

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 $L_n^{6,4,4}$, 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 fomulas 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 $V(\mathcal{G}) = \{v_1, v_2, \dots, v_n\}$ and the edge set $E(\mathcal{G}) = \{e_1, e_2, \dots, e_m\}$. The adjacency matrix $A(\mathcal{G})$ is a $0-1$ $n \times n$ 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 $0 = \mu_1 < \mu_2 \leq \dots \leq \mu_n$.

$$(L(\mathcal{G}))_{st} = \begin{cases} d_s, & s = t; \\ -1, & s \neq t \text{ and } v_s \sim v_t; \\ 0, & \text{otherwise.} \end{cases} \quad (1.1)$$

The normalized Laplacian matrix is given by

$$(\mathcal{L}(\mathcal{G}))_{st} = \begin{cases} 1, & s = t; \\ -\frac{1}{\sqrt{d_s d_t}}, & s \neq t \text{ and } v_s \sim v_t; \\ 0, & \text{otherwise.} \end{cases} \quad (1.2)$$

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 \mathcal{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 \mathcal{G} is expressed by

$$Gut(\mathcal{G}) = \sum_{s < t} d_s d_t d_{st}. \quad (1.3)$$

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 \mathcal{G} is expressed as the sum of the resistance distances between each two vertices, that is

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

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

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

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 nomalized Laplacian matrix, then we make sure the Kirchhoff index, the multiplicative degree-Kirchhoff index and the complexity of L_n . In Section 5, we obtained conciusions 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 $\pi = (1, \tilde{1})(2, \tilde{2}) \cdots (4n, \tilde{4n})$ is an automorphism. Set $V_1 = \{1, 2, \dots, 4n\}$, $V_2 = \{\tilde{1}, \tilde{2}, \dots, \tilde{4n}\}$, $|V(L_n)| = 8n$, $|E(L_n)| = 19n - 4$. Thus the (normalized) Laplacians matrix can be

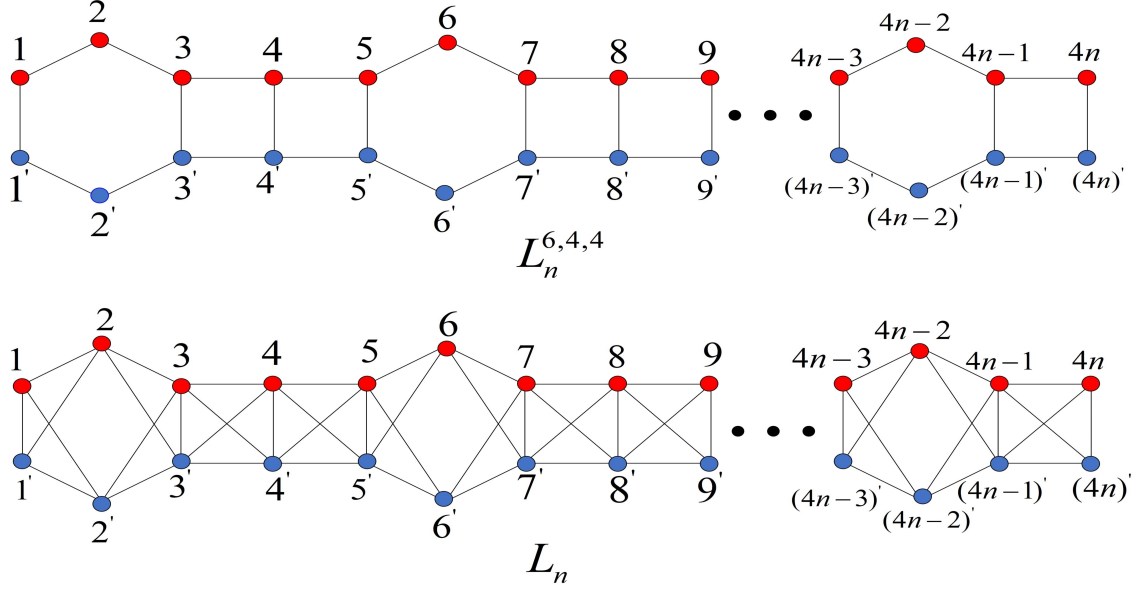


Figure 1: Graphs of $L_n^{6,4,4}$ and L_n .

expressed in the form of block matrix, that is

$$L(L_n) = \begin{pmatrix} L_{V_0V_0} & L_{V_0V_1} & L_{V_0V_2} \\ L_{V_1V_0} & L_{V_1V_1} & L_{V_1V_2} \\ L_{V_2V_0} & L_{V_2V_1} & L_{V_2V_2} \end{pmatrix}, \quad \mathcal{L}(L_n) = \begin{pmatrix} \mathcal{L}_{V_0V_0} & \mathcal{L}_{V_0V_1} & \mathcal{L}_{V_0V_2} \\ \mathcal{L}_{V_1V_0} & \mathcal{L}_{V_1V_1} & \mathcal{L}_{V_1V_2} \\ \mathcal{L}_{V_2V_0} & \mathcal{L}_{V_2V_1} & \mathcal{L}_{V_2V_2} \end{pmatrix},$$

where $L_{V_sV_t}$ and $\mathcal{L}_{V_sV_t}$ 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

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

then

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

and Q' is the transposition of Q .

$$L_A = L_{V_1V_1} + L_{V_1V_2}, \quad L_S = L_{V_1V_1} - L_{V_1V_2}, \quad \mathcal{L}_A = \mathcal{L}_{V_1V_1} + \mathcal{L}_{V_1V_2}, \quad \mathcal{L}_S = \mathcal{L}_{V_1V_1} - \mathcal{L}_{V_1V_2}.$$

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

$$\vartheta_{L(L_n)}(y) = \theta_{L_A(\mathcal{G})}(y)\theta_{L_S(\mathcal{G})}(y), \quad \vartheta_{\mathcal{L}(L_n)}(y) = \theta_{\mathcal{L}_A(\mathcal{G})}(y)\theta_{\mathcal{L}_S(\mathcal{G})}(y).$$

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

$$Kf(\mathcal{G}) = n \sum_{t=2}^n \frac{1}{\xi_t},$$

and the eigenvalues of $L(\mathcal{G})$ are $0 = \xi_1 < \xi_2 \leq \dots \leq \xi_n (n \geq 2)$.

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

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

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

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

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.

$$L_{V_1 V_1} = \begin{pmatrix} 3 & -1 & & & & & & & & & \\ -1 & 4 & -1 & & & & & & & & \\ & -1 & 5 & -1 & & & & & & & \\ & & -1 & 5 & -1 & & & & & & \\ & & & -1 & 5 & -1 & & & & & \\ & & & & -1 & 4 & -1 & & & & \\ & & & & & \ddots & & & & & \\ & & & & & -1 & 5 & -1 & & & \\ & & & & & & -1 & 4 & -1 & & \\ & & & & & & & -1 & 5 & -1 & \\ & & & & & & & & -1 & 3 & \end{pmatrix}_{(4n) \times (4n)},$$

$$L_{V_1 V_2} = \begin{pmatrix} -1 & -1 & & & & & & & & & \\ -1 & 0 & -1 & & & & & & & & \\ & -1 & -1 & -1 & & & & & & & \\ & & -1 & -1 & -1 & & & & & & \\ & & & -1 & -1 & -1 & & & & & \\ & & & & -1 & 0 & -1 & & & & \\ & & & & & \ddots & & & & & \\ & & & & & -1 & -1 & -1 & & & \\ & & & & & & -1 & 0 & -1 & & \\ & & & & & & & -1 & -1 & -1 & \\ & & & & & & & & -1 & -1 & \end{pmatrix}_{(4n) \times (4n)}.$$

Hence,

$$L_A = \begin{pmatrix} 2 & -2 & & & & & & & \\ -2 & 4 & -2 & & & & & & \\ & -2 & 4 & -2 & & & & & \\ & & -2 & 4 & -2 & & & & \\ & & & -2 & 4 & -2 & & & \\ & & & & -2 & 4 & -2 & & \\ & & & & & -2 & 4 & -2 & \\ & & & & & & \ddots & & \\ & & & & & & -2 & 4 & -2 \\ & & & & & & & -2 & 4 & -2 \\ & & & & & & & & -2 & 4 & -2 \\ & & & & & & & & & -2 & 2 \end{pmatrix}_{(4n) \times (4n)},$$

and

$$L_S = \text{diag}(4, 4, 6, 6, 6, 6, 4, \dots, 6, 4, 6, 4)_{(4n)}.$$

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

$$Kf(L_n) = 2(4n) \left(\sum_{i=2}^{4n} \frac{1}{\alpha_i} + \sum_{j=1}^{4n} \frac{1}{\beta_j} \right). \quad (3.4)$$

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

$$\sum_{j=1}^{4n} \frac{1}{\beta_j} = \frac{1}{6} \times (3n - 2) + \frac{1}{4} \times (n + 2) = \frac{9n + 2}{12}. \quad (3.5)$$

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

$$P_{L_A}(x) = \det(xI - L_A) = x(x^{4n-1} + a_1x^{4n-2} + \dots + a_{4n-2}x + a_{4n-1}), \quad a_{4n-1} \neq 0.$$

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

$$m_s = 4m_{s-1} - 4m_{s-2}, \quad 4 \leq s \leq 4n,$$

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

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

where

$$\begin{aligned} M_{s-1} &= \begin{pmatrix} l_{11} & -2 & \cdots & 0 \\ -2 & l_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{s-1,s-1} \end{pmatrix}_{(s-1) \times (s-1)}, \\ U_{4n-s} &= \begin{pmatrix} l_{s+1,s+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{4n-1,4n-1} & -2 \\ 0 & \cdots & -2 & l_{4n,4n} \end{pmatrix}_{(4n-s) \times (4n-s)}. \end{aligned}$$

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

$$\begin{aligned} (-1)^{4n-1}a_{4n-1} &= \sum_{s=1}^{4n} \det m_{s-1} \cdot \det m_{4n-s} \\ &= (4n)2^{4n-1}, \end{aligned}$$

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

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

and

$$\begin{aligned} N_{t-s-1} &= \begin{vmatrix} 4 & -2 & & & \\ -2 & 4 & -2 & & \\ & -2 & 4 & -2 & \\ & & & \ddots & \\ & & & -2 & 4 & -2 \\ & & & & -2 & 4 & -2 \\ & & & & & -2 & 4 \end{vmatrix}_{(t-s-1)} \\ &= (t-s)2^{t-s-1}. \end{aligned}$$

Therefore, we can have

$$\begin{aligned}
(-1)^{4n-2}a_{4n-2} &= \sum_{1 \leq s < t \leq 4n} \det M_{s-1} \cdot \det N_{t-s-1} \cdot \det U_{4n-t} \\
&= \sum_{1 \leq s < t \leq 4n} (t-s)2^{t-s-1} \cdot \det m_{s-1} \cdot m_{4n-t} \\
&= \frac{(4n-1)(4n)(4n+1)2^{4n-3}}{3}.
\end{aligned}$$

The proof is over. ■

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

$$\sum_{i=2}^{4n} \frac{1}{\alpha_i} = \frac{(-1)^{4n-2}a_{4n-2}}{(-1)^{4n-1}a_{4n-1}} = \frac{16n^2 - 1}{12}, \quad (3.6)$$

where the eigenvalues of L_A are $0 = \alpha_1 < \alpha_2 \leq \alpha_3 \leq \dots \leq \alpha_{4n}$.

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

$$\begin{aligned}
Kf(L_n) &= 2(4n) \left(\sum_{i=2}^{4n} \frac{1}{\alpha_i} + \sum_{j=1}^{4n} \frac{1}{\beta_j} \right) \\
&= (8n) \left(\frac{9n+2}{12} + \frac{(4n+1)(4n-1)}{12} \right) \\
&= \frac{32n^3 + 18n^2 + 2n}{3}.
\end{aligned}$$

The result as desired ■

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

Table 1: The Kirchhoff indices of $L_1, L_2 \dots L_{15}$

\mathcal{G}	$Kf(\mathcal{G})$	\mathcal{G}	$Kf(\mathcal{G})$	\mathcal{G}	$Kf(\mathcal{G})$	\mathcal{G}	$Kf(\mathcal{G})$	\mathcal{G}	$Kf(\mathcal{G})$
L_1	17.3	L_4	781.3	L_7	3957.3	L_{10}	11273.3	L_{13}	24457.3
L_2	110.7	L_5	1486.7	L_8	5850.7	L_{11}	14930.7	L_{14}	30454.7
L_3	344.0	L_6	2524.0	L_9	8268.0	L_{12}	19304.0	L_{15}	37360.0

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

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

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 $4j - 3$ ($j = 1, 2, \dots, n$) 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 $4j - 2$ ($j = 1, 2, \dots, n$) 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 $4j - 1$ ($j = 1, 2, \dots, n - 1$) 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 $4j$ ($j = 1, 2, \dots, n - 1$) 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

$$\begin{aligned} W(L_n) &= \frac{4g_1(i) + 2 \sum_{i=4j-3} g_2(i) + 2 \sum_{i=4j-2} g_3(i) + 2 \sum_{i=4j-1} g_4(i) + 2 \sum_{i=4j} g_5(i)}{2} \\ &= \frac{4(1 + 2 \sum_{k=1}^{4n-1} k) + 2 \sum_{j=1}^n \left[1 + 2(\sum_{k=1}^{4j-4} k + \sum_{k=1}^{4n-4j+2} k) \right]}{2} \\ &\quad + \frac{2 \sum_{j=1}^n \left[2 + 2(\sum_{k=1}^{4j-3} k + \sum_{k=1}^{4n-4j+2} k) \right] + 2 \sum_{j=1}^n \left[1 + 2(\sum_{k=1}^{4j-2} k + \sum_{k=1}^{4n-4j+1} k) \right]}{2} \\ &\quad + \frac{2 \sum_{j=1}^{n-1} \left[1 + 2(\sum_{k=1}^{4j-1} k + \sum_{k=1}^{4n-4j} k) \right]}{2} \\ &= \frac{128n^3 + 48n^2 - 5n + 3}{3}. \end{aligned}$$

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

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

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

[illegible]

and

$$\mathcal{L}_{V_1 V_2} = \begin{pmatrix} -\frac{1}{3} & \frac{1}{\sqrt{12}} & & & & & & & \\ \frac{-1}{\sqrt{12}} & 0 & \frac{-1}{\sqrt{20}} & & & & & & \\ & \frac{-1}{\sqrt{20}} & \frac{-1}{5} & \frac{-1}{5} & & & & & \\ & & \frac{-1}{5} & \frac{-1}{5} & \frac{-1}{\sqrt{20}} & & & & \\ & & & \frac{-1}{5} & 0 & \frac{-1}{\sqrt{20}} & & & \\ & & & & \ddots & \ddots & & & \\ & & & & \frac{-1}{5} & \frac{-1}{5} & \frac{-1}{\sqrt{20}} & & \\ & & & & \frac{-1}{\sqrt{20}} & 0 & \frac{-1}{\sqrt{20}} & & \\ & & & & & \frac{-1}{\sqrt{20}} & \frac{-1}{5} & \frac{-1}{\sqrt{15}} & \\ & & & & & & \frac{-1}{\sqrt{15}} & \frac{-1}{3} \end{pmatrix}. \quad (4n) \times (4n)$$

Therefore,

[illegible]

and

$$\mathcal{L}_S = diag\left(\frac{4}{3}, 1, \frac{6}{5}, \frac{6}{5}, \frac{6}{5}, \dots, \frac{6}{5}, 1, \frac{6}{5}, \frac{4}{3}\right)_{(4n)}.$$

Assume that the roots of $P_{\mathcal{L}_A}(x) = 0$ are $0 = \xi_1 < \xi_2 \leq \xi_3 \leq \dots \leq \xi_{3n+2}$, and $0 < \gamma_1 \leq \gamma_2 \leq \gamma_3 \leq \dots \leq \gamma_{3n+2}$ are the roots of $P_{\mathcal{L}_S}(x) = 0$. 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 \mathcal{L}_s is a diagonal matrix. Obviously, its diagonal elements $1, \frac{4}{3}$ and $\frac{6}{5}$ correspond to the eigenvalues of \mathcal{L}_s respectively. Then it can be clearly obtained

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

Let

$$P_{\mathcal{L}_A}(x) = \det(xI - \mathcal{L}_A) = x^{4n} + b_1 x^{4n-1} + \dots + b_{4n-1} x, \quad b_{4n-1} \neq 0,$$

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

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

Based on the Vieta's theorem of $P_{\mathcal{L}_A}(x)$, we can get

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

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

$$\begin{cases} s_{4p} = \frac{4}{5} s_{4p-1} - \frac{4}{25} s_{4p-2}; \\ s_{4p+1} = \frac{4}{5} s_{4p} - \frac{4}{25} s_{4p-1}; \\ s_{4p+2} = s_{4p+1} - \frac{1}{5} s_{4p}; \\ s_{4p+3} = \frac{4}{5} s_{4p+2} - \frac{1}{5} s_{4p+1}. \end{cases}$$

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

$$\begin{cases} s_{4p} = \frac{5}{3} \cdot \left(\frac{4}{125}\right)^p, \quad 1 \leq p \leq n; \\ s_{4p+1} = \frac{2}{3} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n-1; \\ s_{4p+2} = \frac{1}{3} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n-1; \\ s_{4p+3} = \frac{2}{15} \cdot \left(\frac{4}{125}\right)^p, \quad 0 \leq p \leq n-1. \end{cases}$$

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

$$\begin{cases} t_{4p} = \frac{2}{5} t_{4p-1} - \frac{2}{5} t_{4p-2}; \\ t_{4p+1} = \frac{4}{5} t_{4p} - \frac{4}{25} t_{4p-1}; \\ t_{4p+2} = \frac{4}{5} t_{4p+1} - \frac{4}{25} t_{4p}; \\ t_{4p+3} = t_{4p+2} - \frac{1}{5} t_{4p+1}. \end{cases}$$

Therefore, the transformation form of the above formula is obtained.

$$\begin{cases} t_{4p-4} = \frac{5}{3} \cdot (\frac{4}{125})^p, & 1 \leq p \leq n; \\ t_{4p-3} = \frac{2}{3} \cdot (\frac{4}{125})^p, & 0 \leq p \leq n-1; \\ t_{4p-2} = \frac{4}{15} \cdot (\frac{4}{125})^p, & 0 \leq p \leq n-1; \\ t_{4p-1} = \frac{2}{15} \cdot (\frac{4}{125})^p, & 0 \leq p \leq n-1. \end{cases}$$

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

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

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 \mathcal{L}_A is the $(-1)^{4n-2}b_{4n-2}$, then

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

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

Case 1. $i = 4s, j = 4t, 1 \leq s < t \leq n$,

$$\begin{aligned} \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{2}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & \\ & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{2}{\sqrt{5}} & \frac{4}{5} & \\ & & & & & & & -\frac{2}{\sqrt{5}} & \frac{4}{5} \end{vmatrix}_{(4t-4s-1)} \\ &= 10(t-s) \left(\frac{4}{125}\right)^{t-s}. \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & \end{vmatrix}_{(4t-4s)} \\
 &= [4(t-s) + 1] \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & \end{vmatrix}_{(4t-4s+1)} \\
 &= \frac{4}{5} [2(t-s) + 1] \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & \end{vmatrix}_{(4t-4s+2)} \\
 &= \frac{1}{5} [4(t-s) + 3] \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

Case 5. $i \equiv 0, j = 4n, 1 \leq s \leq t,$

$$\begin{aligned}
\det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & & \\ -\frac{2}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & & & \ddots & & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & \\ & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & & & -\frac{2}{\sqrt{5}} & \frac{4}{5} & & \end{vmatrix}_{(4n-4s-1)} \\
&= 10(n-s) \left(\frac{4}{125} \right)^{n-s}.
\end{aligned}$$

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

$$\begin{aligned}
\det \psi &= \begin{vmatrix} 1 & -\frac{1}{\sqrt{5}} & & & & & & & & \\ -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & & & \ddots & & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & \\ & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & & \end{vmatrix}_{(4t-4s-2)} \\
&= \frac{25}{4} (4t - 4s - 1) \left(\frac{4}{125} \right)^{t-s}.
\end{aligned}$$

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

$$\begin{aligned}
\det \psi &= \begin{vmatrix} 1 & -\frac{1}{\sqrt{5}} & & & & & & & & \\ -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & & & \ddots & & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & \\ & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & \\ & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & & \end{vmatrix}_{(4t-4s-1)} \\
&= 10(t-s) \left(\frac{4}{125} \right)^{t-s}.
\end{aligned}$$

Case 8. $i = 4s + 1$, $j = 4t + 2$, $0 \leq s < t \leq n - 1$,

$$\det \psi = \begin{vmatrix} 1 & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & \ddots & & & & \\ & & & -\frac{2}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & \\ & & & & & & & & -\frac{2}{5} \end{vmatrix}_{(4t-4s)} \\ = (4t-4s+1) \left(\frac{4}{125} \right)^{t-s}.$$

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

$$\begin{aligned} \det \psi &= \begin{vmatrix} 1 & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & \ddots & & & & \\ & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & \\ & & & & & & & & 1 \end{vmatrix}_{(4t-4s+1)} \\ &= (2t-2s+1) \left(\frac{4}{125} \right)^{t-s}. \end{aligned}$$

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

$$\begin{aligned} \det \psi &= \begin{vmatrix} 1 & -\frac{1}{\sqrt{5}} & & & & & & & \\ -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} \\ & & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} \end{vmatrix}_{(4n-4s-2)} \\ &= \frac{25}{4}(4n-4s-1)\left(\frac{4}{125}\right)^{n-s}. \end{aligned}$$

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

$$\begin{aligned} \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & & \ddots & \ddots & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} \\ & & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} \end{vmatrix}_{(4l-4s-3)} \\ &= 25(2t-2s-1) \left(\frac{4}{125} \right)^{t-s}. \end{aligned}$$

Case 12. $i = 4s + 2, j = 4t + 1, 0 \leq s < t \leq n - 1,$

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{\sqrt{5}} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} \end{vmatrix}_{(4t-4s-2)} \\
 &= 5(4t - 4s - 1) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{2}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} \end{vmatrix}_{(4t-4s-1)} \\
 &= 8(t - s) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & \\ & & & & & & & -\frac{1}{\sqrt{5}} & \end{vmatrix}_{(4t-4s)} \\
 &= (4t - 4s + 1) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & & \\ & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & \\ & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{1}{\sqrt{5}} \end{vmatrix}_{(4n-4s-3)} \\
 &= 25(2n - 2s - 1) \left(\frac{4}{125} \right)^{n-s}.
 \end{aligned}$$

Case 16. $i = 4s + 3$, $j = 4t$, $0 \leq s < t \leq n$,

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & \\ & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & & \\ & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} \end{vmatrix}_{(4t-4s-4)} \\
 &= \frac{125}{4}(4t-4s-3) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & \\ & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} \end{vmatrix}_{(4t-4s-3)} \\
 &= 25(2t-2s-1) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

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

$$\begin{aligned}
 \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & \\ & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & \\ & & & \ddots & & & & & \\ & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & \\ & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & -\frac{2}{5} & \frac{4}{5} & \\ & & & & & & & -\frac{2}{5} & \frac{4}{5} \end{vmatrix}_{(4t-4s-3)} \\
 &= \frac{25}{3}(4t-4s-1) \left(\frac{4}{125} \right)^{t-s}.
 \end{aligned}$$

Case 19. $i = 4s + 3, j = 4t + 3, 0 \leq s < t \leq n - 1,$

$$\begin{aligned} \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & & & \ddots & & & & & & \\ & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & \\ & & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & \\ & & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & \\ & & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & \\ & & & & & & & & \frac{4}{5} & -\frac{2}{5} \end{vmatrix}_{(4t-4s-1)} \\ &= 10(l-k) \left(\frac{4}{125} \right)^{t-s}. \end{aligned}$$

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

$$\begin{aligned} \det \psi &= \begin{vmatrix} \frac{4}{5} & -\frac{2}{5} & & & & & & & & \\ -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & & & & & \\ & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & & & & & \\ & & & \ddots & & & & & & \\ & & & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & & & & \\ & & & & -\frac{2}{5} & \frac{4}{5} & -\frac{1}{\sqrt{5}} & & & \\ & & & & & -\frac{1}{\sqrt{5}} & 1 & -\frac{1}{\sqrt{5}} & & \\ & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & -\frac{2}{5} & \\ & & & & & & & -\frac{1}{\sqrt{5}} & \frac{4}{5} & \end{vmatrix}_{(4n-4s-4)} \\ &= \frac{125}{4} (4n - 4s - 3) \left(\frac{4}{125} \right)^{n-s}. \end{aligned}$$

Therefore, we can get

$$\begin{aligned} (-1)^{4n-2} b_{4n-2} &= \sum_{1 \leq p < q \leq 4n} \det \mathcal{L}_A[i, j] \cdot s_{i-1} \cdot t_{4n-j} \\ &= E_1 + E_2 + E_3 + E_4, \end{aligned}$$

where

$$\begin{aligned} E_1 &= \sum_{1 \leq s < t \leq n} \det N \mathcal{L}_A[4s, 4t] + \sum_{1 \leq s \leq t \leq n-1} \det N \mathcal{L}_A[4s, 4t + 1] \\ &+ \sum_{1 \leq s \leq t \leq n-1} \det N \mathcal{L}_A[4s, 4t + 2] + \sum_{1 \leq s \leq t \leq n-1} \det N \mathcal{L}_A[4s, 4t + 3] \\ &+ \sum_{1 \leq s \leq n} \det N \mathcal{L}_A[4s, 4n] \\ &= \frac{1}{18} (227n^3 + 347n^2 - 574n + 4) \left(\frac{4}{125} \right)^{n-1}. \end{aligned}$$

$$\begin{aligned} E_2 &= \sum_{0 \leq s < t \leq n} \det N \mathcal{L}_A[4s + 1, 4t] + \sum_{0 \leq s < t \leq n-1} \det N \mathcal{L}_A[4s + 1, 4t + 1] \\ &+ \sum_{0 \leq s \leq t \leq n-1} \det N \mathcal{L}_A[4s + 1, 4t + 2] + \sum_{0 \leq s \leq t \leq n-1} \det N \mathcal{L}_A[4s + 1, 4t + 3] \\ &+ \sum_{0 \leq s \leq n} \det N \mathcal{L}_A[4s + 1, 4n] \\ &= \frac{1}{72} (908n^3 + 3431n^2 + 523n) \left(\frac{4}{125} \right)^n. \end{aligned}$$

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

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

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 $0 = \xi_1 < \xi_2 \leq \xi_3 \leq \dots \leq \xi_{3n+2}$ 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

$$Kf^*(L_n) = \frac{29040n^3 + 8996n^2 - 3198n + 8}{144}.$$

Proof. Together with Eq.(4.7), Theorems 4.1 and 4.2, one can get

$$\begin{aligned}
Kf^*(L_n) &= 2(19n - 4) \left(\sum_{i=2}^{4n} \frac{1}{\xi_i} + \sum_{i=1}^{4n} \frac{1}{\gamma_i} \right) \\
&= 2(19n - 4) \left[\frac{1}{72} \left(\frac{14520n^3 + 4599n^2 - 1496n + 8}{38n - 8} \right) + \frac{21n - 1}{6} \right] \\
&= \frac{29040n^3 + 8996n^2 - 3198n + 8}{144}.
\end{aligned}$$

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 .

Table 2: The multiplicative degree-Kirchhoff indices of $L_1, L_n \dots L_{15}$.

L_n	$Kf^*(L_n)$	L_n	$Kf^*(L_n)$	L_n	$Kf^*(L_n)$	L_n	$Kf^*(L_n)$	L_n	$Kf^*(L_n)$
L_1	241.98	L_4	13817.44	L_7	72077.4	L_{10}	207691.9	L_{13}	45333.08
L_2	1818.86	L_5	26659.15	L_8	107073.9	L_{11}	275733.2	L_{14}	565307
L_3	5940.68	L_6	45675.81	L_9	151875.4	L_{12}	357209.6	L_{15}	694348.2

Theorem 4.4. Suppose that $L_n^{6,4,4}$ 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

$$\lim_{n \rightarrow \infty} \frac{Kf^*(L_n)}{Gut(L_n)} = \frac{1}{4}.$$

Proof. Consider d_{ij} for all vertices, we divide the vertices of L_n into the following four categories.

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

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

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

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

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

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

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

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

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

$$\begin{aligned}
Gut(L_n) &= \frac{f_{4i} + f_{4i-1} + f_{4i-2} + f_{4i-3}}{2} \\
&= \frac{10}{3} n(242n^2 - 63n + 61).
\end{aligned}$$

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

$$\lim_{n \rightarrow \infty} \frac{Kf^*(L_n)}{Gut(L_n)} = \frac{1}{4}.$$

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

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

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 $W_1, W_2 \dots W_{10}$.

\mathcal{G}	$\tau(\mathcal{G})$	\mathcal{G}	$\tau(\mathcal{G})$
W_1	96	W_6	45137758519296
W_2	20736	W_7	9749755840167936
W_3	4478976	W_8	2105947261476274176
W_4	967458816	W_9	454884608478875222016
W_5	208971104256	W_{10}	98255075431437047955456

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.

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