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Kirchhoff Index and Degree Kirchhoff Index of Tetrahedrane-Derived Compounds

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Abstract: Tetrahedrane-derived compounds consist of n crossed quadrilaterals and possess complex three-dimensional structures with high symmetry and dense spatial arrangements. As a result, these compounds hold great potential for applications in materials science, catalytic chemistry, and other related fields. The Kirchhoff index of a graph G is defined as the sum of resistive distances between any two vertices in G. This article focuses on studying a type of tetrafunctional compound with a linear crossed square chain shape. The Kirchhoff index and degree Kirchhoff index of this compound are calculated, and a detailed analysis and discussion is conducted. The calculation formula for the Kirchhoff index is obtained based on the relationship between the Kirchhoff index and Laplace eigenvalue, and the number of spanning trees is derived for linear crossed quadrangular chains. The obtained formula is validated using Ohm's law and Cayley's theorem. Asymptotically, the ratio of Kirchhoff index to Wiener index approaches one-fourth. Additionally, the expression for the degree Kirchhoff index of the linear crossed quadrangular chain is obtained through the relationship between the degree Kirchhoff index and the regular Laplace eigenvalue and matrix decomposition theorem.

Keywords: resistive distance; normal Laplace matrix; Kirchhoff index; degree Kirchhoff index; matrix decomposition theorem; Wiener index

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1. Introduction

The Kirchhoff index and the degree Kirchhoff index are important graph invariants that have been studied extensively in the field of graph theory. They have applications in various fields, including chemistry, physics, and computer science.

In 1993, Klein and Randi put forward the concept of resistive distance on graphs [1]. Various resistance distance calculation formulas such as classical algebraic formulas, probability formulas, combinatorial formulas and functional formulas are deduced one after another. The Kirchhoff index and degree Kirchhoff index discussed in this paper are defined using the resistance distance [2,3]. The Kirchhoff index refers to the sum of the resistance distances between all disordered point pairs in the graph, and it is also known as the total effective resistance [4]. Its research is of great significance in various aspects. For example, in chemistry, it describes the structural characteristics of molecules. In physics, it reflects the scale and connectivity of the network. Mathematically, the Kirchhoff index also occupies an important position. However, direct calculation of the resistance distance and Kirchhoff index is still very difficult, so it is necessary to obtain the Kirchhoff index formula. In the last two decades, many researchers have developed closed-form formulas for Kirchhoff indices for certain types of graphs [5–10]. In their study [5], Li et al. aimed to determine the normalized Laplacian spectrum of H_n using new methods of decomposition theorem and elementary operations that were not previously stated in the existing literature. They then derived explicit formulas for both the degree Kirchhoff index and the number of spanning trees with respect to H_n. These findings can offer valuable insights into the fundamental properties of a particular system and contribute to the development of more advanced materials or applications. Wang et al. investigated the Kirchhoff index of cyclopolyanenes in the literature [6]. They found that the ratio of the Kirchhoff index to the winner index of cyclopolyanenes was approximately 1/3. In their study [7], Liu et al. utilized the recursive method to compute the Kirchhoff index and degree-based Kirchhoff index of random cyclooctane chains. In their study [8], the authors utilized spectral graph theory to derive an exact formula for the Kirchhoff index of hypercube networks. Yang et al. studied the Nordhaus–Gaddum-type Kirchhoff index [9]. In another study [10], the authors proposed exact formulas for calculating the expected values of a random polyomino chain to construct the multiplicative and additive degree Kirchhoff indices. Additionally, they thoroughly examined the highest degree of the expected values through these indices. These formulas can potentially have applications in materials science and other related fields, providing insights into the fundamental properties of electric and heat conductivity in such systems. There is an inseparable relationship between the Kirchhoff index of the graph and the Laplace eigenvalue of the graph, and its value can be obtained by the Laplacian eigenvalue of the graph. In reference [11], Liu et al. used Laplace's characteristic polynomial decomposition theorem to deduce the Kirchhoff index of a linear crossed quadrangular chain. Chen Haiyan and Zhang Fuji gave a new graph parameter based on resistance distance in 2007: degree Kirchhoff index [12]. It is closely related to the regular Laplacian spectrum, which can not only handle the spectral problem of the irregular graph very well, but also has a very close relationship with the random walk on the graph.

Studies on these indices have greatly extended their applications in different fields such as drug design, materials science, and network analysis. In their study [13], Liu et al. began by determining the normalized Laplacian spectra of L_n. They then obtained the multiplicative degree Kirchhoff index and complexity corresponding to L_n. Finally, by comparing these indices with the Wiener index and Gutman index, the researchers observed that the multiplicative degree Kirchhoff index of L_n is nearly one-quarter of its Gutman Wiener index. In their work [14], Feng et al. investigated the Kirchhoff index of phenylenes. In another work [15], they studied the Kirchhoff index and the number of spanning trees of linear pentagonal derivation chains. Meanwhile the authors of [16] compared the winner index and Kirchhoff index of random pentane chains and obtained some conclusions. Yang studied the upper and lower bounds of the Kirchhoff index of planar graphs and fullerene graphs in the literature [17]. In another study [18], the authors derived closed-form formulas for the degree Kirchhoff index of pentagonal cylinders and Möbius chains. Additionally, they investigated the Gutman index and Schultz index of these graphs. These findings shed light on the fundamental properties of these structures, potentially contributing to the development of more advanced materials or applications. Despite their significance, there has been a limited understanding of the Kirchhoff index and the degree Kirchhoff index for complex molecular systems, especially for linear crossed quadrilateral chains. To address this knowledge gap, we aim to investigate the Kirchhoff index and the degree Kirchhoff index of linear crossed quadrilateral chains, which can provide insights into the structural and chemical properties of these systems. Our work builds on previous studies on the Kirchhoff index and the degree Kirchhoff index of other types of molecular systems. This paper deduced the Kirchhoff index of a linear crossed quadrangular chain, counted the formula of spanning tree, obtained its Wiener index, and pointed out that the limit of the ratio of its Kirchhoff index to its Wiener index is one-fourth.

The rest of this paper is organized as follows. Section 2 provides a brief overview of the methods used to calculate the Kirchhoff index and the degree Kirchhoff index. In Sections 3 and 4, we present our results on the Kirchhoff index and the degree Kirchhoff index of linear crossed quadrilateral chains. Finally, we summarize our findings and discuss their implications in Section 5.

2. Preparations

The linear crossed quadrangular chains studied in this paper are all related to an undirected graph. The vertex set and edge set of graph G are expressed by V and E. A binary set consisting of a point set and an edge set is called graph G, namely $G = (V(G), E(G))$ [8]. The difference between the degree diagonal matrix D and the adjacency matrix A of a graph G is called the Laplacian matrix L of the graph, namely $L = D - A$. The degree diagonal matrix D is a diagonal matrix that represents the degrees of each vertex in the graph G. Specifically, the diagonal elements of D are equal to the degree of each vertex, where the degree of a vertex is defined as the number of edges that are incident to the vertex. On the other hand, the adjacency matrix A is a matrix that represents the connections between vertices in the graph. The element $A_{i,j}$ of A is equal to 1 if there exists an edge between vertices i and j in the graph G, and 0 otherwise.

Definition 1 ([19])**.** *The normal Laplace matrix is defined as follows:*

$$NL(G) = \begin{cases} 1, u = v, d_u(G) \neq 0 \\ \frac{-1}{\sqrt{d_u(G)d_v(G)}}, u \text{ is adjacent to } v \\ 0, \text{ otherwise} \end{cases}, \tag{1}$$

where $d_u(G)(d_v(G))$ denotes the degree of vertex $u(v)$ and $NL(G)$ represents the normal Laplacian matrix of graph G.

Definition 2 ([19])**.** *Let the unit resistance be each edge of graph G, then the sum of the resistance distances of all pairs of vertices is called the Kirchhoff index of the graph G.*

$$Kf(G) = \sum_{i<j} r_{ij}, \tag{2}$$

where r_{ij} represents the resistance distance between vertices i and j.

Definition 3 ([20])**.** *The sum of the distances between all point pairs is defined as the Wiener index, namely*

$$W(G) = \sum_{i<j} d_{ij}, \tag{3}$$

where $d_{ij} = d_G(v_i, v_j)$ represents the shortest past between vertex v_i and v_j in graph G.

Lemma 1 ([21])**.** *Let L_A, L_S, NL_A, NL_S be the corresponding Laplace and normal Laplace matrix, then the Laplace and normal Laplace decomposition theorem is*

$$P_{L_{(G)}} = P_{L_A}(\lambda) + P_{L_S}(\lambda), NP_{L_{(G)}} = NP_{L_A}(\lambda) + NP_{L_S}(\lambda). \tag{4}$$

Lemma 2 ([22])**.** *Suppose a graph G is a simple graph, which has m edges and n vertices, then the intrinsic relationship between the number of spanning trees and the normal Laplace eigenvalues of graph G is*

$$\prod_{i=1}^{n} d_G(v_i) \prod_{i=2}^{n} \lambda_i = 2m\tau(G), \tag{5}$$

where $\tau(G)$ denotes a spanning tree of graph G.

Lemma 3 ([22])**.** *Let G be a simple connected graph with m vertices and n edges. The relationship between the Kirchhoff index of a graph G and its normalized Laplacian eigenvalues is given by:*

$$Kf(G) = n \sum_{i=2}^{n} \frac{1}{\mu_i},$$

where $0 = \mu_1 \leq \mu_2 \cdots \leq \mu_m$ is the eigenvalue of matrix L_A .

Lemma 4 ([5]). *Let G be a simple connected graph with m vertices and n edges. The relationship between the degree Kirchhoff index of a graph G and its normalized Laplacian eigenvalues is given by:*

$$Kf^*(G) = 2m\sum_{i=2}^{n}\frac{1}{\lambda_i},$$

where $0 = \lambda_1 \leq \lambda_2 \cdots \leq \lambda_m$ *is the eigenvalue of matrix* L_A *.*

For symbols, definitions and lemmas that are not explained in the text, please refer to [20]. Let $P_M(\lambda) = \det(\lambda I - M)$ denote the characteristic polynomial of a matrix M of order n. Linear crossed quadrilateral chains can be obtained by adding edges to linear quadrilateral chains; that is, adding two pairs of sides to each quadrilateral, as shown in Figure 1.

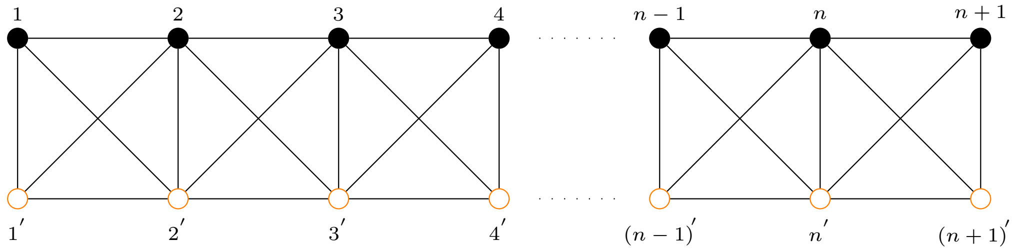

Figure 1. Linear crossed quadrilateral chain.

It could be obtained from the graph that $\pi = (1,1'),(2,2')\cdots(n+1,(n+1)')$ is an automorphic [23], and $|V(G)| = 2n+2, |E(G)| = 5n+1$. So Laplacian and normal Laplacian matrices could be represented by the following block matrices: $L(O_n) = \begin{pmatrix} L_{v_1v_1} & L_{v_1v_2} \\ L_{v_2v_1} & L_{v_2v_2} \end{pmatrix}, NL(O_n) = \begin{pmatrix} NL_{v_1v_1} & NL_{v_1v_2} \\ NL_{v_2v_1} & NL_{v_2v_2} \end{pmatrix}$, and we have $L_{v_1v_1} = L_{v_2v_2}, L_{v_1v_2} = L_{v_2v_1}, NL_{v_1v_1} = NL_{v_2v_2}, NL_{v_1v_2} = NL_{v_2v_1}, P = \begin{pmatrix} \frac{1}{\sqrt{2}}I_n & \frac{1}{\sqrt{2}}I_n \\ \frac{1}{\sqrt{2}}I_n & -\frac{1}{\sqrt{2}}I_n \end{pmatrix}$. From the unitary transformation, we have $P[NL(O_n)]P^T = \begin{pmatrix} NL_A & 0 \\ 0 & NL_S \end{pmatrix}$, $PL(O_n)P^T = \begin{pmatrix} L_A & 0 \\ 0 & L_S \end{pmatrix}$, where P^T is the transpose of P.

Thus,

$$L_A = L_{v_1v_1} + L_{v_1v_2}, L_S = L_{v_1v_1} - L_{v_2v_2}, \tag{6}$$

$$NL_A = NL_{v_1v_1} + NL_{v_1v_2}, NL_S = NL_{v_1v_1} - NL_{v_2v_2}. \tag{7}$$

3. Kirchhoff Indexes for Linear Crossed Quadrilateral Chains

According to the definition of Laplacian matrix, we could obtain the block matrix $L_{v_1v_1}$ and $L_{v_1v_2}$ as follows.

$$L_{v_1v_1} = (l_{ij})_{n+1} = \begin{pmatrix} 3 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -1 & 5 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & 5 & -1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 5 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 5 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 5 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 5 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 3 \end{pmatrix}_{n+1}, \tag{8}$$

where $l_{1,1} = l_{n+1,n+1} = 3, l_{i,i} = 5, i \in \{2, 3, \ldots, n\}$. $l_{i,i+1} = l_{i+1,i} = -1, i \in \{1, 2, 3, \ldots, n\}$.

$$L_{v_1v_2} = (l_{ij})_{n+1} = \begin{pmatrix} -1 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -1 & -1 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -1 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & -1 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & -1 \end{pmatrix}_{n+1}, \tag{9}$$

where $l_{i,i} = -1, i \in \{1, 2, 3, \ldots, n\}$,$l_{i,i+1} = l_{i+1,i} = -1, i \in \{1, 2, 3, \ldots, n\}$. From the formula, we can obtain

$$L_A = (l_{ij})_{n+1} = \begin{pmatrix} 2 & -2 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -2 & 4 & -2 & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -2 & 4 & -2 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 4 & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 4 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -2 & 4 & -2 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -2 & 4 & -2 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -2 & 2 \end{pmatrix}_{n+1}, \tag{10}$$

where $l_{1,1} = l_{n+1,n+1} = 2, l_{i,i} = 4, i \in \{2, 3, \ldots, n\}$, $l_{i,i+1} = l_{i+1,i} = -2, i \in \{1, 2, 3, \ldots, n\}$. Suppose $0 = \alpha_1 \le \alpha_2 \cdots \le \alpha_{n+1}$ and $0 < \beta_1 \le \beta_2 \cdots \le \beta_{n+1}$ are the roots of $P_{L_A}(\lambda) = 0$ and $P_{L_S}(\lambda) = 0$, respectively. Note that if $\eta = (1, 1, 1, \cdots, 1, 1)^T$, $L_A \cdot \eta = 0$. In other words, 0 is the eigenvalue of L_A. From Lemma 3, we can obtain the following lemma.

Lemma 5. *Assume that F_n is a linear crossed quadrilateral chain, then*

$$Kf(F_n) = 2(n+1)\left(\sum_{i=2}^{n+1} \frac{1}{\alpha_i} + \sum_{j=1}^{n+1} \frac{1}{\beta_j}\right). \tag{11}$$

According to the matrix L_S, it is not difficult to obtain

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

Then, according to Lemma 3, we will focus on computing$\sum_{i=2}^{n+1} \frac{1}{\alpha_i}$,where $0 = \alpha_1 \le \alpha_2 \cdots \le \alpha_{n+1}$ is the eigenvalue of matrix L_A . Then, we obtain

$$P_{L_A}(\lambda) = \det(\lambda I - L_A) = \lambda\left(\lambda^n + a_1\lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n\right), a_n \neq 0. \tag{13}$$

From the above equation, we can conclude that $\frac{1}{\alpha_2}, \frac{1}{\alpha_3}, \ldots, \frac{1}{\alpha_{n+1}}$ are the roots of the following equation:

$$a_n x^n + a_{n-1}x^{n-1} + a_1 x + 1 = 0. \tag{14}$$

According to Vieta's theorem [5], we can get

$$\sum_{i=2}^{n+1} \frac{1}{\alpha_i} = \frac{(-1)^{n-1}a_{n-1}}{(-1)^n a_n}. \tag{15}$$

Two facts are given as follows [24].

Fact 1. $(-1)^n a_n = (n+1) \cdot 2^n$.

Proof. For the convenience of description, the i-order main sub-matrix of matrix L_A is expressed as W_i. Let $w_i = \det W_i$, then $w_1 = 2, w_2 = 4, w_3 = 8$. To obtain the n-order main sub-matrix, we eliminate the last row and last column of L_A. Afterward, we compute $\det W_i$ and obtain $w_i = 4w_{i-1} - 4w_{i-2}$ for $3 \leq i \leq n$. Further calculations reveal that $w_i = 2^i$.
Note that $(-1)^n a_n$ is equal to the sum of the determinants of all major submatrices of order n of matrix L_A, namely,

$$(-1)^n a_n = \sum_{i=1}^{n+1} \det L_A = \sum_{i=1}^{n+1} \det \begin{pmatrix} W_{i-1} & 0 \\ 0 & U_{n+1-i} \end{pmatrix} = \sum_{i=1}^{n+1} \det W_{i-1} \cdot \det U_{n+1-i}, \quad (16)$$

where

$$W_{i-1} = \begin{pmatrix} l_{1,1} & -2 & \cdots & 0 \\ -2 & l_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{i-1,i-1} \end{pmatrix}, U_{n+1-i} = \begin{pmatrix} l_{i+1,i+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{n,n} & -2 \\ 0 & \cdots & -2 & l_{n+1,n+1} \end{pmatrix}. \quad (17)$$

Let $w_0 = 1, \det U_0 = 1$. According to the structure of the symmetric matrix L_A, we have $\det U_{n+1-i} = \det W_{n+1-i}$, therefore

$$(-1)^n a_n = \sum_{i=1}^{n+1} \det L_A[i] = \sum_{i=1}^{n+1} w_{i-1} w_{n+1-i} = \sum_{i=2}^{n} w_{i-1} w_{n+1-i} + 2w_n = (n+1) \cdot 2^n. \quad (18)$$

□

Fact 2. $(-1)^{n-1} a_{n-1} = \frac{2^n n(n+1)(n+2)}{12}$.

Proof. Note that $(-1)^{n-1} a_{n-1}$ is equal to the sum of the determinants of all major submatrices of order $n-1$ of matrix L_A , namely,

$$L_A[i,j] = \begin{pmatrix} W_{i-1} & 0 & 0 \\ 0 & X_{j-1-i} & 0 \\ 0 & 0 & U_{n+1-j} \end{pmatrix}, 1 \leq i < j \leq n+1, \quad (19)$$

where $W_{i-1} = \begin{pmatrix} l_{1,1} & -2 & \cdots & 0 \\ -2 & l_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{i-1,i-1} \end{pmatrix}, X_{j-1-i} = \begin{pmatrix} 4 & -2 & \cdots & 0 \\ -2 & 4 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 4 \end{pmatrix},$
$U_{n+1-j} = \begin{pmatrix} l_{j+1,j+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{n,n} & -2 \\ 0 & \cdots & -2 & l_{n+1,n+1} \end{pmatrix}$. If $x_i = \det(X_i)$, we can get $x_i = 4x_{i-1} - 4x_{i-2}$, $x_1 = 4, x_2 = 12, x_3 = 32$, so, $x_i = (1+i)2^i$. Note that

$$\begin{aligned} (-1)^{n-1} a_{n-1} &= \sum_{1 \leq i < j}^{n+1} \det L_A[i,j] = \sum_{1 \leq i < j}^{n+1} \det W_{i-1} \det X_{j-1-i} \det U_{n+1-j} \\ &= \sum_{1 \leq i < j}^{n+1} w_{i-1} w_{n+1-j} x_{j-1-i} = \sum_{1 \leq i < j}^{n} (j-i) \cdot 2^{n-1} \\ &= \frac{2^n n(n+1)(n+2)}{12}. \end{aligned} \quad (20)$$

□

From Facts 1 and 2, the following equation can be obtained:

$$\sum_{i=2}^{n+1} \frac{1}{\alpha_i} = \frac{(-1)^{n-1} a_{n-1}}{(-1)^n a_n} = \frac{n(n+2)}{12}. \tag{21}$$

By substituting Formulas (21) , (12) into (11), we can obtain the following theorem:

Theorem 1. *Assuming F_n is a linear crossed quadrilateral chain, its Kirchhoff index is*

$$Kf(F_n) = \frac{(n+1)(n+2)^2}{6}. \tag{22}$$

Through calculation, we can obtain the partial value of the Kirchhoff index of the linear crossed quadrangular chain, as follows in Table 1.

Table 1. Partial values of Kirchhoff indexes for linear crossed quadrilateral chains.

G	*K f(G)*	*G*	*K f(G)*	*G*	*K f(G)*	*G*	*K f(G)*	*G*	*K f(G)*
F_1	3.00	F_5	49.00	F_9	201.67	F_{13}	525.00	F_{17}	1083.00
F_2	8.00	F_6	74.64	F_{10}	264.00	F_{14}	640.00	F_{18}	1266.67
F_3	16.67	F_7	108.00	F_{11}	338.00	F_{15}	770.67	F_{19}	1470.00
F_4	30.00	F_8	150.00	F_{12}	424.67	F_{16}	918.00	F_{20}	1694.00

In the above table, we list the Kirchhoff indexes of F_n, $1 \leq n \leq 20$. Next, let us calculate the number of spanning trees.

Theorem 2. *Let F_n be a linear crossed quadrilateral chains of length n. The number of distinct spanning trees of F_n, denoted by $\tau(F_n)$, is given by the formula*

$$\tau(F_n) = 2^{2n+2} \cdot 3^{n-1}. \tag{23}$$

Proof. Based on Lemma 2, we obtain

$$\prod_{i=1}^{2n+2} d_i \prod_{i=2}^{n+1} \alpha_i \prod_{i=2}^{n+1} \beta_j = 2|E(F_n)|\tau(F_n). \tag{24}$$

Then,

$$\prod_{i=1}^{2n+2} d_i = 3^4 \cdot 5^{2n-2}, \prod_{i=1}^{n+1} \alpha_i = \frac{2(5n+1)}{9} \cdot \left(\frac{1}{10}\right)^{n-1}, \prod_{j=1}^{n+1} \beta_j = \left(\frac{4}{3}\right)^2 \cdot \left(\frac{6}{5}\right)^{n-1}. \tag{25}$$

Based on the aforementioned analysis, we can obtain the value of $\tau(F_n) = 2^{2n+2} \cdot 3^{n-1}$. □

The number of spanning trees is calculated below in Table 2.

Table 2. Partial value of the number of spanning trees for a linearly crossed quadrilateral chain.

G_0	$\tau(G)$	G	$\tau(G)$
F_1	16	F_5	331,776
F_2	192	F_6	3,981,312
F_3	2304	F_7	47,775,744
F_4	27,648	F_8	573,308,928

Experimental results have confirmed that when $n = 1$, the linear crossed quadrilateral chain F_1 forms a K_4 structure. According to Ohm's law

$$r_{12} = r_{13} = r_{14} = r_{23} = r_{24} = r_{34} = \frac{1}{2}, \tag{26}$$

we find the sum of the resistance distances of F_1 is 3, which represents the Kirchhoff index. According to Theorem 1, we can calculate the Kirchhoff index as follows: $Kf(F_1) = \frac{(1+1)(1+2)^2}{6} = 3$. Using the Cayley formula, we can determine the number of spanning trees for K_4: $\tau(K_4) = 4^{4-2} = 16$. By applying Formula (24), the number of spanning trees for K_4 can also be derived as follows: $\tau(K_4) = 2^{(2+2)} \cdot 3^0 = 16$. Next, we can explore the ratio of the Kirchhoff index of F_n to its Wiener index.

Theorem 3. *Assuming F_n is a linear crossed quadrilateral chain, then*

$$\lim_{n\to\infty} \frac{Kf(F_n)}{W(F_n)} = \frac{1}{4}. \tag{27}$$

Proof. For distance d_{ij}, when we calculate and discuss the Wiener index of F_n, the choice of point i can be divided into the following two cases:
The first vertex of F_n: $g_1(n) = 1 + \sum_{k=1}^{n} 2k = n^2 + n + 1$.
The $s-th$ vertex of F_n, $s = 2, 3, \cdots, n$. $g_2(n) = \sum_{s=2}^{n}\left(1 + \sum_{k=1}^{n-1} 2k + \sum_{k=1}^{n-s+1} 2k\right) = \frac{2n^3+n-1}{3}$.
Therefore, we can conclude

$$W(F_n) = \frac{4g_1(n) + 2g_2(n)}{2} = \frac{2n^3 + 6n^2 + 7n + 5}{3}.$$

Combining the expressions of $W(F_n)$ and $Kf(F_n)$, we can get

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

□

4. Degree Kirchhoff Index of Linear Crossing Quadrilateral Chains

In this section, we first give the normal Laplace spectrum of F_n and then solve the degree Kirchhoff index of F_n. According to the definition of the normal Laplace matrix, we can conclude

$$NL_{v_1v_1} = \left(l_{ij}\right)_{n+1} = \begin{pmatrix} 1 & -\frac{1}{\sqrt{15}} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{15}} & 1 & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{5} & 1 & -\frac{1}{5} & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{5} & 1 & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 1 & -\frac{1}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{5} & 1 & -\frac{1}{5} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & 1 & -\frac{1}{\sqrt{15}} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{\sqrt{15}} & 1 \end{pmatrix}_{n+1},$$

$$NL_{v_1v_2} = \left(l_{ij}\right)_{n+1} = \begin{pmatrix} -\frac{1}{3} & -\frac{1}{\sqrt{15}} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{15}} & -\frac{1}{5} & -\frac{1}{5} & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{5} & -\frac{1}{5} & -\frac{1}{5} & \cdots & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{5} & -\frac{1}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -\frac{1}{5} & -\frac{1}{5} & -\frac{1}{5} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{5} & -\frac{1}{5} & -\frac{1}{\sqrt{15}} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{1}{\sqrt{15}} & -\frac{1}{3} \end{pmatrix}_{n+1},$$

$$NL_A = \left(l_{ij}\right)_{n+1} = \begin{pmatrix} \frac{2}{3} & -\frac{2}{\sqrt{15}} & 0 & 0 & \cdots & 0 & 0 & 0 & 0 \\ -\frac{2}{\sqrt{15}} & \frac{4}{5} & -\frac{2}{5} & 0 & \cdots & 0 & 0 & 0 & 0 \\ 0 & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{2}{5} & \frac{4}{5} & \cdots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & \frac{4}{5} & -\frac{2}{5} & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{5} & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -\frac{2}{5} & \frac{4}{5} & -\frac{2}{\sqrt{15}} \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -\frac{2}{\sqrt{15}} & \frac{2}{3} \end{pmatrix}_{n+1},$$

$NL_S = diag(\frac{4}{3}, \frac{6}{5}, \frac{6}{5}, \cdots, \frac{6}{5}, \frac{4}{3})$, a diagonal matrix of order $n+1$. Suppose $0 = \lambda_1 \le \lambda_2 \le \cdots \lambda_{n+1}$ and $0 < \delta_1 \le \delta_2 \le \cdots \delta_{n+1}$ are the roots of $P_{NL_A}(\lambda) = 0$ and $P_{NL_S}(\lambda) = 0$, respectively. Note that if $\eta(\frac{\sqrt{15}}{5}, 1, 1, \cdots, \frac{\sqrt{15}}{5})^T, NL_A \cdot \eta = 0$. In other words, 0 is an eigenvalue of NL_A. From Lemma 4, we can obtain the following lemma.

Lemma 6. *Suppose F_n is a linear crossed quadrilateral chain, then*

$$Kf^*(F_n) = 2(5n+1)\left(\sum_{i=2}^{n+1} \frac{1}{\lambda_i} + \sum_{j=1}^{n+1} \frac{1}{\delta_j}\right). \tag{28}$$

According to the matrix NL_S, it is not difficult to obtain

$$\sum_{j=1}^{n+1} \frac{1}{\delta_j} = \frac{3}{4} \times 2 + \frac{5}{6}(n-1) = \frac{2}{3} + \frac{5n}{6} = \frac{4+5n}{6}. \tag{29}$$

Next, we will concentrate on computing $\sum_{i=2}^{n+1} \frac{1}{\lambda_i}$. $0 = \lambda_1 \le \lambda_2 \cdots \le \lambda_{n+1}$ are the eigenvalues of matrix NL_S. In that case, we can conclude

$$P_{NL_A}(\lambda) = \det(\lambda I - NL_A) = \lambda\left(\lambda^n + b_1\lambda^{n-1} + \cdots + b_{n-1}\lambda + b_n\right), b_n \ne 0.$$

From the above equation, we can conclude that $\frac{1}{\lambda_2}, \frac{1}{\lambda_3}, \cdots, \frac{1}{\lambda_{n+1}}$ is the root of the following equation

$$b_n x^n + b_{n-1}x^{n-1} + \cdots + b_1 x + 1 = 0. \tag{30}$$

Based on Vieta's theorem, we can obtain

$$\sum_{i=2}^{n+1} \frac{1}{\lambda_i} = \frac{(-1)^{n-1} b_{n-1}}{(-1)^n b_n}. \tag{31}$$

Two facts are given as follows.

Fact 3. $(-1)^n b_n = (\frac{2}{5})^{n-2}[\frac{8}{15} + \frac{4}{9}(n-1)]$.

Proof. The i-order principal submatrix of NL_A matrix is denoted as M_i. Let $m_i = \det(M_i)$, then $m_1 = \frac{2}{3}, m_2 = \frac{2}{3} \times (\frac{2}{5})^2, m_3 = \frac{2}{3} \times (\frac{2}{5})^3, m_3 = \frac{2}{3} \times (\frac{2}{5})^3$ and we can obtain

$m_k = \frac{2}{3} \times (\frac{2}{5})^(k-1), 1 \leq k \leq n.$

Note that $(-1)^n b_n$ is equal to the sum of the determinants of all major submatrices of order n of matrix L_A, namely,

$$(-1)^n b_n = \sum_{i=1}^{n+1} \det NL_A = \sum_{i=1}^{n+1} \det \begin{pmatrix} M_{i-1} & 0 \\ 0 & R_{n+1-i} \end{pmatrix} = \sum_{i=1}^{n+1} \det M_{i-1} \cdot \det R_{n+1-i}, \quad (32)$$

where,

$$M_{i-1} = \begin{pmatrix} l_{1,1} & -\frac{2}{\sqrt{15}} & \cdots & 0 \\ -\frac{2}{\sqrt{15}} & l_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & l_{i-1,i-1} \end{pmatrix}, R_{n+1-i} = \begin{pmatrix} l_{i+1,i+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & l_{n,n} & -\frac{2}{\sqrt{15}} \\ 0 & \cdots & -\frac{2}{\sqrt{15}} & l_{n+1,n+1} \end{pmatrix}.$$

Let $m_0 = 1, \det R_0 = 1$. Since the similarity transformation does not change the determinant of the square matrix, we can conclude $\det R + n + 1 - i = \det M_{n+1-i}$, then

$$\begin{aligned} (-1)^n b_n &= \sum_{i=1}^{n+1} \det NL_A[i] = \sum_{i=1}^{n+1} m_{i-1} m_{n+1-i} = \sum_{i=2}^{n} m_{i-1} m_{n+1-i} + 2m_n \\ &= \left(\frac{2}{5}\right)^{n-2} \cdot \left[\frac{8}{15} + \frac{4}{9}(n-1)\right]. \end{aligned} \quad (33)$$

□

Fact 4. $(-1)^{(n-1)} b_{n-1} = (\frac{2}{5})^{(n-2)} \frac{n^2-3n+2}{3}$.

Proof. Note that $(-1)^{(n-1)} b_{n-1}$ is equal to the sum of the determinants of all major submatrices of order $(n-1)$ of matrix NL_A, namely,

$$L_A[i,j] = \begin{pmatrix} M_{i-1} & 0 & 0 \\ 0 & Y_{j-1-i} & 0 \\ 0 & 0 & R_{n+1-j} \end{pmatrix}, \quad 1 \leq i < j \leq n+1, \quad (34)$$

where

$$M_{i-1} = \begin{pmatrix} c_{1,1} & -\frac{2}{\sqrt{15}} & \cdots & 0 \\ -\frac{2}{\sqrt{15}} & c_{2,2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_{i-1,i-1} \end{pmatrix}, Y_{j-1-i} = \begin{pmatrix} c_{i+1,i+1} & c_{i+1,i+2} & \cdots & 0 \\ c_{i+2,i+1} & c_{i+2,i+2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & c_{j-1,j-1} \end{pmatrix},$$

$$R_{n+1-j} = \begin{pmatrix} c_{j+1,j+1} & \cdots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \cdots & c_{n,n} & -\frac{2}{\sqrt{15}} \\ 0 & \cdots & -\frac{2}{\sqrt{15}} & c_{n+1,n+1} \end{pmatrix}.$$

In summary, we can obtain

$$(-1)^{n-1} b_{n-1} = \sum_{1 \leq i < j}^{n+1} \det NL_A[i,j] = \sum_{1 \leq i < j}^{n+1} M_{i-1} Y_{j-1-i} R_{n+1-j}. \quad (35)$$

Based on Formula (29), all possible values of i and j are as follows.

By derivation, it is not difficult to obtain the following:

$$\det R_{i-1} = \frac{3}{5}\left(\frac{2}{5}\right)^{i-2}, \det Y_{j-1-i} = (j-i)\left(\frac{2}{5}\right)^{j-i-1}, \det M_{n+1-j} = \frac{2}{3}\left(\frac{2}{5}\right)^{n-j}. \quad (36)$$

Case 1: $i = 1, j = n + 1$,

$$\det NL_A = \det Y_{n-1} = n(\frac{2}{5})^(n-1). \tag{37}$$

Case 2: $i = 1, i < j < n + 1$,

$$\det NL_A = \det(Y_{j-2}M_{n+1-j}) = \frac{2}{3}(j-1)(\frac{2}{5})^{(n-2)}, j = 2, 3, \cdots, n. \tag{38}$$

Case 3: $1 < i < j = n + 1$,

$$\det NL_A = (\det R_{i-1}Y_{j-1-i}) = \frac{2}{3}(n+1-i)(\frac{2}{5})^{(n-2)}. \tag{39}$$

Case 4: $1 < i < j < n + 1$,

$$\det NL_A = \det(R_{i-1}Y_{j-1-i}M_{n+1-j}) = \frac{4}{9}(j-i)(\frac{2}{5})^{(n-3)}. \tag{40}$$

It is observed that Cases 3 and 4 are equal.
To sum up, the sum of the determinants of all primary and submatrices of order $n - 1$ is

$$\begin{aligned} &\sum_{i=2}^{n-1}\sum_{j=i+1}^{n}\frac{4}{9}(j-i)\cdot\left(\frac{2}{5}\right)^{n-3} + 2\sum_{j=2}^{n}(j-1)\left(\frac{2}{5}\right)^{n-2} + n\left(\frac{2}{5}\right)^{n-1} \\ &= \frac{2}{3}\left(\frac{2}{5}\right)^{n-2}\sum_{j=2}^{n}(j-1) \\ &= \frac{n^2-3n+2}{3}\left(\frac{2}{5}\right)^{n-2}. \end{aligned} \tag{41}$$

□

From Facts 3 and 4, the following equation can be obtained:

$$\sum_{i=2}^{n+1}\frac{1}{\lambda_i} = \frac{(-1)^{n-1}b_{n-1}}{(-1)^n b_n} = \frac{15}{4}\cdot\frac{n^2-3n+2}{5n+1}. \tag{42}$$

Substituting Formulas (30) and (43) into Formula (29), the following theorem can be obtained.

Theorem 4. *Assuming F_n is a linear crossed quadrilateral chain. Its degree Kirchhoff index is*

$$Kf^*(F_n) = \frac{95n^2 - 85n + 98}{6}. \tag{43}$$

In Table 3 below, we list the degree Kirchhoff index of F_n , $1 \le n \le 20$.

Table 3. Partial values of Kirchhoff indexes for linear crossed quadrilateral chain degrees.

G	$Kf^*(G)$	G	$Kf^*(G)$	G	$Kf^*(G)$
F_1	18	F_5	341.3	F_9	1171.3
F_2	51.3	F_6	501.3	F_{10}	1458
F_3	116.3	F_7	693	F_{11}	1776.3
F_4	213	F_8	916.3	F_{12}	2126.3

5. Discussion

This article focuses on studying a type of tetrafunctional compound with a linear crossed square chain shape and its Kirchhoff index. The Kirchhoff index is an essential parameter for measuring electric and heat conductivity in materials science. The newly derived formula provides a more efficient way to calculate the Kirchhoff index of crossed quadrangular chains than previous methods. The proposed approach could potentially be extended to other graph structures, lending it great practical significance.

One limitation of this study is that it only applies to linear crossed quadrangular chains. More extensive graphs require further investigation. Another potential direction is to explore the relationship between the Kirchhoff index and other topological indices of graphs. Additionally, numerical simulations and experimental verification would help validate the theoretical results obtained in this study.

There are several potential areas for future work on this topic. Firstly, extending the proposed method to other complex structures would be a fruitful avenue for research. Secondly, investigating the interdependence between the Kirchhoff index and other parameters, such as the degree and diameter of the network, remains a crucial question. Thirdly, applying the Kirchhoff index to analyze the properties of real-world networks, such as social, transportation, and biological systems, would have significant implications in various fields. Finally, numerical simulations and empirical experiments are needed to confirm the theoretical results. Overall, the current research presents valuable insights into the fundamental characteristics of electric and heat conductivity in synthetic and natural systems, which could have broad implications for numerous applications.

6. Conclusions

In this research, we studied the Kirchhoff index in the context of a type of tetrafunctional compound with a linear crossed square chain shape. We utilized matrix theory and Laplace's characteristic polynomial decomposition theorem to derive a precise formula for calculating the Kirchhoff index of a linear crossed quadrangular chain. Through comparative analysis with the Kirchhoff index obtained by applying Ohm's law and the number of spanning trees calculated using Cayley's theorem, we verified the accuracy of our formula.

Our findings reveal that the ratio of Kirchhoff index to Wiener index tends towards one-fourth in the asymptotic limit. This sheds new light on the relationship between the Kirchhoff index and other topological indices of graphs, such as the Wiener index. Overall, this study presents a new formula for calculating the Kirchhoff index of a specific type of tetrafunctional compound with a linear crossed square chain shape. This formula could potentially have applications in materials science and related fields, providing insights into the fundamental characteristics of electric and heat conductivity in such systems.

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