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The expected values of Kirchhoff indices in the random polyphenyl and spiro chains*

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Abstract

The Kirchhoff index $Kf(G)$ of a graph G is the sum of resistance distances between all pairs of vertices in G. In this paper, we obtain exact formulas for the expected values of the Kirchhoff indices of the random polyphenyl and spiro chains, which are graphs of a class of unbranched multispiro molecules and polycyclic aromatic hydrocarbons. Moreover, we obtain a relation between the expected values of the Kirchhoff indices of a random polyphenyl and its random hexagonal squeeze, and the average values for the Kirchhoff indices of all polyphenyl chains and all spiro chains with n hexagons, respectively.

Keywords: Expected value, average value, Kirchhoff index, resistance distance, polyphenyl chain, spiro chain.

Math. Subj. Class.: 05C12, 05C80, 05C90, 05D40

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1 Introduction

Based on the electrical network theory, Klein and Randić [13] introduced the concept of resistance distance. A connected graph G with vertex set $\{v_1, v_2, \cdots, v_n\}$ is viewed as an electrical network N by replacing each edge of G with a unit resistor, the resistance distance between v_i and v_j, denoted by $r_G(v_i, v_j)$ or $r(v_i, v_j)$, is the elective resistance between them as computed by the methods of the theory of resistive electrical networks based on Ohm's and Kirchhoff's laws in N.

The Kirchhoff index of G, denoted by $Kf(G)$, is the sum of resistance distances between all pairs of vertices in G, namely,

$$Kf(G) = \sum_{i<j} r_G(v_i, v_j)$$

Like many topological indices, Kirchhoff index is a structure descriptor. The resistance distance is also intrinsic to the graph with some nice purely mathematical and physical interpretations [14] [15]. Also, the Kirchhoff index has been found very useful in chemistry, such as in assessing cyclicity of polycyclic structures including fullerenes, linear hexagonal chains and some special molecular graphs such as circulant graphs, distance-regular graphs and Möbius ladders [1] [18] [22] [24]. Bonchev et al. [4] used it in polymer science and found that the Kirchhoff index in their approach is especially useful for defining the topological radius $R_{top} = \frac{Kf}{n^2}$ of macromolecules containing cyclic fragments. Some closed-form formulae for Kirchhoff index have been given for circulant graphs, linear hexagonal chains and so on [1] [16] [19] [22]. The resistance distance is also well studied in mathematical literatures. Much work has been done to compute Kirchhoff index of some classes of graphs, or give some bounds for Kirchhoff index of graphs and characterize extremal graphs. For instance, unicyclic and bicyclic graphs with extremal Kirchhoff index are characterized and sharp bounds for Kirchhoff index of such graphs are obtained [6] [12] [21] [25] [26].

Polyphenyls and their derivatives, which can be used in organic synthesis, drug synthesis, heat exchangers, etc., attracted the attention of chemists for many years [11] [17] [20]. Spiro compounds are an important class of cycloalkanes in organic chemistry. A spiro union in spiro compounds is a linkage between two rings that consists of a single atom common to both rings and a free spiro union is a linkage that consists of the only direct union between the rings. Some results on energy, Merrifield-Simmons index, Hosoya index and Wiener index of the spiro and polyphenyl chains were reported in [2] [5] [9] [27]. Recently, Deng [7] [8] [10] gave the recurrences or explicit formulae for computing the Wiener index and Kirchhoff index of spiro and polyphenyl chains. Yang and Zhang [23] obtained a simple exact formula for the expected value of the Wiener index of a random polyphenyl chain. In this paper, we will consider the expected values of the Kirchhoff index of random polyphenyl and spiro chains.

A polyphenyl chain PPC_n with n hexagons can be regarded as a polyphenyl chain PPC_{n-1} with $n-1$ hexagons to which a new terminal hexagon has been adjoined by a cut edge, see Figure 1.

Let $PPC_n = H_1 H_2 \cdots H_n$ be a polyphenyl chain with $n (n \geq 2)$ hexagons, where H_k is the k-th hexagon of PPC_n attached to H_{k-1} by a cut edge $u_{k-1}c_k$, $k = 2, 3, \cdots, n$. A vertex v of H_k is said to be ortho-, meta- and para-vertex of H_k if the distance between v and c_k is 1, 2 and 3, denoted by o_k, m_k and p_k, respectively. Examples of ortho-, meta-, and para-vertices are shown in Figure 1. Except the first hexagon, any hexagon in a polyphenyl chain has two ortho-vertices, two meta-vertices and one para-vertex.

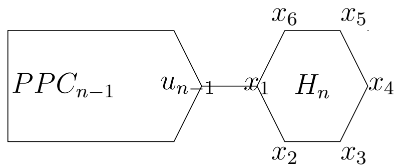

Figure 1: A polyphenyl chain PPC_n with n hexagons, $c_n = x_1$ and ortho-vertices $o_n = x_2, x_6$, meta-vertices $m_n = x_3, x_5$, and para-vertex $p_n = x_4$ in H_n.

A polyphenyl chain PPC_n is a polyphenyl ortho-chain if $u_k = o_k$ for $2 \le k \le n-1$. A polyphenyl chain PPC_n is a polyphenyl meta-chain if $u_k = m_k$ for $2 \le k \le n-1$. A polyphenyl chain PPC_n is a polyphenyl para-chain if $u_k = p_k$ for $2 \le k \le n-1$. The polyphenyl ortho-, meta- and para-chain with n hexagons are denoted by $\overline{O_n}$, $\overline{M_n}$ and $\overline{P_n}$, respectively.

For $n \ge 3$, the terminal hexagon can be attached to meta-, ortho-, or para-vertex in three ways, which results in the local arrangements we describe as PPC^1_{n+1}, PPC^2_{n+1}, PPC^3_{n+1}, see Figure 2.

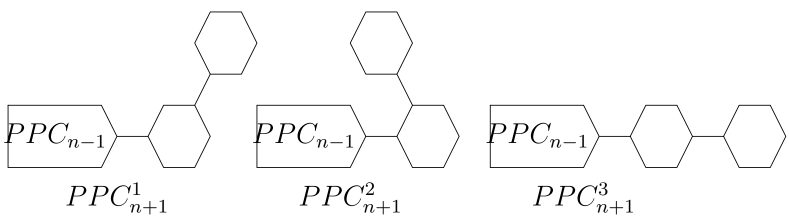

Figure 2: The three types of local arrangements in polyphenyl chains.

A random polyphenyl chain $PPC(n, p_1, p_2)$ with n hexagons is a polyphenyl chain obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \cdots, n)$, a random selection is made from one of the three possible constructions:

(i)$PPC_{k-1} \rightarrow PPC^1_k$ with probability p_1,

(ii)$PPC_{k-1} \rightarrow PPC^2_k$ with probability p_2,

(iii)$PPC_{k-1} \rightarrow PPC^3_k$ with probability $1 - p_1 - p_2$

where the probabilities p_1 and p_2 are constants, irrespective to the step parameter k.

Specially, the random polyphenyl chain $PPC(n, 1, 0)$ is the polyphenyl meta-chain $\overline{M_n}$, $PPC(n, 0, 1)$ is the polyphenyl orth-chain $\overline{O_n}$, and $PPC(n, 0, 0)$ is the polyphenyl para-chain $\overline{P_n}$, respectively.

Also, a spiro chain SPC_n with n hexagons can be regarded as a spiro chain SPC_{n-1} with $n-1$ hexagons to which a new terminal hexagon has been adjoined, see Figure 3.

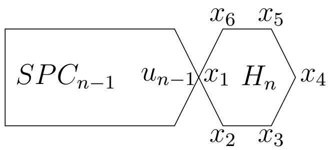

Figure 3: A spiro chain SPC_n with n hexagons.

For $n \geq 3$, the terminal hexagon can also be attached in three ways, which results in the local arrangements we describe as SPC^1_{n+1}, SPC^2_{n+1}, SPC^3_{n+1}, see Figure 4.

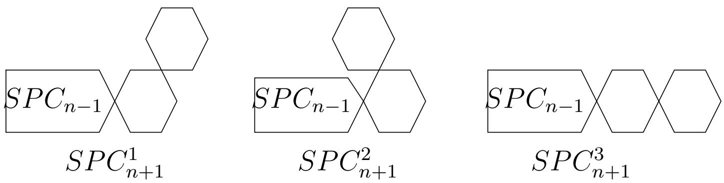

Figure 4: The three types of local arrangements in spiro chains.

A random spiro chain $SPC(n, p_1, p_2)$ with n hexagons is a spiro chain obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \cdots, n)$, a random selection is made from one of the three possible constructions:

(i)$SPC_{k-1} \to SPC^1_k$ with probability p_1,

(ii)$SPC_{k-1} \to SPC^2_k$ with probability p_2,

(iii)$SPC_{k-1} \to SPC^3_k$ with probability $1 - p_1 - p_2$

where the probabilities p_1 and p_2 are constants, irrelative to the step parameter k.

Similarly, the random spiro chain $SPC(n, 1, 0)$, $PPC(n, 0, 1)$ and $PPC(n, 0, 0)$ are the spiro meta-chain M_n, the spiro orth-chain O_n and the spiro para-chain P_n, respectively.

For a random polyphenyl chain $PPC(n, p_1, p_2)$ and a random spiro chain $SPC(n, p_1, p_2)$, their Kirchhoff indices are random variables. In this paper, we will obtain exact formulas for the expected values $E(Kf(PPC(n, p_1, p_2)))$ and $E(Kf(SPC(n, p_1, p_2)))$ of the Kirchhoff indices of random polyphenyl and spiro chains, respectively.

2 Main results

2.1 The Kirchhoff index of the random polyphenyl chain

In this section, we will consider the Kirchhoff index of the random polyphenyl chain.

Theorem 2.1. *For $n \geq 1$, the expected value of the Kirchhoff index of the random polyphenyl chain $PPC(n, p_1, p_2)$ is*

$$E(Kf(PPC(n, p_1, p_2))) = (15 - p_1 - 4p_2)n^3 + (3p_1 + 12p_2 + 8)n^2 - (2p_1 + 8p_2 + \frac{11}{2})n$$

Proof. Note that the polyphenyl chain PPC_n is obtained by attaching PPC_{n-1} a new terminal hexagon by an edge, we suppose that the terminal hexagon is spanned by vertices $x_1, x_2, x_3, x_4, x_5, x_6$, and the new edge is $u_{n-1}x_1$ (see Fig.1). Then

(i) For any $v \in PPC_{n-1}$,

$r(x_1, v) = r(u_{n-1}, v) + 1, r(x_2, v) = r(u_{n-1}, v) + 1 + \frac{5}{6},$
$r(x_3, v) = r(u_{n-1}, v) + 1 + \frac{4}{3}, r(x_4, v) = r(u_{n-1}, v) + 1 + \frac{3}{2},$
$r(x_5, v) = r(u_{n-1}, v) + 1 + \frac{4}{3}, r(x_6, v) = r(u_{n-1}, v) + 1 + \frac{5}{6};$
(ii) PPC_{n-1} has $6(n-1)$ vertices;
(iii) For $k \in \{1, 2, 3, 4, 5, 6\}$, $\sum_{i=1}^{6} r(x_k, x_i) = \frac{35}{6}$.

So, we have
$r(x_1|PPC_n) = r(u_{n-1}|PPC_{n-1}) + 1 \times 6(n-1) + \frac{35}{6}$
$r(x_2|PPC_n) = r(u_{n-1}|PPC_{n-1}) + (1 + \frac{5}{6}) \times 6(n-1) + \frac{35}{6}$
$r(x_3|PPC_n) = r(u_{n-1}|PPC_{n-1}) + (1 + \frac{4}{3}) \times 6(n-1) + \frac{35}{6}$
$r(x_4|PPC_n) = r(u_{n-1}|PPC_{n-1}) + (1 + \frac{3}{2}) \times 6(n-1) + \frac{35}{6}$
$r(x_5|PPC_n) = r(x_3|PPC_{n-1})$
$r(x_6|PPC_n) = r(x_2|PPC_{n-1})$
where $r(x|G) = \sum_{y \in V(G)} r(x, y)$, and

$$\begin{aligned} Kf(PPC_n) &= Kf(PPC_{n-1}) + 6r(u_{n-1}|PPC_{n-1}) + 71n - 36 - \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} r(v_i, v_j) \\ &= Kf(PPC_{n-1}) + 6r(u_{n-1}|PPC_{n-1}) + 71n - 36 - \frac{35}{2} \end{aligned}$$

Then

$$Kf(PPC_{n+1}) = Kf(PPC_n) + 6r(u_n|PPC_n) + 71n + \frac{35}{2} \tag{2.1}$$

For a random polyphenyl chain $PPC(n, p_1, p_2)$, the resistance number $r(u_n|PPC(n, p_1, p_2))$ is a random variable, and its expected value is denoted by

$$U_n = E(r(u_n|PPC(n, p_1, p_2))).$$

By the expectation operator and (1), we can obtain a recursive relation for the expected value of the Kirchhoff number of a random polyphenyl chain $PPC(n, p_1, p_2)$

$$E(Kf(PPC(n+1, p_1, p_2)) = E(Kf(PPC(n, p_1, p_2))) + 6U_n + 71n + \frac{35}{2} \tag{2.2}$$

Now, we consider computing U_n.

(i) If $PPC_n \to PPC_{n+1}^1$ with probability p_1, then u_n coincides with the vertex x_3 or x_5. Consequently, $r(u_n|PPC_n)$ is given by $r(x_3|PPC_n)$ with probability p_1.

(ii) If $PPC_n \to PPC_{n+1}^2$ with probability p_2, then u_n coincides with the vertex x_2 or x_6. Consequently, $r(u_n|PPC_n)$ is given $r(x_2|PPC_n)$ with probability p_2.

(iii) If $PPC_n \to PPC_{n+1}^3$ with probability $1 - p_1 - p_2$, then u_n coincides with the vertex x_4. Consequently, $r(u_n|PPC_n)$ is given by $r(x_4|PPC_n)$ with probability $1 - p_1 - p_2$.

From (i)-(iii) above, we immediately obtain

$$
\begin{aligned}
U_n =& r(x_3|PPC_n)p_1 + r(x_2|PPC_n)p_2 + r(x_4|PPC_n)(1-p_1-p_2) \\
=& p_1[r(u_{n-1}|PPC(n-1,p_1,p_2)) + 14(n-1) + \frac{35}{6}] \\
&+ p_2[r(u_{n-1}|PPC(n-1,p_1,p_2)) + 11(n-1) + \frac{35}{6}] \\
&+ (1-p_1-p_2)[r(u_{n-1}|PPC(n-1,p_1,p_2)) + 15(n-1) + \frac{35}{6}]
\end{aligned}
$$

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

$$
U_n = U_{n-1} + (15 - p_1 - 4p_2)n + p_1 + 4p_2 - \frac{55}{6}
$$

And $U_1 = E(r(u_1|PPC(1,p_1,p_2))) = \frac{35}{6}$, using the above recurrence relation, we have

$$
U_n = \frac{(15-p_1-4p_2)}{2}n^2 + (\frac{p_1}{2} + 2p_2 - \frac{5}{3})n
$$

From (2),

$$
\begin{aligned}
&E(Kf(PPC(n+1,p_1,p_2)) \\
&= E(Kf(PPC(n,p_1,p_2))) + 6[\tfrac{(15-p_1-4p_2)}{2}n^2 + (\tfrac{p_1}{2} + 2p_2 - \tfrac{5}{3})n] + 71n + \tfrac{35}{2} \\
&= E(Kf(PPC(n,p_1,p_2))) + (45 - 3p_1 - 12p_2)n^2 + (3p_1 + 12p_2 + 61)n + \tfrac{35}{2}
\end{aligned}
$$

and $E(Kf(PPC(1,p_1,p_2))) = \frac{35}{2}$.

Using the above recurrence relation, we have

$$
E(Kf(PPC(n,p_1,p_2))) = (15-p_1-4p_2)n^3 + (3p_1+12p_2+8)n^2 - (2p_1+8p_2+\frac{11}{2})n.
$$

□

Specially, by taking $(p_1,p_2) = (1,0),(0,1)$ or $(0,0)$, respectively, and Theorem 2.1, we have

Corollary 2.2. *([8]) The Kirchhoff indices of the polyphenyl meta-chain $\overline{M_n}$, the polyphenyl ortho-chain $\overline{O_n}$ and the polyphenyl para-chain $\overline{P_n}$ are*

$$
Kf(\overline{M_n}) = 14n^3 + 11n^2 - \frac{15}{2}n
$$

$$
Kf(\overline{O_n}) = 11n^3 + 20n^2 - \frac{27}{2}n
$$

$$
Kf(\overline{P_n}) = 15n^3 + 8n^2 - \frac{11}{2}n
$$

2.2 The Kirchhoff index of the random spiro chain

In this section, we will consider the Kirchhoff index of the random spiro chain.

Theorem 2.3. *For $n \geq 1$, the expected value of the Kirchhoff index of the random spiro chain $SPC(n, p_1, p_2)$ is*

$$E(Kf(SPC(n,p_1,p_2))) = (\frac{25}{4} - \frac{25}{36}p_1 - \frac{25}{9}p_2)n^3 + (\frac{25}{12}p_1 + \frac{25}{3}p_2 + \frac{125}{12})n^2 - (\frac{25}{18}p_1 + \frac{50}{9}p_2 - \frac{5}{6})n.$$

Proof. Note that the spiro chain SPC_n is obtained by attaching SPC_{n-1} a new terminal hexagon, we suppose that the terminal hexagon is spanned by vertices x_1, x_2, x_3, x_4, x_5, x_6, and the vertex x_1 is u_{n-1} (see Fig.3). Then

(i) For any $v \in SPC_{n-1}$,
$r(x_1, v) = r(u_{n-1}, v)$, $r(x_2, v) = r(u_{n-1}, v) + \frac{5}{6}$,
$r(x_3, v) = r(u_{n-1}, v) + \frac{4}{3}$, $r(x_4, v) = r(u_{n-1}, v) + \frac{3}{2}$,
$r(x_5, v) = r(u_{n-1}, v) + \frac{4}{3}$, $r(x_6, v) = r(u_{n-1}, v) + \frac{5}{6}$;
(ii) SPC_{n-1} has $5(n-1)+1$ vertices;
(iii) For $k \in \{1,2,3,4,5,6\}$, $\sum_{i=1}^{6} r(x_k, x_i) = \frac{35}{6}$.

So, we have
$r(x_1|SPC_n) = r(u_{n-1}|SPC_{n-1}) + \frac{35}{6}$
$r(x_2|SPC_n) = r(u_{n-1}|SPC_{n-1}) + \frac{5}{6}\times(5n-4) + \frac{5}{6} + \frac{4}{3} + \frac{3}{2} + \frac{4}{3} = r(u_{n-1}|SPC_{n-1}) + \frac{25}{6}\times(n-1) + \frac{35}{6}$
$r(x_3|SPC_n) = r(u_{n-1}|SPC_{n-1}) + \frac{20}{3}\times(n-1) + \frac{35}{6}$
$r(x_4|SPC_n) = r(u_{n-1}|SPC_{n-1}) + \frac{15}{2}\times(n-1) + \frac{35}{6}$
$r(x_5|SPC_n) = r(x_3|SPC_{n-1})$
$r(x_6|SPC_n) = r(x_2|SPC_{n-1})$
where $r(x|G) = \sum_{y \in V(G)} r(x, y)$, and

$$\begin{aligned} Kf(SPC_n) &= Kf(SPC_{n-1}) + 5r(u_{n-1}|SPC_{n-1}) + \\ &\quad \frac{175(n-1)}{6} + 35 - \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6} r(v_i, v_j) \\ &= Kf(SPC_{n-1}) + 5r(u_{n-1}|SPC_{n-1}) + \frac{175n}{6} - \frac{35}{3} \end{aligned} \tag{2.3}$$

Then

$$Kf(SPC_{n+1}) = Kf(SPC_n) + 5r(u_n|SPC_n) + \frac{175n}{6} + \frac{35}{2} \tag{2.4}$$

For a random spiro chain $SPC(n, p_1, p_2)$, the resistance number $r(u_n|SPC(n, p_1, p_2))$ is a random variable, and its expected value is denoted by

$$U_n = E(r(u_n|SPC(n, p_1, p_2))).$$

By the expectation operator and (3), we can obtain a recursive relation for the expected value of the Kirchhoff number of a random spiro chain $SPC(n, p_1, p_2)$

$$E(Kf(SPC(n+1, p_1, p_2)) = E(Kf(SPC(n, p_1, p_2))) + 5U_n + \frac{175n}{6} + \frac{35}{2} \tag{2.5}$$

Now, we consider computing U_n.

(i) If $SPC_n \to SPC_{n+1}^1$ with probability p_1, then u_n is the vertex x_3 or x_5. Consequently, $r(u_n|SPC_n)$ is given by $r(x_3|SPC_n)$ with probability p_1.

(ii) If $SPC_n \to SPC_{n+1}^2$ with probability p_2, then u_n is the vertex x_2 or x_6. Consequently, $r(u_n|SPC_n)$ is given $r(x_2|SPC_n)$ with probability p_2.

(iii) If $SPC_n \to SPC_{n+1}^3$ with probability $1 - p_1 - p_2$, then u_n is the vertex x_4. Consequently, $r(u_n|SPC_n)$ is given by $r(x_4|SPC_n)$ with probability $1 - p_1 - p_2$.

From (i)-(iii) above, we immediately obtain

$$\begin{aligned}U_n =& r(x_3|SPC_n)p_1 + r(x_2|SPC_n)p_2 + r(x_4|SPC_n)(1 - p_1 - p_2)\\ =& p_1[r(u_{n-1}|SPC(n-1, p_1, p_2)) + \frac{20}{3}(n-1) + \frac{35}{6}]\\ &+ p_2[r(u_{n-1}|SPC(n-1, p_1, p_2)) + \frac{25}{6}(n-1) + \frac{35}{6}]\\ &+ (1 - p_1 - p_2)[r(u_{n-1}|SPC(n-1, p_1, p_2)) + \frac{15}{2}(n-1) + \frac{35}{6}]\end{aligned}$$

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

$$U_n = U_{n-1} + (\frac{15}{2} - \frac{5}{6}p_1 - \frac{10}{3}p_2)n + \frac{5}{6}p_1 + \frac{10}{3}p_2 - \frac{5}{3}$$

And $U_1 = E(r(u_1|SPC(1, p_1, p_2))) = \frac{35}{6}$, using the above recurrence relation, we have

$$U_n = (\frac{15}{4} - \frac{5}{12}p_1 - \frac{5}{3}p_2)n^2 + (\frac{25}{12} + \frac{5}{12}p_1 + \frac{5}{3}p_2)n$$

From (4),

$$\begin{aligned}&E(Kf(SPC(n+1, p_1, p_2)) =\\ &= E(Kf(SPC(n, p_1, p_2))) + 5[(\tfrac{15}{4} - \tfrac{5}{12}p_1 - \tfrac{5}{3}p_2)n^2 +\\ &\quad(\tfrac{25}{12} + \tfrac{5}{12}p_1 + \tfrac{5}{3}p_2)n] + \tfrac{175}{6}n + \tfrac{35}{2}\end{aligned}$$

and $E(Kf(SPC(1, p_1, p_2))) = \frac{35}{2}$.

Using the above recurrence relation, we have

$$\begin{aligned}E(Kf(SPC(n, p_1, p_2))) = (\frac{25}{4} - \frac{25}{36}p_1 - \frac{25}{9}p_2)n^3 + (\frac{25}{12}p_1 + \frac{25}{3}p_2 + \frac{125}{12})n^2\\ -(\frac{25}{18}p_1 + \frac{50}{9}p_2 - \frac{5}{6})n.\end{aligned}$$

□

Specially, by taking $(p_1, p_2) = (1, 0), (0, 1)$ or $(0, 0)$, respectively, and Theorem 2.3, we have

Corollary 2.4. *([8]) The Kirchhoff indices of the spiro meta-chain M_n, the spiro ortho-chain O_n and the spiro para-chain P_n are*

$$\begin{aligned}Kf(M_n) &= \frac{50}{9}n^3 + \frac{25}{2}n^2 - \frac{5}{9}n\\ Kf(O_n) &= \frac{125}{36}n^3 + \frac{75}{4}n^2 - \frac{85}{18}n\\ Kf(P_n) &= \frac{25}{4}n^3 + \frac{125}{12}n^2 + \frac{5}{6}n.\end{aligned}$$

2.3 A relation between $E(Kf(PPC))$ and $E(Kf(SPC))$

Since a spiro chain can be obtained from a polyphenyl chain by squeezing off its cut edges, it is straightforward by Rayleigh short-cut principle in the classical theory of electricity that the Kirchhoff index of the spiro chain is less than the polyphenyl chain. In fact, a relation between the Kirchhoff indices of a polyphenyl chain and its corresponding spiro chain obtained by squeezing off its cut edges was given in [8]. Here, we can also obtain a relation between the expected values of their Kirchhoff indices of the random polyphenyl chain $PPC(n, p_1, p_2)$ and the random spiro chain $SPC(n, p_1, p_2)$ with the same probabilities p_1 and p_2 from Theorems 2.1 and 2.3.

Theorem 2.5. *For a random polyphenyl chain $PPC(n, p_1, p_2)$ and a random spiro chain $SPC(n, p_1, p_2)$ with n hexagons, the expected values of their Kirchhoff indices are related as*

$$50E(Kf(PPC(n, p_1, p_2))) = 72E(Kf(SPC(n, p_1, p_2))) + 300n^3 - 350n^2 - 335n.$$

Theorem 2.5 also shows that the expected value of Kirchhoff index of the random spiro chain is less than the random polyphenyl chain. In fact, for $n \geq 2$, $E(Kf(SPC(n, p_1, p_2))) < \frac{25}{36}E(Kf(PPC(n, p_1, p_2)))$. The reason is quite obvious. Dividing both sides of the equation in Theorem 2.5 yields

$$E(Kf(PPC(n, p_1, p_2))) = \frac{36}{25}E(Kf(SPC(n, p_1, p_2))) + 6n^3 - 7n^2 - \frac{67}{10}n$$

and it is easily seen that for $n \geq 2$, $6n^3 - 7n^2 - \frac{67}{10}n > 0$.

2.4 The average value of the Kirchhoff index

Let $\overline{\mathcal{G}}_n$ is the set of all polyphenyl chains with n hexagons. The average value of the Kirchhoff indices with respect to $\overline{\mathcal{G}}_n$ is

$$Kf_{avr}(\overline{\mathcal{G}}_n) = \frac{1}{|\overline{\mathcal{G}}_n|} \sum_{G \in \overline{\mathcal{G}}_n} Kf(G).$$

In order to obtain the average value of the Kirchhoff indices with respect to $\overline{\mathcal{G}}_n$, we only need to take $p_1 = p_2 = \frac{1}{3}$ in the random polyphenyl chain $PPC(n, p_1, p_2)$, i.e., the average value of the Kirchhoff indices with respect to $\overline{\mathcal{G}}_n$ is just the expected value of the Kirchhoff index of the random polyphenyl chain $PPC(n, p_1, p_2)$ for $p_1 = p_2 = \frac{1}{3}$. From Theorem 2.1, we have

Theorem 2.6. *The average value of the Kirchhoff indices with respect to $\overline{\mathcal{G}}_n$ is*

$$Kf_{avr}(\overline{\mathcal{G}}_n) = \frac{40}{3}n^3 + 13n^2 - \frac{53}{6}n.$$

Similarly, let $\mathcal{G}_n$ is the set of all spiro chains with n hexagons. The average value of the Kirchhoff indices with respect to $\mathcal{G}_n$ is

$$Kf_{avr}(\mathcal{G}_n) = \frac{1}{|\mathcal{G}_n|} \sum_{G \in \mathcal{G}_n} Kf(G).$$

And the average value of the Kirchhoff indices with respect to $\mathcal{G}_n$ is just the the expected value of the Kirchhoff index of the random spiro chain $SPC(n, p_1, p_2)$ for $p_1 = p_2 = \frac{1}{3}$. From Theorem 2.3, we have

Theorem 2.7. *The average value of the Kirchhoff indices with respect to $\mathcal{G}_n$ is*

$$Kf_{avr}(\mathcal{G}_n) = \frac{275}{54}n^3 + \frac{125}{9}n^2 - \frac{40}{27}n.$$

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