Research Article

Comparison of the Wiener and Kirchhoff Indices of Random Pentachains

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Let G be a connected (molecule) graph. The Wiener index $W(G)$ and Kirchhoff index $Kf(G)$ of G are defined as the sum of distances and the resistance distances between all unordered pairs of vertices in G , respectively. In this paper, explicit formulae for the expected values of the Wiener and Kirchhoff indices of random pentachains are derived by the difference equation and recursive method. Based on these formulae, we then make comparisons between the expected values of the Wiener index and the Kirchhoff index in random pentachains and present the average values of the Wiener and Kirchhoff indices with respect to the set of all random pentachains with n pentagons.

1. Introduction

All graphs considered in this paper are simple, undirected, and connected. All notations not defined in this paper can be found in [1]. Let G be a graph with the vertex set $V(G) = \{v_1, v_2, \dots, v_n\}$ and edge set $E(G)$. The traditional distance $d(v_r, v_s)$ between vertices v_r and v_s is the number of edges of a shortest path connecting these vertices in G . In 1993, Klein and Randić [2] conceived the novel concept of resistance distance based on the electric resistance in an electrical network N corresponding to the considered graph G , in which the resistance between any two adjacent nodes is 1 Ohm. Similar to the long recognized shortest path distance, the resistance distance is also intrinsic to the graph, not only with some nice purely mathematical and physical interpretations [2, 3], but also with a substantial potential for chemical applications. Denote by $r(v_i, v_j)$ the resistance distance between the vertices v_i and v_j in G , which is computed by Ohm's and Kirchhoff's laws in N .

For the resistance distance of a connected graph, a formula for computing it was presented by Klein and Randić [2] in 1993. We may compute the distance of two

vertices in a connected graph G of order n from its Laplacian matrix. Precisely, let L be the Laplacian matrix of G and J be the $n \times n$ matrix whose entries are 1. Let $X = (L + (1/n)J)^{-1}$. Then, the resistance distance between vertices i and j of G is

$$r(i, j) = X_{i,i} + X_{j,j} - 2X_{i,j}. \quad (1)$$

The Wiener index $W(G)$ [4, 5] of a graph G was first introduced by Wiener in the study of paraffin boiling points and a graph invariant based on distances in 1947. This is the oldest topological index related to molecular branching [6]. It is defined as the sum of distances between all unordered pairs of vertices in G , i.e.,

$$W(G) = \frac{1}{2} \sum_{r=1}^n \sum_{s=1}^n d(v_r, v_s) = \frac{1}{2} \sum_{r=1}^n d(v_r | G), \quad (2)$$

where $d(v_i | G)$ denotes the sum of distances between v_i and all other vertices of G , defined by

$$d(v_i | G) = \sum_{j=1}^n r(v_i, v_j). \quad (3)$$

For a survey of results and bibliography on the chemical applications and the mathematical literature of the Wiener index, see [7–15] and the references cited therein.

Similar to the Wiener index, the Kirchhoff index $Kf(G)$ of a graph G [2, 16] is defined as

$$Kf(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n r(v_i, v_j) = \frac{1}{2} \sum_{i=1}^n r(v_i|G), \quad (4)$$

where $r(v_i|G)$ denotes the sum of resistance distances between v_i and all other vertices of G , defined by

$$r(v_i|G) = \sum_{j=1}^n r(v_i, v_j). \quad (5)$$

Klein and Randić [2] proved that $r(v_i, v_j) \leq d(v_i, v_j)$ and $Kf(G) \leq W(G)$ with equality if and only if G is a tree. Like many topological indices, the Kirchhoff index based on resistance distance is also a graph invariant and molecular structure descriptor. Unfortunately, it is difficult to implement some algorithms [2, 17, 18] to compute resistant distance and Kirchhoff index in a graph from their computational complexity. Hence, it makes sense to find explicit closed-form formula for the Kirchhoff index. Up to now, the Kirchhoff index has been found to have noteworthy applications in chemistry, such as in assessing cyclicity of polycyclic structures including fullerenes, linear hexagonal chains, and some special molecular graphs such as distance-regular graphs and Möbius ladders [17–21]. Bonchev et al. in [16] considered the polymer science by using it and found that the Kirchhoff index in their approach is especially useful for defining the topological radius $R_{\text{top}} = (Kf/n^2)$ of macromolecules containing cyclic fragments. Many mathematical properties have also been established (see [22–41] and the references cited therein).

Motivated by the works in [42–44], in this paper, we derive explicit formulae for the expected values of the Kirchhoff indices of random alpha-pentachain [43] and spiro-pentachain as shown in Figure 1 and Wiener index of random spiro-pentachain. Based on these formulae, we then make comparisons between the expected values of the Wiener index and the Kirchhoff index in random pentachains and present the average values of the Wiener and Kirchhoff indices with respect to the set of all random pentachains with n pentagons. In fact, there also exist numerous research results for a general pentachain. For example, Xiao et al. [45] studied a connection between the Kekulé structures of pentachains and the Hosoya index of caterpillar trees, and a general expression for calculating the bond incident degree indices of pentachains was established in [46]. Denote by $E[\Xi]$ the expected value of a random variable.

2. Wiener and Kirchhoff Indices in Alpha-Pentachains

An *alpha-pentachain* of length n is obtained from a sequence of 5 cycles (pentagons) $C_1, C_2, \dots, C_n$ by adding a bridge to each pair of consecutive 5 cycles, which is denoted by P_n^α . The cycle C_i will be called the i -th pentagon of P_n^α , $1 \leq i \leq n$.

Figure 2 shows the unique alpha-pentachains for $n = 1, 2$ and all the alpha-pentachains for $n = 3$, and Figure 3 shows a general case, where v_{n-1} is a vertex of C_{n-1} in P_{n-1}^α . Note that there are two ways to add a bridge between two consecutive cycles. So, P_n^α may not be unique when $n \geq 3$.

Consider P_{n-1}^α for $n \geq 3$. Let $C_{n-1} = x_1x_2x_3x_4x_5x_1$, and there is a bridge connecting x_1 and v_{n-2} which is a vertex in C_{n-2} . There are two possible constructions of getting P_n^α from P_{n-1}^α by the symmetry of the structure of an alpha-pentachain (see Figure 4). Precisely, let $P_n^{\alpha_1}$ and $P_n^{\alpha_2}$ be obtained by adding a bridge connecting a vertex of the extra pentagon C_n with the vertices x_2 and x_3 of C_{n-1} , respectively (see Figure 4). We may assume that for getting a P_n^α from a fixed P_{n-1}^α is a random process, namely, the probability of getting $P_n^{\alpha_1}$ and $P_n^{\alpha_2}$ from a fixed P_{n-1}^α is p and $1 - p$, respectively.

We assume that the probability p is constant and independent of n , i.e., the process described above is a zeroth-order Markov process. After associating probabilities, such an alpha-pentachain is called a *random alpha-pentachain* and denoted by $P_{n;p}^\alpha$. Gutman et al. [47, 48] considered the Wiener indices of random benzenoid chain graphs in 1990s. Chen and Zhang [49] obtained explicit analytical expressions for the expected value of the Wiener index and the number of perfect matchings in a random phenylene chain. Yang and Zhang [15] studied the Wiener indices of random polyphenyl chain graphs in 2012. Wei et al. [44, 50, 51] obtained simple formulae for the expected value of the Wiener indices of random polygonal chains. Wang et al. [43] studied the expected value of the Wiener indices of random alpha-pentachains.

Theorem 1 (see [43]). *Let $P_{n;p}^\alpha$ be a random alpha-pentachain. Then,*

$$E[W(P_{n;p}^\alpha)] = \frac{5}{6} (15 - 5p)n^3 + \left(5 + \frac{25}{2}p\right)n^2 - \left(\frac{5}{2} + \frac{25}{3}p\right)n. \quad (6)$$

In addition, Huang et al. [42] considered the problem about the Kirchhoff index in random alpha-pentachains. Wei and Ke [44] presented a simple formula for the expected value of Kirchhoff index in random generalized polyomino chain. For more details concerning random chain graphs, one may refer to [52–55] and the references cited therein. In this section, we will further consider the Kirchhoff index of random alpha-pentachain and have the following recurrence formula for computing it.

Lemma 1 (see [2]). *Let y be a cut vertex of a connected graph G , and let a and b be vertices occurring in different components which arise upon deletion of y . Then,*

$$r(a, b) = r(a, y) + r(y, b). \quad (7)$$

Lemma 2. *Let P_n^α be an alpha-pentachain of length n , where $n \geq 2$. Then,*

$$Kf(P_n^\alpha) = Kf(P_{n-1}^\alpha) + 5r(v_{n-1}|P_{n-1}^\alpha) + 45n - 35. \quad (8)$$

FIGURE 1: Two types of pentachains considered in this paper: (a) alpha-pentachain; (b) spiro-pentachain.

FIGURE 2: The alpha-pentachains for $n = 1, 2, 3$. FIGURE 3: An alpha-pentachain P_n^α with n pentagons.

Proof. Keeping the notation defined in Figure 3, note that by (1), the resistance distance matrix of the graph induced by $\{v_{n-1}, x_1, x_2, x_3, x_4, x_5\}$ is

$$\begin{pmatrix}
 0 & 1 & \frac{9}{5} & \frac{11}{5} & \frac{11}{5} & \frac{9}{5} \\
 1 & 0 & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} & \frac{4}{5} \\
 \frac{9}{5} & \frac{4}{5} & 0 & \frac{4}{5} & \frac{4}{5} & \frac{6}{5} \\
 \frac{11}{5} & \frac{6}{5} & \frac{4}{5} & 0 & \frac{4}{5} & \frac{6}{5} \\
 \frac{11}{5} & \frac{6}{5} & \frac{4}{5} & \frac{4}{5} & 0 & \frac{4}{5} \\
 \frac{9}{5} & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & 0
 \end{pmatrix}. \quad (9)$$

By Lemma 1 and the matrix above, it is easy to check that

$$r(x_j, v) = \begin{cases} r(v_{n-1}, v) + 1, & \text{for } j = 1, \\ r(v_{n-1}, v) + \frac{9}{5}, & \text{for } j = 2, 5, \\ r(v_{n-1}, v) + \frac{11}{5}, & \text{for } j = 3, 4, \end{cases} \quad (10)$$

for any vertex v of P_{n-1}^α . Also, for a fixed vertex j , we have

$$\sum_{i=1}^5 r(x_j, x_i) = \frac{4}{5} + \frac{6}{5} + \frac{6}{5} + \frac{4}{5} = 4, \quad (11)$$

where $1 \leq j \leq 5$. Note that P_{n-1}^α has $5(n-1)$ vertices. Combining the above formulae, we obtain the following formulae:

$$r(x_1 | P_n^\alpha) = r(v_{n-1} | P_{n-1}^\alpha) + 1 \times 5(n-1) + 4 = r(v_{n-1} | P_{n-1}^\alpha) + 5n - 1, \quad (12)$$

$$r(x_2 | P_n^\alpha) = r(x_5 | P_n^\alpha) = r(v_{n-1} | P_{n-1}^\alpha) + \frac{9}{5} \times 5(n-1) + 4 = r(v_{n-1} | P_{n-1}^\alpha) + 9n - 5,$$

$$r(x_3 | P_n^\alpha) = r(x_4 | P_n^\alpha) = r(v_{n-1} | P_{n-1}^\alpha) + \frac{11}{5} \times 5(n-1) + 4 = r(v_{n-1} | P_{n-1}^\alpha) + 11n - 7. \quad (13)$$

FIGURE 4: Two types of local arrangements in an alpha-pentachain.

Hence,

$$Kf(P_n^\alpha) = Kf(P_{n-1}^\alpha) + 5r(v_{n-1}|P_{n-1}^\alpha) + 45n - 25$$

$$- \frac{1}{2} \sum_{i=1}^5 \sum_{j=1}^5 r(x_i, x_j) \quad (14)$$

$$= Kf(P_{n-1}^\alpha) + 5r(v_{n-1}|P_{n-1}^\alpha) + 45n - 35.$$

This completes the proof.

Note that both $Kf(P_{n;p}^\alpha)$ and $r(v_{n-1}|P_{n-1;p}^\alpha)$ are random variables. For convenience, let $R_{n-1}^\alpha = E[r(v_{n-1}|P_{n-1;p}^\alpha)]$ for $n \geq 2$. We will keep these notations throughout this section. In order to obtain the explicit expression of $E[Kf(P_{n;p}^\alpha)]$, we need to find the explicit expression of R_{n-1}^α from Lemma 2. $\square$

Lemma 3. Let $P_{n;p}^\alpha$ be a random alpha-pentachain of length n , where $n \geq 2$. Then,

$$R_{n-1}^\alpha = p\{E[r(v_{n-2}|P_{n-2;p}^\alpha)] + 9(n-1) - 5\} + (1-p)\{E[r(v_{n-2}|P_{n-2;p}^\alpha)] + 11(n-1) - 7\}. \quad (17)$$

Note that $E[R_{n-1}^\alpha] = R_{n-1}^\alpha$. By applying the expectation operator to the above equation, we get

$$\begin{aligned} R_{n-1}^\alpha &= E[R_{n-1}^\alpha] = E[p(R_{n-2}^\alpha + 9(n-1) - 5) + (1-p)(R_{n-2}^\alpha + 11(n-1) - 7)] \\ &= p(R_{n-2}^\alpha + 9(n-1) - 5) + (1-p)(R_{n-2}^\alpha + 11(n-1) - 7). \end{aligned} \quad (18)$$

That is,

$$R_{n-1}^\alpha = R_{n-2}^\alpha + (11-2p)(n-1) + (2p-7), \quad \text{for } n \geq 3. \quad (19)$$

Note that equation (19) is a first-order nonhomogeneous linear difference equation with constant coefficients. It is clear that the general solution of the homogeneous part of equation (19) is $R^\alpha = c$, a constant.

$$R_{n-1}^\alpha = \left(\frac{11}{2} - p\right)(n-1)^2 + \left(p - \frac{3}{2}\right)(n-1). \quad (15)$$

Proof. When $n = 2$, $P_{1;p}^\alpha$ is isomorphic to a pentagon. So,

$$R_1^\alpha = E[r(v_1|P_{1;p}^\alpha)] = \frac{4}{5} + \frac{6}{5} + \frac{6}{5} + \frac{4}{5} = 4. \quad (16)$$

When $n \geq 3$, there are two cases to be considered as shown in Figure 4. If $P_{n-1}^\alpha \rightarrow P_{n-1}^{\alpha_1}$, then v_{n-1} coincides with the vertex labeled x_2 or x_5 . Consequently, $r(v_{n-1}|P_{n-1;p}^\alpha)$ is given by equation (12). If $P_{n-1}^\alpha \rightarrow P_{n-1}^{\alpha_2}$, then v_{n-1} coincides with the vertex labeled x_3 or x_4 . Consequently, $r(v_{n-1}|P_{n-1;p}^\alpha)$ is given by equation (13). By symmetry, we may only consider v_{n-1} which coincides with the vertex labeled x_{i+1} for $i = 1, 2$.

Recall that the above two cases occur in random alpha-pentachains with probabilities p and $1-p$. From equations $(2 \cdot i)$ ($i = 1, 2$), we obtain that

Let $R^{\alpha*} = (n-1)[a(n-1) + b] = a(n-1)^2 + b(n-1)$ be a particular solution of equation (19). By substituting $R^{\alpha*}$ into equation (19), we have

$$\begin{aligned} a(n-1)^2 + b(n-1) - a(n-2)^2 - b(n-2) \\ = 2a(n-1) + b - a = (11-2p)(n-1) + (2p-7). \end{aligned} \quad (20)$$

By comparing the coefficients of n and the constant term, we have

$$\begin{aligned} a &= \frac{11}{2} - p, \\ b &= p - \frac{3}{2}. \end{aligned} \quad (21)$$

Consequently, the general solution of equation (19) is

$$R_{n-1}^\alpha = R^{\alpha*} + R^\alpha = \left(\frac{11}{2} - p\right)(n-1)^2 + \left(p - \frac{3}{2}\right)(n-1) + c, \quad \text{for } n \geq 2. \quad (22)$$

By substituting the initial condition, we obtain that $c = 0$. Hence, we get the lemma. $\square$

Theorem 2. Let $P_{n,p}^\alpha$ be a random alpha-pentachain of length n , where $n \geq 1$. Then,

$$E[Kf(P_{n,p}^\alpha)] = \left(\frac{55}{6} - \frac{5}{3}p\right)n^3 + (5p+5)n^2 - \left(\frac{10}{3}p + \frac{25}{6}\right)n. \quad (23)$$

Proof. Since P_1^α is unique, E_1 is exactly the Kirchhoff index of P_1^α , namely, $E_1 = Kf(P_1^\alpha) = 10$. So, the theorem holds when $n = 1$. When $n \geq 2$, by Lemmas 2 and 3, we have

$$\begin{aligned} E_n &= E[Kf(P_{n,p}^\alpha)] \\ &= E[Kf(P_{n-1,p}^\alpha) + 5r(v_{n-1}|P_{n-1,p}^\alpha) + 45n - 35] \\ &= E_{n-1} + 5R_{n-1}^\alpha + 45n - 35 \\ &= E_{n-1} + 5\left[\left(\frac{11}{2} - p\right)(n-1)^2 + \left(p - \frac{3}{2}\right)(n-1)\right] + 45n - 35 \\ &= E_{n-1} + \left(\frac{55}{2} - 5p\right)n^2 + \left(15p - \frac{35}{2}\right)n - 10p. \end{aligned} \quad (24)$$

Clearly, $E = c$, a constant, is the general solution for the homogeneous part of equation (24).

Let $E^* = a_0n^3 + a_1n^2 + a_2n$ be a particular solution of equation (24). By substituting E^* into equation (24), we have

$$\begin{aligned} &a_0n^3 + a_1n^2 + a_2n - [a_0(n-1)^3 + a_1(n-1)^2 + a_2(n-1)] \\ &= 3a_0n^2 + (2a_1 - 3a_0)n + (a_0 - a_1 + a_2) \\ &= \left(\frac{55}{2} - 5p\right)n^2 + \left(15p - \frac{35}{2}\right)n - 10p. \end{aligned} \quad (25)$$

By comparing the coefficients of n^i term for $0 \leq i \leq 2$, we have

$$\begin{aligned} a_0 &= \frac{55}{6} - \frac{5}{3}p, \\ a_1 &= 5p + 5, \\ a_2 &= -\frac{10}{3}p - \frac{25}{6}. \end{aligned} \quad (26)$$

Combining the result and the initial condition, we get that the general solution of equation (24) is

$$E_n = E^* + E = \left(\frac{55}{6} - \frac{5}{3}p\right)n^3 + (5p+5)n^2 - \left(\frac{10}{3}p + \frac{25}{6}\right)n. \quad (27)$$

Theorems 1 and 2 show that both the function $E[W(P_{n,p}^\alpha)]$ and $E[Kf(P_{n,p}^\alpha)]$ are asymptotic to a cubic in n and linear in p . In particular, it is easy to obtain the Wiener and Kirchhoff indices of two special alpha-pentachains $P_{n,1}^\alpha$ and $P_{n,0}^\alpha$ when setting $p = 1$ and $p = 0$ from Theorems 1 and 2. $\square$

Corollary 1. The Wiener indices of the alpha-pentachains $P_{n,1}^\alpha$ and $P_{n,0}^\alpha$ are

$$\begin{aligned} W(P_{n,1}^\alpha) &= \frac{25}{3}n^3 + \frac{35}{2}n^2 - \frac{65}{6}n, \\ W(P_{n,0}^\alpha) &= \frac{25}{2}n^3 + 5n^2 - \frac{5}{2}n. \end{aligned} \quad (28)$$

Corollary 2. The Kirchhoff indices of the alpha-pentachains $P_{n,1}^\alpha$ and $P_{n,0}^\alpha$ are

$$\begin{aligned} Kf(P_{n,1}^\alpha) &= \frac{15}{2}n^3 + 10n^2 - \frac{15}{2}n, \\ Kf(P_{n,0}^\alpha) &= \frac{55}{6}n^3 + 5n^2 - \frac{25}{6}n. \end{aligned} \quad (29)$$

Klein and Randić [2] proved that $Kf(G) \leq W(G)$ with equality if and only if G is a tree. Combining Theorem 1 with Theorem 2, we can also verify that $E[Kf(P_{n,p}^\alpha)] < E[W(P_{n,p}^\alpha)]$.

Theorem 3. Let $P_{n,p}^\alpha$ be a random alpha-pentachain. Then,

$$E[Kf(P_{n,p}^\alpha)] < E[W(P_{n,p}^\alpha)]. \quad (30)$$

Proof. By Theorems 1 and 2, we have

$$\begin{aligned} 6E[W(P_{n,p}^\alpha)] - 6E[Kf(P_{n,p}^\alpha)] &= (20 - 20p)n^3 + 45pn^2 + (10 - 30p)n \\ &= (20 - 20p)n^3 + n[(45n - 30)p + 10]. \end{aligned} \quad (31)$$

Since $0 \leq p \leq 1$, $(20 - 20p)n^3 + n[(45n - 30)p + 10] > 0$, which implies that

$$E[Kf(P_{n;p}^\alpha)] < E[W(P_{n;p}^\alpha)]. \quad (32)$$

Hence, this completes the proof. $\square$

3. Wiener and Kirchhoff Indices in Spiro-Pentachains

The notation not defined in this section can be found in Section 2. A spiro-pentachain of length n , denoted by P_n^s , can be obtained from an alpha-pentachain P_n^α by contracting each bridge between each pair of consecutive pentagons in P_n^α . Figure 5 shows a general spiro-pentachain, where v_{n-1} is a vertex of C_{n-1} in P_{n-1}^s . Clearly, P_n^s may not be unique when $n \geq 3$. Corresponding to the structure of alpha-pentachain P_n^α , the spiro-pentachain P_n^s has also two types of local arrangements which are denoted by $P_n^{s_1}$ and $P_n^{s_2}$ (see Figure 6). We may also assume that for getting P_n^s from fixed P_{n-1}^s is a random process, namely, the probability of getting $P_n^{s_1}$ and $P_n^{s_2}$ from fixed P_{n-1}^s is p and $1 - p$, respectively.

We assume that the probability p is constant and independent of n , i.e., the process described above is a zeroth-order Markov process. After associating probabilities, such a spiro-pentachain is called a *random spiro-pentachain* and denoted by $P_{n;p}^s$. In this section, we will consider the Wiener and Kirchhoff indices of random spiro-pentachain.

Lemma 4. Let P_n^s be a spiro-pentachain of length n , where $n \geq 2$. Then, the Wiener index $W(P_n^s)$ of P_n^s is

$$d(x_1|P_n^s) = d(v_{n-1}|P_n^s) = d(v_{n-1}|P_{n-1}^s) + 6, \quad (36)$$

$$d(x_2|P_n^s) = d(x_5|P_n^s) = d(v_{n-1}|P_{n-1}^s) + 4(n-1) + 6 = d(v_{n-1}|P_{n-1}^s) + 4n + 2,$$

$$d(x_3|P_n^s) = d(x_4|P_n^s) = d(v_{n-1}|P_{n-1}^s) + 2 \times 4(n-1) + 6 = d(v_{n-1}|P_{n-1}^s) + 8n - 2. \quad (37)$$

Hence,

$$W(P_n^s) = W(P_{n-1}^s) + 6 + 4 d(v_{n-1}|P_{n-1}^s) + 24n$$

$$- \frac{1}{2} \sum_{i=1}^5 \sum_{j=1}^5 d(x_i, x_j) \quad (38)$$

$$= W(P_{n-1}^s) + 4 d(v_{n-1}|P_{n-1}^s) + 24n - 9.$$

This completes the proof.

Note that both $W(P_{n;p}^s)$ and $r(v_{n-1}|P_{n-1;p}^s)$ are also random variables. In order to obtain the explicit expression of $E[W(P_{n;p}^s)]$, we need to find the explicit expression of $D_{n-1}^s \triangleq E[d(v_{n-1}|P_{n-1}^s)]$ for $n \geq 2$ from Lemma 4. $\square$

Lemma 5. Let $P_{n;p}^s$ be a random spiro-pentachain of length n , where $n \geq 2$. Then,

FIGURE 5: A spiro-pentachain P_n^s with n pentagons.

$$W(P_{n-1}^s) + 4 d(v_{n-1}|P_{n-1}^s) + 24n - 9. \quad (33)$$

Proof. Keeping the notation defined in Figure 5, it is easy to check that

$$d(x_j, v) = \begin{cases} d(v_{n-1}, v), & \text{for } j = 1, \\ d(v_{n-1}, v) + 1, & \text{for } j = 2, 5, \\ d(v_{n-1}, v) + 2, & \text{for } j = 3, 4, \end{cases} \quad (34)$$

for any vertex v of P_{n-1}^s . Also, for a fixed vertex j , we have

$$\sum_{i=1}^5 d(x_j, x_i) = 1 + 1 + 2 + 2 = 6, \quad (35)$$

where $1 \leq j \leq 5$. Note that P_{n-1}^s has $5(n-1) - (n-2) = 4n - 3$ vertices and x_1 coincides with v_{n-1} in P_{n-1}^s . Combining the above formulae, we obtain the following formulae:

$$D_{n-1}^s = (4 - 2p)(n-1)^2 + (2p+2)(n-1). \quad (39)$$

Proof. When $n = 2$, $P_{1;p}^s$ is isomorphic to a pentagon. So,

$$D_1^s = E[d(v_1|P_{1;p}^s)] = 6. \quad (40)$$

When $n \geq 3$, there are two cases to be considered as shown in Figure 6. If $P_{n-1}^s \rightarrow P_{n-1}^{s_1}$, then v_{n-1} coincides with the vertex labeled x_2 or x_5 . Consequently, $d(v_{n-1}|P_{n-1;p}^s)$ is given by equation (36). If $P_{n-1}^s \rightarrow P_{n-1}^{s_2}$, then v_{n-1} coincides with the vertex labeled x_3 or x_4 . Consequently, $d(v_{n-1}|P_{n-1;p}^s)$ is given by equation (37). By symmetry, we may only consider v_{n-1} which coincides with the vertex labeled x_{i+1} for $i = 1, 2$.

Recall that the above two cases occur in random spiro-pentachains with probabilities p and $1 - p$. From equations (3·i) ($i = 1, 2$), we obtain that

FIGURE 6: Two types of local arrangements in a spiro-pentachain.

$$D_{n-1}^s = p\{E[d(v_{n-2}|P_{n-2;p}^s)] + 4(n-1) + 2\} + (1-p)\{E[d(v_{n-2}|P_{n-2;p}^s)] + 8(n-1) - 2\}. \quad (41)$$

Note that $E[D_{n-1}^s] = D_{n-1}^s$. By applying the expectation operator to the above equation, we get

$$\begin{aligned} D_{n-1}^s &= E[D_{n-1}^s] = E[p(D_{n-2}^s + 4(n-1) + 2) + (1-p)(D_{n-2}^s + 8(n-1) - 2)] \\ &= p[D_{n-2}^s + 4(n-1) + 2] + (1-p)[D_{n-2}^s + 8(n-1) - 2]. \end{aligned} \quad (42)$$

That is,

$$D_{n-1}^s = D_{n-2}^s + (8-4p)(n-1) + (4p-2), \quad \text{for } n \geq 2. \quad (43)$$

Using recurrence relation (43) and the initial condition, we have

$$D_{n-1}^s = (4-2p)(n-1)^2 + (2p+2)(n-1). \quad (44)$$

Hence, we get the lemma. $\square$

Theorem 4. Let $P_{n;p}^s$ be a random spiro-pentachain of length n , where $n \geq 1$. Then,

$$E[W(P_{n;p}^s)] = \left(\frac{16}{3} - \frac{8}{3}p\right)n^3 + (8p+8)n^2 + \left(\frac{5}{3} - \frac{16}{3}p\right)n. \quad (45)$$

Proof. For convenience, let $E_n^w = E[W(P_{n;p}^s)]$. Since P_1^s is unique, E_1^w is exactly the Wiener index of P_1^s , namely, $E_1^w = W(P_1^s) = 15$. So, the theorem holds when $n = 1$. When $n \geq 2$, by Lemmas 4 and 5, we have

$$\begin{aligned} E_n^w &= E[W(P_{n;p}^s)] \\ &= E[W(P_{n-1;p}^s) + 4d(v_{n-1}|P_{n-1;p}^s) + 24n - 9] \\ &= E_{n-1}^w + 4D_{n-1}^s + 24n - 9 \\ &= E_{n-1}^w + 4[(4-2p)(n-1)^2 + (2p+2)(n-1)] + 24n - 9 \\ &= E_{n-1}^w + (16-8p)n^2 + 24pn - (1+16p). \end{aligned} \quad (46)$$

Using recurrence relation (46) and the initial condition, we have

$$E[W(P_{n;p}^s)] = \left(\frac{16}{3} - \frac{8}{3}p\right)n^3 + (8p+8)n^2 + \left(\frac{5}{3} - \frac{16}{3}p\right)n. \quad (47)$$

We now give the formula for the expected value of the Kirchhoff index of a random spiro-pentachain. $\square$

Lemma 6. Let P_n^s be a spiro-pentachain of length n , where $n \geq 2$. Then,

$$Kf(P_n^s) = Kf(P_{n-1}^s) + 4r(v_{n-1}|P_{n-1}^s) + 16n - 6. \quad (48)$$

Proof. Keeping the notation defined in Figure 5, note that the resistance distance matrix of the graph induced by $\{x_1, x_2, x_3, x_4, x_5\}$ is

$$\begin{pmatrix} 0 & \frac{4}{5} & \frac{6}{5} & \frac{6}{5} & \frac{4}{5} \\ \frac{4}{5} & 0 & \frac{6}{5} & \frac{6}{5} & \frac{4}{5} \\ \frac{6}{5} & \frac{4}{5} & 0 & \frac{4}{5} & \frac{6}{5} \\ \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & 0 & \frac{4}{5} \\ \frac{4}{5} & \frac{6}{5} & \frac{6}{5} & \frac{4}{5} & 0 \end{pmatrix}, \quad (49)$$

by (1). By Lemma 1 and the matrix above, it is easy to check that

$$r(x_j, v) = \begin{cases} r(v_{n-1}, v), & \text{for } j = 1, \\ r(v_{n-1}, v) + \frac{4}{5}, & \text{for } j = 2, 5, \\ r(v_{n-1}, v) + \frac{6}{5}, & \text{for } j = 3, 4, \end{cases} \quad (50)$$

for any vertex v in P_{n-1}^s . From the proof of Lemma 2, we have

$$\sum_{i=1}^5 r(x_j, x_i) = 4, \quad (51)$$

for a fixed j , $1 \leq j \leq 5$. Note that P_{n-1}^s has $5(n-1) - (n-2) = 4n-3$ vertices and x_1 coincides with v_{n-1} in P_{n-1}^s . Combining the formulae above, we obtain the following formulae:

$$\begin{aligned} r(x_1|P_n^s) &= r(v_{n-1}|P_n^s) = r(v_{n-1}|P_{n-1}^s) + 4, \\ r(x_2|P_n^s) &= r(x_5|P_n^s) = r(v_{n-1}|P_{n-1}^s) + \frac{4}{5} \times 4(n-1) + 4 \\ &= r(v_{n-1}|P_{n-1}^s) + \frac{4}{5}(4n+1), \end{aligned} \quad (52)$$

$$\begin{aligned} r(x_3|P_n^s) &= r(x_4|P_n^s) = r(v_{n-1}|P_{n-1}^s) + \frac{6}{5} \times 4(n-1) + 4 \\ &= r(v_{n-1}|P_{n-1}^s) + \frac{4}{5}(6n-1). \end{aligned} \quad (53)$$

Hence,

$$\begin{aligned} Kf(P_n^s) &= Kf(P_{n-1}^s) + 4 + \left[r(v_{n-1}|P_{n-1}^s) + \frac{4}{5}(4n+1) \right] \times 2 \\ &\quad + \left[r(v_{n-1}|P_{n-1}^s) + \frac{4}{5}(6n-1) \right] \times 2 - \frac{1}{2} \sum_{i=1}^5 \sum_{j=1}^5 r(x_i, x_j) \\ &= Kf(P_{n-1}^s) + 4r(v_{n-1}|P_{n-1}^s) + 16n - 6. \end{aligned} \quad (54)$$

This completes the proof. $\square$

Lemma 7. Let $P_{n;p}^s$ be a random spiro-pentachain of length n , where $n \geq 2$. Then,

$$R_{n-1}^s = \frac{4}{5}(3-p)(n-1)^2 + \frac{4}{5}(2+p)(n-1), \quad (55)$$

where $R_{n-1}^s = E[r(v_{n-1}|P_{n-1;p}^s)]$.

Proof. When $n = 2$,

$$R_1^s = E[r(v_1|P_{1;p}^s)] = \frac{4}{5} + \frac{6}{5} + \frac{6}{5} + \frac{4}{5} = 4. \quad (56)$$

When $n \geq 3$, there are two cases to be considered as shown in Figure 6. If $P_{n-1}^s \rightarrow P_n^{s_1}$, then v_{n-1} coincides with the vertex labeled x_2 or x_5 . Consequently, $r(v_{n-1}|P_{n-1;p}^s)$ is given by equation (52). If $P_{n-1}^s \rightarrow P_n^{s_2}$, then v_{n-1} coincides with the vertex labeled x_3 or x_4 . Consequently, $r(v_{n-1}|P_{n-1;p}^s)$ is given by equation (53). By symmetry, we may only consider v_{n-1} which coincides with the vertex labeled x_{i+1} for $i = 1, 2$.

Recall that the above two cases occur in random spiro-pentachains with probabilities p and $1-p$. From equations (3·i) ($i = 5, 6$), we obtain that

$$R_{n-1}^s = E\left\{p\left[r(v_{n-2}|P_{n-2;p}^s) + \frac{4}{5}[4(n-1)+1]\right] + (1-p)\left[r(v_{n-2}|P_{n-2;p}^s) + \frac{4}{5}[6(n-1)-1]\right]\right\}. \quad (57)$$

By applying the expectation operator to the above equation, we get

$$R_{n-1}^s = R_{n-2}^s + \frac{8}{5}(3-p)(n-1) + \frac{4}{5}(2p-1), \quad \text{for } n \geq 2. \quad (58)$$

Using recurrence relation (58) and the initial condition, we have

$$R_{n-1}^s = \frac{4}{5}(3-p)(n-1)^2 + \frac{4}{5}(2+p)(n-1). \quad (59)$$

Hence, we get the lemma.

Similar to the proof in Theorem 2, now we have the following result by Lemmas 6 and 7. $\square$

Theorem 5. Let $P_{n;p}^s$ be a random spiro-pentachain of length n , where $n \geq 1$. Then,

$$E[Kf(P_{n;p}^s)] = \frac{16}{15}(3-p)n^3 + \frac{16}{5}(2+p)n^2 + \frac{2}{15}(3-16p)n. \quad (60)$$

Similarly, Theorems 4 and 5 show that both the functions $E[W(P_{n;p}^s)]$ and $E[Kf(P_{n;p}^s)]$ are asymptotic to a cubic in n and linear in p . Then, we easily get the Wiener and Kirchhoff indices of two special spiro-pentachains $P_{n;1}^s$ and $P_{n;0}^s$ when setting $p = 1$ and $p = 0$ from Theorems 4 and 5.

Corollary 3. The Wiener indices of the spiro-pentachains $P_{n;1}^s$ and $P_{n;0}^s$ are

$$\begin{aligned} W(P_{n;1}^s) &= \frac{8}{3}n^3 + 16n^2 - \frac{11}{3}n, \\ W(P_{n;0}^s) &= \frac{16}{3}n^3 + 8n^2 + \frac{5}{3}n. \end{aligned} \quad (61)$$

Corollary 4. The Kirchhoff indices of the spiro-pentachains $P_{n;1}^s$ and $P_{n;0}^s$ are

$$\begin{aligned} Kf(P_{n;1}^s) &= \frac{32}{15}n^3 + \frac{48}{5}n^2 - \frac{26}{15}n, \\ Kf(P_{n;0}^s) &= \frac{48}{15}n^3 + \frac{32}{5}n^2 + \frac{2}{5}n. \end{aligned} \quad (62)$$

By Theorems 4 and 5, similar to Theorem 3, we also have the following result.

Theorem 6. Let $P_{n;p}^s$ be a random spiro-pentachain. Then,

$$E[Kf(P_{n;p}^s)] < E[W(P_{n;p}^s)]. \quad (63)$$

4. The Average Values of the Kirchhoff and Wiener Indices in Random Pentachains

In this section, we present the average values of the Kirchhoff and Wiener indices in random pentachains with respect to the set of all alpha-pentachains and all spiro-pentachains with n

pentagons. Let $\mathcal{P}_n^\alpha$ and $\mathcal{P}_n^s$ be the sets of all alpha-pentachains and all spiro-pentachains with n pentagons. The average values of Wiener indices of $\mathcal{P}_n^\alpha$ and $\mathcal{P}_n^s$ are defined by

$$W_{\text{avr}}(\mathcal{P}_n^\alpha) = \frac{1}{|\mathcal{P}_n^\alpha|} \sum_{G \in \mathcal{P}_n^\alpha} W(G), \quad (64)$$

$$W_{\text{avr}}(\mathcal{P}_n^s) = \frac{1}{|\mathcal{P}_n^s|} \sum_{G \in \mathcal{P}_n^s} W(G),$$

respectively. Similarly, the average values of Kirchhoff indices of $\mathcal{P}_n^\alpha$ and $\mathcal{P}_n^s$ are defined by

$$Kf_{\text{avr}}(\mathcal{P}_n^\alpha) = \frac{1}{|\mathcal{P}_n^\alpha|} \sum_{G \in \mathcal{P}_n^\alpha} Kf(G), \quad (65)$$

$$Kf_{\text{avr}}(\mathcal{P}_n^s) = \frac{1}{|\mathcal{P}_n^s|} \sum_{G \in \mathcal{P}_n^s} Kf(G),$$

respectively.

Actually, these are the population means of the Wiener and Kirchhoff indices of all elements in $\mathcal{P}_n^\alpha$ or $\mathcal{P}_n^s$. Since every element occurring in $\mathcal{P}_n^\alpha$ or $\mathcal{P}_n^s$ has the same probability, we have $p = 1 - p$. Thus, we may apply Theorems 1, 2, 4, and 5 by putting $p = 1 - p = (1/2)$ and obtain the following results.

Theorem 7. The average values of the Wiener indices with respect to $\mathcal{P}_n^s$ and $\mathcal{P}_n^\alpha$ are

$$\begin{aligned} W_{\text{avr}}(\mathcal{P}_n^\alpha) &= \frac{125}{12}n^3 + \frac{45}{4}n^2 - \frac{20}{3}n, \\ W_{\text{avr}}(\mathcal{P}_n^s) &= 4n^3 + 12n^2 - n. \end{aligned} \quad (66)$$

Theorem 8. The average values of the Kirchhoff indices with respect to $\mathcal{P}_n^s$ and $\mathcal{P}_n^\alpha$ are

$$\begin{aligned} Kf_{\text{avr}}(\mathcal{P}_n^\alpha) &= \frac{25}{3}n^3 + \frac{15}{2}n^2 - \frac{35}{6}n, \\ Kf_{\text{avr}}(\mathcal{P}_n^s) &= 4n^3 + 12n^2 - n. \end{aligned} \quad (67)$$

It is not difficult to note that the average values of the Wiener indices with respect to $\{P_{n;1}^\alpha, P_{n;0}^\alpha\}$ and $\{P_{n;1}^s, P_{n;0}^s\}$ are

$$\begin{aligned} \frac{W(P_{n;1}^\alpha) + W(P_{n;0}^\alpha)}{2} &= \frac{125}{12}n^3 + \frac{45}{4}n^2 - \frac{20}{3}n, \\ \frac{W(P_{n;1}^s) + W(P_{n;0}^s)}{2} &= \frac{8}{3}n^3 + 8n^2 - \frac{2}{3}n, \end{aligned} \quad (68)$$

from Corollaries 1 and 3 and Theorem 8. We also can find that the average values of the Kirchhoff indices with respect to $\{P_{n;1}^\alpha, P_{n;0}^\alpha\}$ and $\{P_{n;1}^s, P_{n;0}^s\}$ are

$$\frac{Kf(P_{n,1}^\alpha) + Kf(P_{n,0}^\alpha)}{2} = \frac{25}{3}n^3 + \frac{15}{2}n^2 - \frac{35}{6}n, \quad (69)$$

$$\frac{Kf(P_{n,1}^s) + Kf(P_{n,0}^s)}{2} = \frac{8}{3}n^3 + 8n^2 - \frac{2}{3}n,$$

from Corollaries 2 and 4 and Theorem 8. The interesting results show that both the average values of the Wiener indices and the average values of the Kirchhoff indices with respect to $\mathcal{P}_n^\alpha$ and $\mathcal{P}_n^s$ are exactly equal to the average value of the Wiener and Kirchhoff indices with respect to $\{P_{n,1}^\alpha, P_{n,0}^\alpha\}$ and $\{P_{n,1}^s, P_{n,0}^s\}$, respectively.

Data Availability

No data were used to support this study.

Conflicts of Interest

The authors declare that they have no potential conflicts of interest.

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