<th>( Kf(G) )</th>
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<th>( Kf(G) )</th>
</tr>
</thead>
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<tr>
<td>( L_1 )</td>
<td>17.3</td>
<td>( L_4 )</td>
<td>781.3</td>
<td>( L_7 )</td>
<td>3957.3</td>
<td>( L_{10} )</td>
<td>11273.3</td>
<td>( L_{13} )</td>
<td>24457.3</td>
</tr>
<tr>
<td>( L_2 )</td>
<td>110.7</td>
<td>( L_5 )</td>
<td>1486.7</td>
<td>( L_8 )</td>
<td>5850.7</td>
<td>( L_{11} )</td>
<td>14930.7</td>
<td>( L_{14} )</td>
<td>30454.7</td>
</tr>
<tr>
<td>( L_3 )</td>
<td>344.0</td>
<td>( L_6 )</td>
<td>2524.0</td>
<td>( L_9 )</td>
<td>8268.0</td>
<td>( L_{12} )</td>
<td>19304.0</td>
<td>( L_{15} )</td>
<td>37360.0</td>
</tr>
</tbody>
</table>

Next, we will further consider the Wiener index of \( L_n \).

**Theorem 3.4.** Let \( L_n^{6,4,4} \) be the dicyclobutadieno derivative of \([n]\)phenylenes and the graph \( L_n \) be obtained from the transformation of the graph \( L_n^{6,4,4} \), then

\[
\lim_{n \to \infty} \frac{Kf(L_n)}{W(L_n)} = \frac{1}{4}.
\]

**Proof.** Consider \( d_{st} \) for all vertices. For the calculation of convenience, we divide the vertices of the graph into the following five categories.

**Case 1.** Vertex 1 of \( L_n \):

\[
g_1(i) = 1 + 2 \left( \sum_{k=1}^{4n-1} k \right).
\]
Case 2. Vertex $4j - 3 (j = 1, 2, \ldots, n)$ of $L_n$, $i = 4j - 3$:

$$g_2(i) = 1 + 2 \left( \sum_{k=1}^{i-1} k + \sum_{k=1}^{4n-i} k \right).$$

Case 3. Vertex $4j - 2 (j = 1, 2, \ldots, n)$ of $L_n$, $i = 4j - 2$:

$$g_3(i) = 1 + 2 \left( \sum_{k=1}^{i-1} k + \sum_{k=1}^{4n-i} k \right).$$

Case 4. Vertex $4j - 1 (j = 1, 2, \ldots, n - 1)$ of $L_n$, $i = 4j - 1$:

$$g_4(i) = 1 + 2 \left( \sum_{k=1}^{i-1} k + \sum_{k=1}^{4n-i} k \right).$$

Case 5. Vertex $4j (j = 1, 2, \ldots, n - 1)$ of $L_n$, $i = 4j$:

$$g_5(i) = 1 + 2 \left( \sum_{k=1}^{i-1} k + \sum_{k=1}^{4n-i} k \right).$$

Hence, we have

$$W(L_n) = \frac{4g_1(i) + 2 \sum_{i=4j-3} g_2(i) + 2 \sum_{i=4j-2} g_3(i) + 2 \sum_{i=4j-1} g_4(i) + 2 \sum_{i=4j} g_5(i)}{2}$$

$$= \frac{4(1 + 2 \sum_{k=1}^{4n-1} k) + 2 \sum_{j=1}^{n} \left[ 1 + 2(\sum_{k=1}^{4j-4} k + \sum_{k=1}^{4n-4j+1} k) \right] + 2 \sum_{j=1}^{n} \left[ 1 + 2(\sum_{k=1}^{4j-3} k + \sum_{k=1}^{4n-4j+2} k) \right] + 2 \sum_{j=1}^{n} \left[ 1 + 2(\sum_{k=1}^{4j-2} k + \sum_{k=1}^{4n-4j+3} k) \right] + 2 \sum_{j=1}^{n-1} \left[ 1 + 2(\sum_{k=1}^{4j-1} k + \sum_{k=1}^{4n-4j} k) \right]}{2} + \frac{2 \sum_{j=1}^{n-1} \left[ 1 + 2(\sum_{k=1}^{4j-1} k + \sum_{k=1}^{4n-4j} k) \right]}{3}.$$  

Consider the above results of Kirchhoff index and Wiener index, we can get following equation when $n$ tends to infinity.

$$\lim_{n \to \infty} Kf(L_n) = \frac{1}{4}.$$  

The result as desired.
4. Multiplicative degree-Kirchhoff index and complexity of $L_n$

In this section, we use the eigenvalues of normalized Laplacian matrix to determine the multiplicative degree-Kirchhoff index of $L_n$. Besides, we calculate the complexity of $L_n$. Then

$$
\mathcal{L}_{V_1V_1} = \begin{pmatrix}
1 & -\frac{1}{\sqrt{12}} & -\frac{1}{\sqrt{20}} & \frac{1}{5} & \frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} \\
-\frac{1}{\sqrt{12}} & 1 & -\frac{1}{\sqrt{20}} & -\frac{1}{5} & \frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} \\
-\frac{1}{\sqrt{20}} & -\frac{1}{\sqrt{20}} & 1 & -\frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} \\
\frac{1}{5} & -\frac{1}{5} & -\frac{1}{5} & 1 & \frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} \\
-\frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} & -\frac{1}{\sqrt{20}} & -\frac{1}{\sqrt{20}} & 1 & \frac{1}{\sqrt{20}} \\
\frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} & -\frac{1}{\sqrt{20}} & \frac{1}{\sqrt{20}} & -\frac{1}{\sqrt{20}} & 1
\end{pmatrix}_{(4n) \times (4n)}$

and

$$
\mathcal{L}_{V_1V_2} = \begin{pmatrix}
\frac{1}{3} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{2} & -\frac{2}{5} & \frac{2}{5} \\
-\frac{1}{\sqrt{2}} & 1 & -\frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
-\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{2} & 0 & -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\
\frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1 & -\frac{1}{\sqrt{2}} \\
\frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 1
\end{pmatrix}_{(4n) \times (4n)}$

Therefore,

$$
\mathcal{L}_A = \begin{pmatrix}
\frac{2}{3} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-\frac{1}{\sqrt{3}} & \frac{1}{3} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{3} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{3} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
-\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{3} & -\frac{1}{\sqrt{3}} \\
-\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{3}
\end{pmatrix}_{(4n) \times (4n)}$

and

$$
\mathcal{L}_S = \text{diag}(\frac{4}{3}, 1, \frac{6}{5}, \frac{6}{5}, \frac{6}{5}, \frac{6}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5}, \frac{4}{5})_{(4n)}.
$$
Assume that the roots of $P(x) = 0$ are $0 = \xi_1 < \xi_2 \leq \xi_3 \leq \cdots \leq \xi_{3n+2}$, and $0 < \gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \cdots \leq \gamma_{3n+2}$ are the roots of $P(x) = 0$. By Lemma 2.3, we can get

$$Kf^*(L_n) = 2(19n - 4) \left( \sum_{i=2}^{4n} \frac{1}{\xi_i} + \sum_{i=1}^{4n} \frac{1}{\gamma_i} \right).$$

Since $L_n$ is a diagonal matrix. Obviously, its diagonal elements $1, \frac{4}{3}, \frac{6}{5}$ correspond to the eigenvalues of $L_n$ respectively. Then it can be clearly obtained

$$\sum_{i=1}^{4n} \frac{1}{\gamma_i} = \frac{21n - 1}{6} \quad (4.7)$$

Let

$$P(x) = det(xI - L_A) = x^{4n} + b_1 x^{4n-1} + \cdots + b_{4n-1} x, \ b_{4n-1} \neq 0,$$

i.e., $\frac{1}{\xi_2}, \frac{1}{\xi_3}, \cdots, \frac{1}{\xi_{4n}}$ are the roots of the following equation

$$b_{4n-1} x^{4n-1} + b_{4n-2} x^{4n-2} + \cdots + b_1 x + 1 = 0.$$

Based on the Vieta’s theorem of $P(x)$, we can get

$$\sum_{i=2}^{4n} \frac{1}{\xi_i} = (-1)^{4n-2} b_{4n-2} \quad (4.8)$$

Similarly, we can get another two interesting facts.

**Theorem 4.1.** $(-1)^{4n-1} b_{4n-1} = \frac{25}{9} (38n - 8) \left( \frac{4}{125} \right)^n$.

**Proof.** Let $s_p = det F_p$, then we have $s_1 = \frac{2}{3}$, $s_2 = \frac{1}{3}$, $s_3 = \frac{2}{15}$, $s_4 = \frac{4}{75}$, $s_5 = \frac{8}{375}$, $s_6 = \frac{4}{375}$, $s_7 = \frac{8}{1875}$, $s_8 = \frac{16}{9375}$, and

$$\begin{align*}
s_4 &= s_4p - \frac{4}{3} s_4p-1 - \frac{8}{25} s_4p-2; \\
s_4p+1 &= \frac{4}{3} s_4p - \frac{1}{25} s_4p-1; \\
s_4p+2 &= s_4p+1 - \frac{4}{3} s_4p; \\
s_4p+3 &= \frac{4}{3} s_4p+2 - \frac{8}{25} s_4p+1.
\end{align*}$$

After further simplification, the transformation form of the above formula is obtained.

$$\begin{align*}
s_4p &= \frac{5}{3} \cdot \left( \frac{4}{125} \right)^p, \quad 1 \leq p \leq n; \\
s_4p+1 &= \frac{2}{3} \cdot \left( \frac{4}{125} \right)^p, \quad 0 \leq p \leq n - 1; \\
s_4p+2 &= \frac{1}{3} \cdot \left( \frac{4}{125} \right)^p, \quad 0 \leq p \leq n - 1; \\
s_4p+3 &= \frac{2}{3} \cdot \left( \frac{4}{125} \right)^p, \quad 0 \leq p \leq n - 1.
\end{align*}$$

Similarly, we have $t_1 = \frac{2}{3}$, $t_2 = \frac{4}{5}$, $t_3 = \frac{2}{15}$, $t_4 = \frac{4}{75}$, $t_5 = \frac{8}{375}$, $t_6 = \frac{16}{1875}$, $t_7 = \frac{4}{1875}$, $t_8 = \frac{16}{9375}$, and

$$\begin{align*}
t_4p &= \frac{5}{3} t_4p - 2 \frac{4}{5} t_4p-1; \\
t_4p+1 &= \frac{8}{3} t_4p - \frac{4}{25} t_4p-1; \\
t_4p+2 &= \frac{4}{5} t_4p+1 - \frac{4}{25} t_4p; \\
t_4p+3 &= t_4p+2 - \frac{1}{5} t_4p+1.
\end{align*}$$
Therefore, the transformation form of the above formula is obtained.

\[
\begin{align*}
    t_{4p-4} &= \frac{5}{3} \cdot \left(\frac{4}{125}\right)^p, \quad 1 \leq p \leq n; \\
    t_{4p-3} &= \frac{2}{3} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n - 1; \\
    t_{4p-2} &= \frac{4}{15} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n - 1; \\
    t_{4p-1} &= \frac{2}{15} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n - 1.
\end{align*}
\]

Since the \((-1)^{3n+1}b_{3n+1}\) is the total of all the principal minors of order \(3n + 1\) of \(L_A\), we have

\[
(-1)^{4n-1}b_{4n-1} = \sum_{i=2}^{4n} \det NL_A[i] + s_{4n} + t_{4n} \\
= \sum_{q=1}^{n} \det NL_A[4q] + \sum_{q=1}^{n-1} \det NL_A[4q + 1] + \sum_{q=0}^{n-1} \det NL_A[4q + 2] \\
= \sum_{q=0}^{n-1} \det NL_A[4q + 3] + s_{4n} + t_{4n} + \sum_{q=1}^{n} s_{4(q-1)+3}t_{4(n-q)+1} \\
= \sum_{q=1}^{n-1} s_{4q}t_{4(n-q)} + \sum_{q=0}^{n-1} s_{4q+1}t_{4(n-q+1)+3} + \sum_{q=0}^{n-1} s_{4q+2}t_{4(n-q+1)+2} + s_{4n} + t_{4n} \\
= \frac{1}{45}(38n - 8)\left(\frac{4}{125}\right)^n.
\]

The proof of Theorem 4.1 completed.

**Theorem 4.2.** \((-1)^{4n-2}b_{4n-2} = \frac{1}{3240}(14520n^3 + 4599n^2 - 1496n + 3)\left(\frac{4}{125}\right)^n\).

**Proof.** We observe that the sum of all the principal minors of order \(4n\) of \(L_A\) is the \((-1)^{4n-2}b_{4n-2}\), then

\[
(-1)^{4n-2}b_{4n-2} = \sum_{1 \leq s < t \leq 4n} \det L_A[s, t] \cdot f_{s-1} \cdot f'_{4n-t}. \quad (4.8)
\]

By Eq.(4.8), we know that the result of \(\det L_A[s, t]\) will change with the values of \(s\) and \(t\). Then we can get the following twenty cases.

**Case 1.** \(i = 4s, j = 4t, \quad 1 \leq s < t \leq n,\)

\[
\begin{vmatrix}
    \frac{4}{5} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
    -\frac{2}{\sqrt{5}} & 1 & -\frac{1}{5} & -\frac{1}{\sqrt{5}} \\
    -\frac{2}{\sqrt{5}} & -\frac{4}{5} & 1 & -\frac{1}{\sqrt{5}} \\
    -\frac{2}{\sqrt{5}} & -\frac{4}{5} & -\frac{1}{5} & 1 \\
    -\frac{2}{\sqrt{5}} & -\frac{4}{5} & -\frac{1}{5} & 1 \\
    -\frac{2}{\sqrt{5}} & -\frac{4}{5} & -\frac{1}{5} & 1 \\
\end{vmatrix}
\]

\[
\det \psi = 10(t-s)\left(\frac{4}{125}\right)^{t-s} \quad (4t-4s-1).
\]
Case 2.  \( i = 4s, j = 4t + 1, 1 \leq s \leq t \leq n - 1, \)

\[
\begin{vmatrix}
\frac{4}{5} & -\frac{1}{\sqrt{5}} & 0 & \cdots \\
-\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & 1 & \cdots \\
\cdots & \cdots & \cdots & \ddots
\end{vmatrix}
\]

\[
det\psi = \frac{4}{5} (4t - 4s + 1) \left( \frac{4}{125} \right)^{t-s}.
\]

Case 3.  \( i = 4s, j = 4t + 2, 1 \leq s \leq t \leq n - 1, \)

\[
\begin{vmatrix}
\frac{4}{5} & -\frac{1}{\sqrt{5}} & 0 & \cdots \\
-\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & 1 & \cdots \\
\cdots & \cdots & \cdots & \ddots
\end{vmatrix}
\]

\[
det\psi = \frac{4}{5} (2(t - s) + 1) \left( \frac{4}{125} \right)^{t-s}.
\]

Case 4.  \( i = 4s, j = 4t + 3, 1 \leq s \leq t \leq n - 1, \)

\[
\begin{vmatrix}
\frac{4}{5} & -\frac{1}{\sqrt{5}} & 0 & \cdots \\
-\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & 1 & \cdots \\
\cdots & \cdots & \cdots & \ddots
\end{vmatrix}
\]

\[
det\psi = \frac{1}{5} (4(t - s) + 3) \left( \frac{4}{125} \right)^{t-s}.
\]
Case 5. \( i \equiv 0, \ j = 4n, \ 1 \leq s \leq t, \)

\[
\begin{vmatrix}
\frac{4}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{5} \\
-\frac{2}{\sqrt{5}} & \frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{5} & -\frac{2}{5}
\end{vmatrix}
= 10(n - s) \left( \frac{4}{125} \right)^{n-s}.
\]

Case 6. \( i = 4s + 1, \ j = 4t, \ 0 \leq s < t \leq n, \)

\[
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{2}{\sqrt{5}} & \frac{4}{5} & \frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{2}{5} & -\frac{1}{5}
\end{vmatrix}
= \frac{25}{4} (4t - 4s - 1) \left( \frac{4}{125} \right)^{t-s}.
\]

Case 7. \( i = 4s + 1, \ j = 4t + 1, \ 0 \leq s < t \leq n - 1, \)

\[
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{5} \\
-\frac{2}{\sqrt{5}} & \frac{4}{5} & \frac{2}{5} \\
-\frac{1}{\sqrt{5}} & -\frac{2}{5} & -\frac{1}{5}
\end{vmatrix}
= 10(t - s) \left( \frac{4}{125} \right)^{t-s}.
\]
Case 8. $i = 4s + 1$, $j = 4t + 2$, $0 \leq s < t \leq n - 1$,

$$
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} & -\frac{5}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{5}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} \\
\end{vmatrix}
$$

$$
\det \psi = \left(4t - 4s + 1\right) \left(\frac{4}{125}\right)^{t-s}.
$$

Case 9. $i = 4s + 1$, $j = 4t + 3$, $0 \leq s \leq t \leq n - 1$,

$$
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} & -\frac{5}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{5}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} \\
\end{vmatrix}
$$

$$
\det \psi = \left(2t - 2s + 1\right) \left(\frac{4}{125}\right)^{t-s}.
$$

Case 10. $i \equiv 1$, $j = 4n + 1$, $0 \leq s \leq n$,

$$
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} & -\frac{5}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{5}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} \\
\end{vmatrix}
$$

$$
\det \psi = \frac{25}{4} \left(4n - 4s - 1\right) \left(\frac{4}{125}\right)^{n-s}.
$$

Case 11. $i = 4s + 2$, $j = 4t$, $0 \leq s < t \leq n$,

$$
\begin{vmatrix}
1 & -\frac{1}{\sqrt{5}} & -\frac{2}{\sqrt{5}} & -\frac{5}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\
-\frac{5}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{2}{\sqrt{5}} & \frac{4}{\sqrt{5}} \\
\end{vmatrix}
$$

$$
\det \psi = 25(2t - 2s - 1) \left(\frac{4}{125}\right)^{t-s}.
$$
Case 12. $i = 4s + 2$, $j = 4t + 1$, $0 \leq s < t \leq n - 1,$

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{2}{5} & -\frac{2}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
\end{vmatrix}
\]

\[= 5(4t - 4s - 1) \left( \frac{4}{125} \right)^{t-s} .\]

Case 13. $i = 4s + 2$, $j = 4t + 2$, $0 \leq s < t \leq n - 1,$

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{2}{5} & -\frac{2}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
\end{vmatrix}
\]

\[= 8(t - s) \left( \frac{4}{125} \right)^{t-s} .\]

Case 14. $i = 4s + 2$, $j = 4t + 3$, $0 \leq s \leq t \leq n - 1,$

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{2}{5} & -\frac{1}{\sqrt{5}} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{1}{\sqrt{5}} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
\end{vmatrix}
\]

\[= (4t - 4s + 1) \left( \frac{4}{125} \right)^{t-s} .\]

Case 15. $i \equiv 2$, $j = 4n + 2$, $0 \leq s \leq n - 1,$

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{2}{5} & -\frac{2}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
-\frac{2}{5} & \frac{4}{5} & \frac{4}{5} & \frac{4}{5} \\
\end{vmatrix}
\]

\[= 25(2n - 2s - 1) \left( \frac{4}{125} \right)^{n-s} .\]
Case 16. \( i = 4s + 3, j = 4t, 0 \leq s < t \leq n, \)

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{1}{\sqrt{5}} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & \ldots \\
-\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \ldots \\
\end{vmatrix}
\]

\[
= \frac{125}{4} (4t - 4s - 3) \left( \frac{4}{125} \right)^{t-s}.
\]

Case 17. \( i = 4s + 3, j = 4t + 1, 0 \leq s < t \leq n - 1, \)

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{1}{\sqrt{5}} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & \ldots \\
-\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \ldots \\
\end{vmatrix}
\]

\[
= 25(2t - 2s - 1) \left( \frac{4}{125} \right)^{t-s}.
\]

Case 18. \( i = 4s + 3, j = 4t + 2, 0 \leq s < t \leq n - 1, \)

\[
\det \psi = \begin{vmatrix}
\frac{4}{5} & -\frac{2}{5} & -\frac{1}{\sqrt{5}} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & \ldots \\
-\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \ldots \\
\end{vmatrix}
\]

\[
= \frac{25}{3} (4t - 4s - 1) \left( \frac{4}{125} \right)^{t-s}.
\]
Case 19. \( i = 4s + 3, j = 4t + 3, 0 \leq s < t \leq n - 1, \)

\[
\begin{vmatrix}
\frac{4}{5} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
\vdots & \vdots & \vdots & \vdots \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{4}{5} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
\end{vmatrix}
\]

\[= 10(l - k) \left( \frac{4}{125} \right)^{t-s}. \]

Case 20. \( i \equiv 3, j = 4t, 0 \leq s \leq n - 1, \)

\[
\begin{vmatrix}
\frac{4}{5} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
\vdots & \vdots & \vdots & \vdots \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{4}{5} & \frac{2}{5} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \\
\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
-\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & -\frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \\
\end{vmatrix}
\]

\[= \frac{125}{4} (4n - 4s - 3) \left( \frac{4}{125} \right)^{n-s} . \]

Therefore, we can get

\[-1)^{n-2}b_{4n-2} = \sum_{1 \leq p < q \leq 4n} detN_{\mathcal{L}_A}[i, j] \cdot s_{i-1} \cdot t_{4n-j} \]

\[= E_1 + E_2 + E_3 + E_4, \]

where

\[E_1 = \sum_{1 \leq s < t \leq n} detN_{\mathcal{L}_A}[4s, 4t] + \sum_{1 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s, 4t + 1] + \sum_{1 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s, 4t + 2] + \sum_{1 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s, 4t + 3] + \sum_{1 \leq s \leq n} detN_{\mathcal{L}_A}[4s, 4n]
\]

\[= \frac{1}{18} (227n^3 + 347n^2 - 574n + 4) \left( \frac{4}{125} \right)^{n-1}. \]

\[E_2 = \sum_{0 \leq s < t \leq n} detN_{\mathcal{L}_A}[4s + 1, 4t] + \sum_{0 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s + 1, 4t + 1] + \sum_{0 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s + 1, 4t + 2] + \sum_{0 \leq s \leq t \leq n-1} detN_{\mathcal{L}_A}[4s + 1, 4t + 3] + \sum_{0 \leq s \leq n} detN_{\mathcal{L}_A}[4s + 1, 4n]
\]

\[= \frac{1}{72} (908n^3 + 3431n^2 + 523n) \left( \frac{4}{125} \right)^{n}. \]
\[ E_3 = \sum_{0 \leq s < t \leq n} \det \mathcal{N} \mathcal{L}_A[4s + 2, 4t] + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 2, 4t + 1] \]
\[ + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 2, 4t + 2] + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 2, 4t + 3] \]
\[ + \sum_{0 \leq s \leq n} \det \mathcal{N} \mathcal{L}_A[4s + 2, 4n] \]
\[ = \frac{1}{45} (454n^3 + 1375n^2 - 1079n) \left( \frac{4}{125} \right)^n. \]

\[ E_4 = \sum_{0 \leq s < t \leq n} \det \mathcal{N} \mathcal{L}_A[4s + 3, 4t] + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 3, 4t + 1] \]
\[ + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 3, 4t + 2] + \sum_{0 \leq s < t \leq n-1} \det \mathcal{N} \mathcal{L}_A[4s + 3, 4t + 3] \]
\[ + \sum_{0 \leq s \leq n} \det \mathcal{N} \mathcal{L}_A[4s + 3, 4n] \]
\[ = \frac{1}{81} (92n^3 + 561n^2 - 611n) \left( \frac{4}{125} \right)^{n-1}. \]

Hence
\[ (-1)^{4n-2}b_{4n-2} = E_1 + E_2 + E_3 + E_4 = \frac{1}{3240} (14520n^3 + 4599n^2 - 1496n + 4) \left( \frac{4}{125} \right)^n. \]

The proof of Theorem 4.2 completed.

Let \(0 = \xi_1 < \xi_2 \leq \xi_3 \leq \cdots \leq \xi_{3n+2}\) are the eigenvalues of \(\mathcal{L}_A\), we can get the following exact equation
\[ \sum_{i=2}^{4n} \frac{1}{\xi_i} = \frac{(-1)^{4n-2}b_{4n-2}}{(-1)^{4n-1}b_{4n-1}} = \frac{1}{72} \left( \frac{14520n^3 + 4599n^2 - 1496n + 8}{38n - 8} \right). \]

**Theorem 4.3.** Set \(L_n^{6,4,4}\) be the derivative \([n]\)pheylenes, and the expression of the multiplicative degree-Kirchhoff index is
\[ K_f^*(L_n) = \frac{29040n^3 + 8996n^2 - 3198n + 8}{144}. \]

**Proof.** Together with Eq.(4.7), Theorems 4.1 and 4.2, one can get
\[ K_f^*(L_n) = 2(19n - 4) \left( \sum_{i=2}^{4n} \frac{1}{\xi_i} + \sum_{i=1}^{4n} \frac{1}{\gamma_i} \right) \]
\[ = 2(19n - 4) \left[ \frac{1}{72} \left( \frac{14520n^3 + 4599n^2 - 1496n + 8}{38n - 8} \right) + \frac{21n - 1}{6} \right] \]
\[ = \frac{29040n^3 + 8996n^2 - 3198n + 8}{144}. \]

The result as desired.

The multiplicative degree-Kirchhoff indices of \(L_n\) from \(L_1\) to \(L_{15}\), see Table 2.

Then we want to calculate the Gutman index of \(L_n\).
Consider $L_n$ be obtained from the transformation of the graph $L_n$ into the following four categories.

\textbf{Case 1.} Vertex $4i - 2 (i = 1, 2, \ldots, n)$ of $L_n$:

\[
\begin{align*}
f_{4i-2} &= 2 \sum_{i=1}^{n} \left[ 4 \times 4 \times 2 + 2 \times 3 \times 4 \times (4i - 3) + 2 \times 3 \times 4 \times (4n - 4i + 2) + 2 \sum_{t=1}^{i-1} 4 \times 4 \times 4 \times (i-t) \\
&+ 2 \sum_{t=i+1}^{n} 4 \times 4 \times 4 \times (t-i) + 2 \sum_{t=2}^{i} 4 \times 5 \times (4i - 4t + 1) + 2 \sum_{t=i+1}^{n} 4 \times 5 \times (4t - 4i - 1) \\
&+ 2 \sum_{t=2}^{i} 4 \times 5 \times (4i - 4t + 2) + 2 \sum_{t=i+1}^{n} 4 \times 5 \times (4t - 4i - 2) + 2 \sum_{t=1}^{i-1} 4 \times 5 \times (4i - 4t - 1) \\
&+ 2 \sum_{t=i+1}^{n} 4 \times 5 \times (4t - 4i + 1) \right] \\
&= \frac{10}{3} n(56n^2 - 24n + 37).
\end{align*}
\]

\textbf{Case 2.} Vertex $4i - 1 (i = 2, 3, \ldots, n)$ of $L_n$:

\[
\begin{align*}
f_{4i-1} &= 2 \sum_{i=1}^{n} \left[ 5 \times 5 \times 1 + 2 \times 3 \times 5 \times (4i - 1) + 2 \times 3 \times 5 \times (4n - 4i + 1) + 2 \sum_{t=1}^{i} 5 \times 4 \times (4i - 4t + 1) \\
&+ 2 \sum_{t=i+1}^{n} 5 \times 4 \times (4t - 4i - 1) + 2 \sum_{t=2}^{i} 5 \times 5 \times (4i - 4t + 3) + 2 \sum_{t=i+1}^{n} 5 \times 5 \times (4t - 4i - 3) \\
&+ 2 \sum_{t=2}^{i} 5 \times 5 \times (4i - 4t + 2) + 2 \sum_{t=i+1}^{n} 5 \times 5 \times (4t - 4i - 2) + 2 \sum_{t=1}^{i-1} 5 \times 5 \times 4 \times (i-t) \\
&+ 2 \sum_{t=i+1}^{n} 5 \times 5 \times 4 \times (t-i) \right] \\
&= \frac{10}{3} n(152n^2 - 48n - 29).
\end{align*}
\]

\textbf{Theorem 4.4.} Suppose that $L_5^{4,4,4}$ be the dicyclobutadieno derivative of $[n]$phenylenes and the graph $L_n$ be obtained from the transformation of the graph $L_n^{6,4,4}$, then

\[
\lim_{n \to \infty} \frac{Kf^*(L_n)}{Gut(L_n)} = \frac{1}{4}.
\]

\textbf{Proof.} Consider $d_{ij}$ for all vertices, we divide the vertices of $L_n$ into the following four categories.
Case 3. Vertex $4i(i = 2, 3, \cdots, n)$ of $L_n$:

\[
\begin{align*}
\sum_{i=1}^{n} f_{4i} &= 2 \sum_{i=2}^{n} \left[ 5 \times 5 \times 1 + 2 \times 3 \times 5 \times (4i - 1) + 2 \times 3 \times 5 \times (4n - 4i + 1) + 2 \sum_{t=1}^{i} 5 \times 4 \times (4i - 4t + 2) \\
&\quad + 2 \sum_{t=1}^{n} 5 \times 4 \times (4t - 4i - 2) + 2 \sum_{t=2}^{i} 5 \times 5 \times (4i - 4t + 5) + 2 \sum_{t=i+1}^{n} 5 \times 5 \times (4t - 4i - 3) \\
&\quad + 2 \sum_{t=2}^{i} 5 \times 5 \times (4i - 4t + 1) + 2 \sum_{t=1}^{n} 5 \times 5 \times (4t - 4i - 3) + 2 \sum_{t=i+1}^{n} 5 \times 5 \times 4 \times (i - t) \\
&\quad + 2 \sum_{t=i+1}^{n} 5 \times 5 \times 4 \times (t - i) \\
&= \frac{10}{3} n (140n^2 - 48n + 43).
\end{align*}
\]

Case 4. Vertex $4i - 3(i = 2, 3, \cdots, n)$ of $L_n$:

\[
\begin{align*}
\sum_{i=2}^{n} f_{4i-3} &= 2 \sum_{i=2}^{n} \left[ 5 \times 5 \times 1 + 2 \times 3 \times 5 \times (4i - 4) + 2 \times 3 \times 5 \times (4n - 4i + 4) + 2 \sum_{t=1}^{i-1} 5 \times 4 \times (4i - 4t - 1) \\
&\quad + 2 \sum_{t=1}^{n} 5 \times 4 \times (4t - 4i + 1) + 2 \sum_{t=2}^{i-1} 5 \times 5 \times (4i - 4t) + 2 \sum_{t=i+1}^{n} 5 \times 5 \times (4t - 4i) \\
&\quad + 2 \sum_{t=1}^{i-1} 5 \times 5 \times (4i - 4t - 2) + 2 \sum_{t=1}^{n} 5 \times 5 \times (4t - 4i + 2) + 2 \sum_{t=1}^{i-1} 5 \times 5 \times (4i - 4t + 1) \\
&\quad + 2 \sum_{t=1}^{n} 5 \times 5 \times (4t - 4i + 1) \\
&= \frac{10}{3} n (136n^2 - 6n + 71).
\end{align*}
\]

According to Eq.(1.3), the Gutman index of $L_n$ is

\[
Gut(L_n) = \frac{f_{4i} + f_{4i-1} + f_{4i-2} + f_{4i-3}}{2} = \frac{10}{3} n (242n^2 - 63n + 61).
\]

Therefore, combining with $Kf^*(L_n)$ and $Gut(L_n)$, we have

\[
\lim_{n \to \infty} \frac{Kf^*(L_n)}{Gut(L_n)} = \frac{1}{4}
\]

The result as desired.

Finally, we want to get the complexity of $L_n$.

**Theorem 4.5.** For the graph $L_n$, we have

\[
\tau(L_n) = 2^{3n^2} \cdot 3^{3n-2}
\]

**Proof.** Based on Lemma 2.4, we can get

\[
\prod_{i=1}^{8n} d_i \prod_{i=2}^{4n} \alpha_i \prod_{j=1}^{4n} \beta_j = 2(19n - 4) \cdot \tau(L_n)
\]

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Note that
\[
\prod_{i=1}^{8n} d_i = 3^4 \cdot 4^{2n} \cdot 5^{6n-4}
\]
\[
\prod_{i=2}^{4n} \alpha_i = \frac{25}{9} \cdot (38n - 8) \cdot \left(\frac{4}{125}\right)^n
\]
\[
\prod_{j=1}^{4n} \beta_j = \left(\frac{4}{3}\right)^2 \cdot \left(\frac{6}{5}\right)^{3n-2}
\]
Hence,
\[
\tau(L_n) = 2^{3n+2} \cdot 3^{3n-2}
\]
The proof is over.
Thus we can get the complexity of $L_n$ from $W_1$ to $W_{10}$ which are listed in Table 3.

Table 3: The complexity of $W_1, W_2...W_{10}$.

<table>
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<tr>
<th>$\mathcal{G}$</th>
<th>$\tau(\mathcal{G})$</th>
<th>$\mathcal{G}$</th>
<th>$\tau(\mathcal{G})$</th>
</tr>
</thead>
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<td>$W_6$</td>
<td>451377585192996</td>
</tr>
<tr>
<td>$W_2$</td>
<td>20736</td>
<td>$W_7$</td>
<td>974975580167936</td>
</tr>
<tr>
<td>$W_3$</td>
<td>4478976</td>
<td>$W_8$</td>
<td>2105947261476274176</td>
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<td>$W_4$</td>
<td>967458816</td>
<td>$W_9$</td>
<td>45488460847887522016</td>
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<tr>
<td>$W_5$</td>
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<td>$W_{10}$</td>
<td>98255075431437047955456</td>
</tr>
</tbody>
</table>

5. Conclusion

In this paper, the linear chain network with $n$ hexagons and $2n - 1$ squares is considered. We have devoted to calculate the (multiplicative degree) Kirchhoff index, Wiener index Gutman index and complexity. In the meantime, we deduced that the ratio of (multiplicative degree) Kirchhoff index of to (Gutman) Wiener index is nearly a quarter when $n$ tends to infinity. Furthermore, we got some important rules of $L_n^{6,4,4}$. These rules also apply to some other graphs.

References


[40] Y.G. Pan, C. Liu, J.P. Li, Kirchhoff indices and numbers of spanning trees of molecular graphs derived from linear crossed polyomino chain, Polycyclic Aromatic Compounds 42.1 (2021): 218-225