Computing the Kirchhoff index of linear phenylenes *

Yujun Yang
School of Mathematics and Information Science, Yantai University,
Yantai, Shandong 264005, P.R. China.
E-mail address: young229@sina.com

Abstract

The Laplacian eigenvalues of linear phenylenes PH_n are partially determined, and a simple closed-form formula for the Kirchhoff index of PH_n is derived in terms of the index n.

Key words: resistance distance; Kirchhoff index; Laplacian matrix; Linear phenylenes

1 Introduction

Let G be a connected graph with vertex-set $V(G) = \{1, 2, \cdots, n\}$. On the basis of electrical network theory, Klein and Randić [7] proposed the novel concept of the resistance distance. They view G as an electrical network by viewing each edge of G as a unit resistor. Then the resistance distance between vertices i and j, denoted by r_{ij}, is defined to be the net effective resistance between them. The Kirchhoff index of G, denoted by $Kf(G)$ [7], is defined as the sum of resistance distances between all pairs of vertices in G, i.e.,

$$Kf(G) = \sum_{i<j} r_{ij}.$$

As an analogy to the famous Wiener index [10], the Kirchhoff index is an important molecular structure-descriptor [11], and thus it is well studied in both mathematical and chemical literatures [2, 3, 5, 8]. So far, the Kirchhoff index have been computed for some classes of graphs with symmetries, see for instance [6, 9, 13-16] and the references therein.

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The Laplacian matrix of G is $L(G) = D(G) - A(G)$, where $A(G)$ is the adjacency matrix and $D(G)$ is the digonal matrix of vertex degrees. The Laplacian polynomial of G is defined as

$$P_{L(G)}(x) = \det(xI_n - L(G)),$$

where I_n denote the identity matrix of order n. Let $0 = \lambda_0 < \lambda_1 \leq \cdots \leq \lambda_{n-1}$ be the eigenvalues of $L(G)$, called the Laplacian eigenvalues of G. Gutman and Mohar [4], and Zhu, Klein and Lukovits [17] obtained the following amazing formula.

Theorem 1.1. *[4, 17] For any connected n-vertex graph G, $n \geq 2$,*

$$Kf(G) = n\sum_{k=1}^{n-1}\frac{1}{\lambda_k}. \tag{1}$$

Consider the linear phenylenes PH_n, consisting of $n-1$ four-membered (cyclobutadiene) and n six-membered (benzene) rings, in which each cyclobutadiene unit is adjacent to two benzene rings, whereas benzene rings are not adjacent to each other, see Fig. 1. In this paper, firstly the decomposition theorem of the Laplacian polynomial is stated. Then according to this theorem, we decompose the Laplacian polynomial of PH_n into the product of two polynomials: the Laplacian polynomial of the path P_{3n} with $3n$ vertices and the characteristic polynomial of a symmetric tridiagonal matrix L_S of order $3n$. Hence the Laplacian eigenvalues of PH_n contains the Laplacian eigenvalues of P_{3n}. Though there are still $3n$ Laplacian eigenvalues of PH_n left to be unknown, the sum of their reciprocals can be determined according to the relationship between roots and coefficients of the characteristic polynomial of L_S. Hence simple closed-form formula for the Kirchhoff index of PH_n is derived by Theorem 1.1.

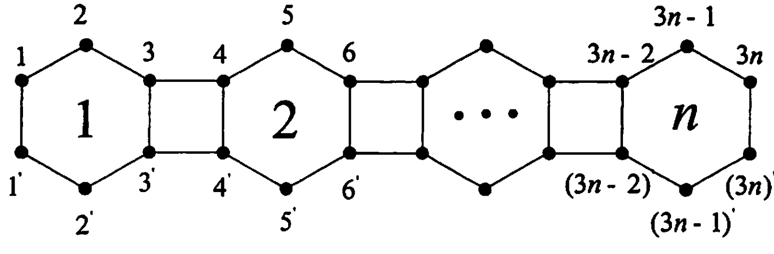

Fig. 1. The linear phenylenes PH_n.

2 Laplacian spectrum of PH_n

An *automorphism* of G is a permutation π of $V(G)$ which has the property that uv is an edge of G if and only if $\pi(u)\pi(v)$ is an edge of G.

Suppose that G has an automorphism π which can be written as the product of disjoint 1-cycles and transpositions, that is

$$\pi = (1^0)(2^0)\cdots(m^0)(1,1')(2,2')\cdots(k,k').$$

Let $V_0 = \{1^0, 2^0, \cdots, m^0\}$, $V_1 = \{1, 2, \cdots, k\}$, $V_2 = \{1', 2', \cdots, k'\}$. Then by a suitable arrangement of vertices in G, $L(G)$ can be written as the following block matrix

$$L(G) = \begin{bmatrix} L_{V_0V_0} & L_{V_0V_1} & L_{V_0V_2} \\ L_{V_1V_0} & L_{V_1V_1} & L_{V_1V_2} \\ L_{V_2V_0} & L_{V_2V_1} & L_{V_2V_2} \end{bmatrix},$$

where $L_{V_iV_j}$ is the sub-matrix formed by rows corresponding to vertices in V_i and columns corresponding to vertices in V_j for $i, j = 0, 1, 2$.

Let

$$L_A(G) = \begin{bmatrix} L_{V_0V_0} & \sqrt{2}L_{V_0V_1} \\ \sqrt{2}L_{V_1V_0} & L_{V_1V_1} + L_{V_1V_2} \end{bmatrix}, \quad L_S(G) = L_{V_2V_2} - L_{V_1V_2}$$

Yang and Yu [12] obtained the following decomposition theorem of the Laplacian polynomial, which is restated in [14] in a somewhat different way as follows:

Theorem 2.1. *Let $L(G)$, $L_A(G)$ and $L_S(G)$ be defined as above. Then*

$$P_{L(G)}(x) = P_{L_A(G)}(x)P_{L_S(G)}(x). \tag{2}$$

In particular, if π can be written only as the product of disjoint transpositions (i.e. $V_0 = \emptyset$), then $L_A = L_{V_1V_1} + L_{V_1V_2}$, $L_S = L_{V_2V_2} - L_{V_1V_2}$ and $L_{V_1V_1} = L_{V_2V_2}$.

Now we compute the Laplacian spectrum of PH_n according to Theorem 2.1. For convenience, we abbreviate $L_A(PH_n)$ and $L_S(PH_n)$ to L_A and L_S.

We label the vertices of PH_n as in Fig. 1. Obviously, $\pi = (1,1')(2,2')\ldots(3n,(3n)')$ is an automorphism of PH_n. Thus $V_1 = \{1, 2, \ldots, 3n\}$ and $V_2 = \{1', 2', \ldots, (3n)'\}$. Accordingly, $L_{V_1V_1}$ $(L_{V_2V_2})$ and

$L_{V_1V_2}$ are given as follows:

$$\begin{bmatrix} 2 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 3 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 3 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 3 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 2 \end{bmatrix},$$

$$\begin{bmatrix} -1 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & -1 \end{bmatrix}$$

Hence we can obtain L_A and L_S as given in the blow

$$\begin{bmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 1 \end{bmatrix},$$

$$\begin{bmatrix} 3 & -1 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 4 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 2 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & -1 & 4 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & -1 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 & -1 & 3 \end{bmatrix}$$

By Theorem 2.1,

$$P_{L(PH_n)}(x) = P_{L_A}(x)P_{L_S}(x).$$

Observe that L_A is the Laplacian matrix of the path P_{3n}. Hence the Laplacian polynomial of PH_n is the product of the Laplacian polynomial of P_{3n} and the characteristic polynomial of L_S.

It is well known that the eigenvalues of L_A are [1] $\lambda_i = 4\sin^2(\frac{k\pi}{6n})$, $k = 0, 1, 2, \cdots, 3n-1$. Suppose that the eigenvalues of L_S are μ_j, $j = 1, 2, \cdots, 2n$. Then the Laplacian eigenvalues of PH_n are $\lambda_0, \lambda_1, \cdots, \lambda_{3n-1}, \mu_1, \mu_2, \cdots, \mu_{3n}$.

3 The Kirchhoff index of PH_n

Suppose that $\det(xI_{3n} - L_S) = x^{3n} + \alpha_1 x^{3n-1} + \cdots + \alpha_{3n-1}x + \alpha_{3n}$. Then

Theorem 3.1.

$$Kf(PH_n) = 9n^3 - n + 6n\frac{(-1)^{3n-1}\alpha_{3n-1}}{\det L_S}. \tag{3}$$

Proof. Since $\lambda_0 = 0$, by Theorem 1.1,

$$Kf(PH_n) = 6n(\sum_{i=1}^{3n-1}\frac{1}{\lambda_i} + \sum_{j=1}^{3n}\frac{1}{\mu_j}).$$

On the one hand,

$$6n(\sum_{i=1}^{3n-1}\frac{1}{\lambda_i}) = 2 \times 3n\sum_{i=1}^{3n-1}\frac{1}{\lambda_i} = 2Kf(P_{3n}),$$

on the other hand,

$$\sum_{j=1}^{3n}\frac{1}{\mu_j} = \frac{\sum\limits_{i=1}^{3n}\prod\limits_{\substack{j=1\\ j\neq i}}^{3n}\mu_j}{\prod\limits_{j=1}^{3n}\mu_j} = \frac{(-1)^{3n-1}\alpha_{3n-1}}{\alpha_{3n}}.$$

Noticing that $Kf(P_{3n}) = \frac{(3n)^3-3n}{6} = \frac{9n^3-n}{2}$ by the formula that $Kf(P_n) = \frac{n^3-n}{6}$, we complete the proof. □

For $1 \le i \le 3n$, let D_i be the ith order principal sub-matrix formed by the first i rows and columns of L_S and d_i be the value of determinant of D_i. Then by expanding the determinate of D_i with respect to its last row, we readily have

Lemma 3.2. *$d_1 = 3$, $d_2 = 5$ and for $3 \le i \le 3n-1$,*

$$d_i = \begin{cases} 4d_{i-1} - d_{i-2}, & \text{if } i \equiv 0,1 \pmod 3, \\ 2d_{i-1} - d_{i-2}, & \text{otherwise,} \end{cases}$$

$d_{3n} = \det L_S = 3d_{3n-1} - d_{3n-2}$.

Now we construct a sequence $\{d_i\}_{i\geq 0}$ such that $d_0 = 1$, $d_1 = 3$, $d_2 = 5$ and for $i \geq 3$,

$$d_i = \begin{cases} 4d_{i-1} - d_{i-2}, & \text{if } i \equiv 0,1 \pmod 3, \\ 2d_{i-1} - d_{i-2}, & \text{otherwise.} \end{cases}$$

In order to find the explicit formula for the n-th term of sequence $\{d_i\}_{i\geq 0}$, we construct three new sequences $\{a_i\}_{i\geq 0}$, $\{b_i\}_{i\geq 0}$ and $\{c_i\}_{i\geq 0}$ from $\{d_i\}_{i\geq 0}$ such that for $i \geq 0$, $a_i = d_{3i}$, $b_i = d_{3i+1}$ and $c_i = d_{3i+2}$. We first show the following result:

Lemma 3.3. *$a_0 = 1$, $a_1 = 17$ and for $i \geq 1$,*

$$a_i = 22a_{i-1} - a_{i-2}. \tag{4}$$

In addition, b_i and c_i satisfy the same recurrence formula.

Proof. It is easy to verify that $a_0 = 1$ and $a_1 = 17$. Since $a_0 = d_0 = 1$, $a_1 = d_1 = 3$ and $a_2 = d_2 = 5$ and for $i \geq 1$,

$$\begin{cases} a_i = 4c_{i-1} - b_{i-1}, & (*) \\ b_i = 4a_i - c_{i-1}, & (**) \\ c_i = 2b_i - a_i. & (***) \end{cases}$$

Substituting Eq. (***) into Eqs. (*) and (**), we have

$$\begin{cases} a_i = 7b_{i-1} - 4a_{i-1}, & \text{(i)} \\ b_i = 4a_i - 2b_{i-1} + a_{i-1}. & \text{(ii)} \end{cases}$$

By Eq. (i), $b_{i-1} = \frac{a_i + 4a_{i-1}}{7}$. Substituting b_{i-1} and b_i into Eq. (ii) we have $\frac{a_{i+1}+4a_i}{7} = 4a_i - 2\frac{a_i+4a_{i-1}}{7} + a_{i-1}$, that is $a_{i+1} = 22a_i - a_{i-1}$. We can obtain $b_{i+1} = 22b_i - b_{i-1}$ and $c_{i+1} = 22c_i - c_{i-1}$ in the similar way. □

Lemma 3.4. *For $i \geq 0$,*

$$a_i = \frac{10+\sqrt{30}}{20}(11+2\sqrt{30})^n + \frac{10-\sqrt{30}}{20}(11-2\sqrt{30})^n; \tag{5}$$

$$b_i = \frac{6+\sqrt{30}}{20}(11+2\sqrt{30})^n + \frac{6-\sqrt{30}}{20}(11-2\sqrt{30})^n; \tag{6}$$

$$c_i = \frac{10+\sqrt{30}}{20}(11+2\sqrt{30})^{n+1} + \frac{10-\sqrt{30}}{20}(11-2\sqrt{30})^{n+1}. \tag{7}$$

Proof. We only show the expression for a_i, Eqs. (6) and (7) can be proved in the same way. The characteristic equations of $(a_i)_{i\geq 0}$ is $x^2 = 22x - 1$ with $x_1 = 11 + 2\sqrt{30}$, $x_2 = 11 - 2\sqrt{30}$ as its roots. Suppose that

$$a_i = (11+2\sqrt{30})^i y_1 + (11-2\sqrt{30})^i y_2. \tag{8}$$

Then the initial conditions $a_0 = 1$ and $a_1 = 4$ lead to the system of equations

$$\begin{cases} y_1 + y_2 = 1 \\ (11+2\sqrt{30})\, y_1 + (11-2\sqrt{30})\, y_2 = 17 \end{cases}$$

Solving it we obtain $y_1 = \frac{10+\sqrt{30}}{20}$, $y_2 = \frac{10-\sqrt{30}}{20}$. The desired result follows by substituting y_1 and y_2 back into Eq. (8). □

Bearing in mind that

$$\det L_S = 3d_{3n-1} - d_{3n-2} = 3c_{n-1} - b_{n-1},$$

by Lemma 3.4, we immediately have

Lemma 3.5.

$$det\ L_S = \frac{\sqrt{30}}{10}((11+2\sqrt{30})^n - (11-2\sqrt{30})^n). \tag{9}$$

The only thing left is to calculate α_{3n-1}. For convenience, we denote the diagonal entries of L_s by l_{ii}, $i = 1, 2, \cdots, 3n$. For $1 \le i \le 3n$, let

$$L_i = \begin{vmatrix} -l_{11} & 1 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 1 & -l_{22} & \cdots & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & -l_{i-1,i-1} & 0 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & -l_{i+1,i+1} & 1 & \cdots & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & -l_{3n-1,3n-1} & 1 \\ 0 & 0 & \cdots & 0 & 0 & \cdots & 1 & -l_{3n,3n} \end{vmatrix}.$$

Then α_{3n-1} can be computed as in the following lemma.

Lemma 3.6.

$$a_{3n-1} = (-1)^{3n-1}[\frac{29n}{40}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n) + \frac{61\sqrt{30}}{2400}((11+2\sqrt{30})^n - (11-2\sqrt{30})^n)]. \tag{10}$$

Proof. First notice that

$$a_{3n-1} = \sum_{i=1}^{3n} L_i = (-1)^{3n-1}\sum_{i=1}^{3n} d_{i-1}d_{3n-i} = (-1)^{3n-1}\sum_{i=0}^{3n-1} d_i d_{3n-1-i}.$$

Thus,

$$
\begin{aligned}
a_{3n-1} &= (-1)^{3n-1}\sum_{i=0}^{3n-1} d_i d_{3n-1-i} \\
&= (-1)^{3n-1}\sum_{k=0}^{n-1}(d_{3k}d_{3n-1-3k} + d_{3k+1}d_{3n-1-3k-1}d_{3k+2}d_{3n-1-3k-2}) \\
&= (-1)^{3n-1}\sum_{k=0}^{n-1}(a_k c_{n-k-1} + b_k b_{n-k-1} + c_k a_{n-k-1}).
\end{aligned}
$$

By Eqs. (5), (6) and (7), simple computations show that

$$
\begin{aligned}
a_k c_{n-k-1} &= \frac{7}{40}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n) \\
&+ \frac{23-4\sqrt{30}}{40}(11+2\sqrt{30})^k \times (11-2\sqrt{30})^{n-1-k} \\
&+ \frac{23+4\sqrt{30}}{40}(11+2\sqrt{30})^{n-1-k}(11-2\sqrt{30})^k. \\
b_k b_{n-k-1} &= \frac{3}{8}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n \\
&+ (11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k} \\
&+ (11+2\sqrt{30})^{n-1-k}(11-2\sqrt{30})^k). \\
c_k a_{n-k-1} &= \frac{7}{40}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n) \\
&+ \frac{23+4\sqrt{30}}{40}(11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k} \\
&+ \frac{23-4\sqrt{30}}{40}(11+2\sqrt{30})^{n-1-k}(11-2\sqrt{30})^k.
\end{aligned}
$$

Hence

$$
\begin{aligned}
a_{3n-1} &= (-1)^{3n-1}(\frac{29n}{40}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n) \\
&+ \frac{61}{40}\sum_{k=0}^{n-1}((11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k} \\
&+ (11+2\sqrt{30})^{n-1-k}(11-2\sqrt{30})^k)) \\
&= (-1)^{3n-1}(\frac{29n}{40}((11+2\sqrt{30})^n + (11-2\sqrt{30})^n) \\
&+ \frac{61}{20}\sum_{k=0}^{n-1}(11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k}). \qquad (11)
\end{aligned}
$$

Now we show that

$$\sum_{k=0}^{n-1}(11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k} = \frac{\sqrt{30}}{120}((11+2\sqrt{30})^n-(11-2\sqrt{30})^n). \tag{12}$$

We only show the assertion holds if n is even, and the case that n is odd can be proved in the same way. If n is even, since $(11+2\sqrt{30})(11-2\sqrt{30}) = 1$, then

$$\begin{aligned}
&\sum_{k=0}^{n-1}(11+2\sqrt{30})^k(11-2\sqrt{30})^{n-1-k} \\
=&\sum_{i=1}^{\frac{n}{2}}((11+2\sqrt{30})^{2i-1}+(11-2\sqrt{30})^{2i-1}) \\
=&\sum_{i=1}^{\frac{n}{2}}(11+2\sqrt{30})^{2i-1}+\sum_{i=1}^{\frac{n}{2}}(11-2\sqrt{30})^{2i-1} \\
=&\frac{11+2\sqrt{30}-(11+2\sqrt{30})^{n+1}}{1-(11+2\sqrt{30})^2}+\frac{11-2\sqrt{30}-(11-2\sqrt{30})^{n+1}}{1-(11-2\sqrt{30})^2} \\
=&\frac{(11+2\sqrt{30})^{n+1}-(11+2\sqrt{30})}{240+44\sqrt{30}}+\frac{(11-2\sqrt{30})^{n+1}-(11-2\sqrt{30})}{240-44\sqrt{30}} \\
=&\frac{(11+2\sqrt{30})^n-1}{4\sqrt{30}}+\frac{1-(11-2\sqrt{30})^n}{4\sqrt{30}} \\
=&\frac{\sqrt{30}}{120}((11+2\sqrt{30})^n-(11-2\sqrt{30})^n).
\end{aligned}$$

Combining Eq. (11) with Eq. (12), we can obtain Eq. (10) □

Now we are arriving at our main result:

Theorem 3.7.

$$Kf(PH_n) = 9n^3 + \frac{29\sqrt{30}}{20}\frac{(11+2\sqrt{30})^{2n}+1}{(11+2\sqrt{30})^{2n}-1}n^2 + \frac{21}{40}n. \tag{13}$$

Proof. Substituting Eqs. (9) and (10) into Eq. (3), we have Eq. (13). □

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