Kirchhoff Index of Cyclopolyacenes

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The resistance distance between two vertices of a connected graph G is computed as the effective resistance between them in the corresponding network constructed from G by replacing each edge with a unit resistor. The Kirchhoff index of G is the sum of resistance distances between all pairs of vertices. In this paper, following the method of Y. J. Yang and H. P. Zhang in the proof of the Kirchhoff index of the linear hexagonal chain, we obtain the Kirchhoff index of cyclopolyacenes, denoted by HR_n, in terms of its Laplacian spectrum. We show that the Kirchhoff index of HR_n is approximately one third of its Wiener index.

Key words: Resistance Distance; Kirchhoff Index; Laplacian Spectrum; Cyclopolyacenes.

1. Introduction

The concept of resistance distance was introduced a few years ago by Klein and Randić [1]. Let G be a connected graph with vertices labeled as $1,2,\dots,n$. They defined

$$R(G)=\sum_{i<j} r_{ij},$$

where r_{ij} is the effective resistance between vertices i and j as computed with Ohm's law when all the edges of G are considered to be unit resistors. Later $R(G)$ was called the Kirchhoff index of G labeled by $Kf(G)$. The famous Wiener index $W(G)$ [2] was given by

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

where d_{ij} is the length of a shortest path connecting i and j. Klein and Randić proved that $r_{ij}\le d_{ij}$ and $Kf(G)\le W(G)$ and the equality holds if and only if G is a tree.

Like the Wiener index, the Kirchhoff index is a graph structure-descriptor [3]. It is difficult to give closed-form formulae for general graphs [1, 4 – 7]. But the Kirchhoff index has been given for some classes of graphs, such as cycles [8, 9], complete graphs [9], geodetic graphs [7], distance-transitive graphs [7], circulant graphs [10], linear hexagonal chains [11], and so on [4, 7, 12, 13]. In this paper, we devote ourselves to cyclopolyacenes. For a more general family of 'cyclopolyphenacenes', we refer the reader to [14].

Let G be a connected graph with vertices labeled by $1,2,\dots,n$. The Laplacian matrix of G, denoted by $L(G)$, is a square matrix of order n whose (i,j)-entry l_{ij} is defined by

$$l_{ij}=\begin{cases}-1 & \text{if } i\neq j \text{ and the vertices } i \text{ and } j \text{ are adjacent},\\ 0 & \text{if } i\neq j \text{ and the vertices } i \text{ and } j \text{ are not adjacent},\\ d_i & \text{if } i=j \text{ and } d_i \text{ is the degree of the vertex } i.\end{cases} \quad (1)$$

The characteristic polynomial of $L(G)$ is defined as

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

where I_n denotes the identity matrix of order n. This polynomial is regarded as the Laplacian polynomial of G. Let $\lambda_0\le\lambda_1\le\dots\le\lambda_{n-1}$ be the eigenvalues of $L(G)$ which are called the Laplacian eigenvalues of G, then $\lambda_0=0$ and $\lambda_k>0$ for each $k>0$ [15]. The spectrum of $L(G)$ is $S(G)=(\lambda_0,\lambda_1,\dots,\lambda_{n-1})$. Gutman and Mohar [16], and Zhu et al. [17] obtained the Kirchhoff index of a graph in terms of its Laplacian spectrum as follows:

Lemma 1.1. *For any connected graph G of order $n\ge 2$,*

$$Kf(G)=n\sum_{k=1}^{n-1}\frac{1}{\lambda_k}. \quad (2)$$

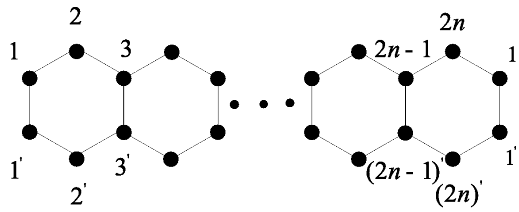

Fig. 1. HR_n and its vertex labeling.

Let HR_n denote the cyclopolyacenes with n hexagons, we refer the reader to Figure 1 for this graph. In the paper of Zhang and Yang [11], they computed the Kirchhoff index of the linear hexagonal chains. In the present article, we compute the Kirchhoff index of HR_n (Theorem 3.8) and show that the Kirchhoff index of HR_n is approximately one third of its Wiener index (Theorem 3.9).

2. Laplacian Polynomial Decomposition

Two graphs G_1 and G_2 are isomorphic if there exists a one to one correspondence Φ from $V(G_1)$ to $V(G_2)$ such that $u_1v_1 \in E(G_1)$ if and only if $\Phi(u_1)\Phi(v_1) \in E(G_2)$. If $G_1 = G_2$, then the isomorphism is called an automorphism of G. In fact, an automorphism of G is a permutation Φ of $V(G)$ which preserves the adjacency of G.

We label the vertices of HR_n as in Figure 1 and denote $V_1 = \{1,2,\ldots,2n\}$ and $V_2 = \{1',2'\ldots,(2n)'\}$. Then,

$$\Phi = (1,1')(2,2')\ldots(2n,(2n)')$$

is an automorphism of HR_n. The Laplacian matrix L of HR_n can be written as the following block matrix:

$$L = \begin{bmatrix} L_{V_1V_1} & L_{V_1V_2} \\ L_{V_2V_1} & L_{V_2V_2} \end{bmatrix},$$

where $L_{V_iV_j}$ is the submatrix formed by rows corresponding to vertices in V_i and columns corresponding to vertices in V_j for $i,j = 1,2$. Let be

$$T = \begin{bmatrix} \left(\frac{1}{\sqrt{2}}\right)I_{2n} & \left(\frac{1}{\sqrt{2}}\right)I_{2n} \\ \left(\frac{1}{\sqrt{2}}\right)I_{2n} & -\left(\frac{1}{\sqrt{2}}\right)I_{2n} \end{bmatrix}.$$

By the unitary transformation TLT, we obtain

$$TLT = \begin{bmatrix} L_A & 0 \\ 0 & L_S \end{bmatrix},$$

where

$$L_A = L_{V_1V_1} + L_{V_1V_2},\ L_S = L_{V_2V_2} - L_{V_1V_2}.$$

As a result of linear algebra, we have

Lemma 2.1. *Let L, L_A, and L_S be defined as above. Then*

$$P_L(x) = P_{L_A}(x)P_{L_S}(x). \tag{3}$$

For simplicity, we define two $2n \times 2n$ matrices I_0 and I_e with all elements 0 except 1 in the odd and even diagonal positions, respectively. And likewise we could let C be the $2n \times 2n$ 'cyclic' matrix with all elements 0 except 1s just above the diagonal as well as a 1 in the lower left corner, and let $C^\dagger$ $(= C^{-1})$ be its transpose. A direct calculation shows that $I = I_0 + I_e$, $L_{V_1V_2} = L_{V_2V_1} = -I_0$, $L_{V_1V_1} = 3I_0 + 2I_e - C - C^\dagger$, $L_A = 2I - C - C^\dagger$, and $L_S = 4I_0 + 2I_e - C - C^\dagger$.

By Lemma 2.1, the Laplacian spectrum of HR_n consists of eigenvalues of L_A and L_S. Assume that the eigenvalues of L_A and L_S are λ_i, $0 \le i \le 2n-1$ and μ_j, $1 \le j \le 2n$, respectively. Then, $S(HR_n) = (\lambda_0,\ \lambda_1,\ \ldots,\ \lambda_{2n-1},\ \mu_1,\ \mu_2,\ \ldots,\ \mu_{2n})$. Note that L_A is the Laplacian matrix of the cycle C_{2n} of order $2n$.

3. Kirchhoff Index of Cyclopolyacenes

Assume that $\det(xI - L_S) = x^{2n} + \alpha_1 x^{2n-1} + \cdots + \alpha_{2n-2}x^2 + \alpha_{2n-1}x + \alpha_{2n}$.

Theorem 3.1.

$$Kf(HR_n) = 2Kf(C_{2n}) - 4n\frac{\alpha_{2n-1}}{\det L_S}. \tag{4}$$

Proof: By Lemma 1.1,

$$\begin{aligned} Kf(HR_n) &= 4n\left(\sum_{i=1}^{2n-1}\frac{1}{\lambda_i} + \sum_{j=1}^{2n}\frac{1}{\mu_j}\right) \\ &= 2 \times 2n\sum_{i=1}^{2n-1}\frac{1}{\lambda_i} + 4n\frac{\sum_{j'=1}^{2n}\prod_{j=1,\ j\neq j'}^{2n}\mu_j}{\prod_{j=1}^{2n}\mu_j} \\ &= 2Kf(C_{2n}) + 4n\frac{(-1)^{2n-1}\alpha_{2n-1}}{(-1)^{2n}\alpha_{2n}} \\ &= 2Kf(C_{2n}) - 4n\frac{\alpha_{2n-1}}{\det L_S}. \end{aligned}$$ □

By [10], $Kf(C_{2n}) = \frac{4n^3-n}{6}$. For $i < 2n$, let S_i be the ith-order principal submatrix formed by the first i rows and columns of L_S and $c_i = \det S_i$.

Lemma 3.2. *For $i < 2n$, the integers c_i satisfy the recurrence*

$$c_i = 6c_{i-2} - c_{i-4}, \tag{5}$$

with initial conditions $c_0 = 1$, $c_1 = 4$, $c_2 = 7$, and $c_3 = 24$.

Proof: A direct calculation shows that $c_0 = 1, c_1 = 4, c_2 = 7$, and $c_3 = 24$. For $2 \le i < 2n$, expanding $\det S_i$ with regard to its last row we obtain

$$c_i = \begin{cases} 4c_{i-1} - c_{i-2} & \text{if } i \text{ is odd,} \\ 2c_{i-1} - c_{i-2} & \text{if } i \text{ is even.} \end{cases}$$

For $0 \le i < n$, let $a_i = c_{2i}$ and for $0 \le i < n$, let $b_i = c_{2i+1}$. Then $a_0 = 1, b_0 = 4$ and for $i \ge 1$

$$\begin{cases} a_i = 2b_{i-1} - a_{i-1}, \\ b_i = 4a_i - b_{i-1}. \end{cases}$$

Hence, $a_i = 6a_{i-1} - a_{i-2}$ and $b_i = 6b_{i-1} - b_{i-2}$. Therefore, c_i satisfies the recurrence

$$c_i = 6c_{i-2} - c_{i-4}$$

with the initial conditions $c_0 = 1, c_1 = 4, c_2 = 7$, and $c_3 = 24$. □

Lemma 3.3. *Let c_i, $0 \le i < 2n$ be the sequence as above. Then*

$$c_i = \frac{1}{4}\big[(3+2\sqrt{2}-(-1)^i)(\sqrt{2}+1)^i + (3-2\sqrt{2}-(-1)^i)(1-\sqrt{2})^i\big]. \tag{6}$$

Proof: The characteristic equations of c_i is $x^4 = 6x^2 - 1$ whose roots are $x_1 = \sqrt{2}+1$, $x_2 = -(\sqrt{2}+1)$, $x_3 = \sqrt{2}-1$, and $x_4 = -(\sqrt{2}-1)$. Assume that

$$c_i = (\sqrt{2}+1)^i y_1 + (-(\sqrt{2}+1))^i y_2 + (\sqrt{2}-1)^i y_3 + (-(\sqrt{2}-1))^i y_4.$$

Considering of the initial conditions $c_0 = 1, c_1 = 4, c_2 = 7$, and $c_3 = 24$, we obtain the systems of equations

$$\begin{aligned} & y_1 + y_2 + y_3 + y_4 = 1 \\ & (\sqrt{2}+1)y_1 - (\sqrt{2}+1)y_2 + (\sqrt{2}-1)y_3 - (\sqrt{2}-1)y_4 = 4 \\ & (\sqrt{2}+1)^2 y_1 + (\sqrt{2}+1)^2 y_2 + (\sqrt{2}-1)^2 y_3 + (\sqrt{2}-1)^2 y_4 = 7 \\ & (\sqrt{2}+1)^3 y_1 - (\sqrt{2}+1)^3 y_2 + (\sqrt{2}-1)^3 y_3 - (\sqrt{2}-1)^3 y_4 = 24. \end{aligned} \tag{7}$$

A direct computation shows that $y_1 = \frac{3+2\sqrt{2}}{4}$, $y_2 = -\frac{1}{4}$, $y_3 = -\frac{1}{4}$, and $y_4 = \frac{3-2\sqrt{2}}{4}$ and the result follows. □

Because $\det(L_S) = 2(c_{2n-1} - c_{2n-2} - 1)$. By Lemma 3.3, we have

$$\det(L_S) = (3+2\sqrt{2})^n + (3-2\sqrt{2})^n - 2. \tag{8}$$

Considering $\det(xI - L_S) = -2 + (x-2)A_{2n-1} - 2B_{2n-2}$, where A_{2n-1} is the determinant of a $(2n-1)\times(2n-1)$ matrix with all elements 0 except $x-4$ and $x-2$ in the odd and even diagonal positions, respectively, as well as 1 just above and under the diagonal, and B_{2n-2} is the determinant of a $(2n-2)\times(2n-2)$ matrix that results from the deletion of the last row and column of A_{2n-1}. In this way, $B_{2n-2} = (x-2)A_{2n-3} - 2B_{2n-4}$ and by the recurrence

$$B_{2n-2} = \begin{cases} (x-2)(A_{2n-3} - A_{2n-5} + A_{2n-7} - \cdots \\ \quad - A_5 + A_3 - A_1) + 1, & \text{if } n \text{ is odd,} \\ (x-2)(A_{2n-3} - A_{2n-5} + A_{2n-7} - \cdots \\ \quad + A_5 - A_3 + A_1) - 1, & \text{if } n \text{ is even.} \end{cases}$$

If $n \ge 3$ is odd, the constant of A_{2n-1} is

$$c_{2n-1} = \frac{1}{4}\big[(4+2\sqrt{2})(1+\sqrt{2})^{2n-1} + (4-2\sqrt{2})(1-\sqrt{2})^{2n-1}\big] = \frac{1}{2}\big[(4+3\sqrt{2})(3+2\sqrt{2})^{n-1} + (4-3\sqrt{2})(3-2\sqrt{2})^{n-1}\big]$$

and the constant of $A_{2n-3} - A_{2n-5} + A_{2n-7} - \cdots - A_5 + A_3 - A_1$ is

$$\frac{4+2\sqrt{2}}{4}\big[-(\sqrt{2}+1) + (\sqrt{2}+1)^3 - (\sqrt{2}+1)^5 + \cdots + (\sqrt{2}+1)^{2n-3}\big] + \frac{4-2\sqrt{2}}{4}\big[-(1-\sqrt{2}) + (1-\sqrt{2})^3 - (1-\sqrt{2})^5 + \cdots + (1-\sqrt{2})^{2n-3}\big] = \frac{1}{4}\big[(\sqrt{2}+1)(3+2\sqrt{2})^{n-1} + (1-\sqrt{2})(3-2\sqrt{2})^{n-1}\big] - \frac{1}{2}.$$

To determine the coefficient of x in A_{2n-1}, we assume that

$$A_{2n-1} = x^{2n-1} + \beta_1 x^{2n-2} + \cdots + \beta_{2n-2}x + \beta_{2n-1}.$$

Obviously, β_{2n-2} is the coefficient of x in A_{2n-1}.

Lemma 3.4. [11] $\beta_{2n-2} = \sum_{i=0}^{2n-2} c_i c_{2n-2-i}$.

Assume that $f(x)$ is the ordinary generating function of c_i, that is $f(x) = \sum_{i\ge 0} c_i x^i$. Lemma 3.4 indicates that

β_{2n-2} is the coefficient of x^{2n-2} in $f(x)\cdot f(x)=f^2(x)$. We simplify $f(x)$ as

$$f(x)=\sum_{i\geq 0}c_ix^i=1+4x+7x^2+24x^3+\sum_{i\geq 4}c_ix^i=$$
$$1+4x+7x^2+24x^3+\sum_{i\geq 4}(6c_{i-2}-c_{i-4})x^i$$
$$=1+4x+7x^2+24x^3+6x^2(f(x)-1-4x)-x^4f(x).$$

Hence, $f(x)=\frac{x^2+4x+1}{x^4-6x^2+1}$.

Lemma 3.5.

$$\beta_{2n-2}=$$
$$(3-2\sqrt{2})^{n-1}\left[\frac{1}{8}(2n-1)(9-6\sqrt{2})+\frac{9\sqrt{2}-10}{16}\right]$$
$$+(3+2\sqrt{2})^{n-1}\left[\frac{1}{8}(2n-1)(9+6\sqrt{2})-\frac{9\sqrt{2}+10}{16}\right].$$

Proof: The function $f(x)=\frac{x^2+4x+1}{x^4-6x^2+1}$ can be decomposed as

$$f(x)=\frac{x+1}{2(x^2-2x-1)}-\frac{x+3}{2(x^2+2x-1)}.$$

So $f^2(x)=\frac{(x+1)^2}{4(x^2-2x-1)^2}+\frac{(x+3)^2}{4(x^2+2x-1)^2}-\frac{x^2+4x+3}{2(x^4-6x^2+1)}$. Since the roots of $x^2-2x-1=0$ are $1+\sqrt{2}$ and $1-\sqrt{2}$, one can assume that

$$\frac{(x+1)^2}{4(x^2-2x-1)^2}=\frac{A}{(x-1-\sqrt{2})^2}+\frac{B}{x-1-\sqrt{2}}+\frac{C}{(x-1+\sqrt{2})^2}+\frac{D}{x-1+\sqrt{2}}.$$

Comparing the coefficients between the left and the right, we have

$$A=\frac{3+2\sqrt{2}}{16},\ B=-\frac{\sqrt{2}}{32},\ C=\frac{3-2\sqrt{2}}{16},\ D=\frac{\sqrt{2}}{32}.$$

Since

$$\frac{3+2\sqrt{2}}{16(x-1-\sqrt{2})^2}=\frac{3+2\sqrt{2}}{16}\left[\frac{1}{1+\sqrt{2}}\right]^2\left[\frac{1}{1-\frac{x}{1+\sqrt{2}}}\right]^2=\frac{1}{16}\left[\sum_{i=0}^{\infty}\left(\frac{1}{1+\sqrt{2}}\right)^i x^i\right]^2,$$

the coefficient of x^{2n-2} in $\frac{3+2\sqrt{2}}{16(x-1-\sqrt{2})^2}$ is

$$\frac{1}{16}\sum_{i=0}^{2n-2}\left[\frac{1}{1+\sqrt{2}}\right]^i\left[\frac{1}{1+\sqrt{2}}\right]^{2n-2-i}=\frac{1}{16}(2n-1)(3-2\sqrt{2})^{n-1}.$$

Similarly, one can get the coefficients of x^{2n-2} in $\frac{-\sqrt{2}}{32(x-1-\sqrt{2})}$, $\frac{3-2\sqrt{2}}{16(x-1+\sqrt{2})^2}$, and $\frac{\sqrt{2}}{32(x-1+\sqrt{2})}$. They are $\frac{2-\sqrt{2}}{32}(3-2\sqrt{2})^{n-1}$, $\frac{1}{16}(2n-1)(3+2\sqrt{2})^{n-1}$ and $\frac{2+\sqrt{2}}{32}(3+2\sqrt{2})^{n-1}$, respectively. So the coefficient of x^{2n-2} in $\frac{(x+1)^2}{4(x^2-2x-1)^2}$ is

$$(3-2\sqrt{2})^{n-1}\left(\frac{2n-1}{16}+\frac{2-\sqrt{2}}{32}\right)+(3+2\sqrt{2})^{n-1}\left(\frac{2n-1}{16}+\frac{2+\sqrt{2}}{32}\right). \tag{9}$$

A direct computation shows that

$$\frac{(x+3)^2}{4\left(x^2+2x-1\right)^2}=\frac{3+2\sqrt{2}}{16\left(x+1-\sqrt{2}\right)^2}-\frac{\sqrt{2}}{32\left(x+1-\sqrt{2}\right)}+\frac{3-2\sqrt{2}}{16\left(x+1+\sqrt{2}\right)^2}+\frac{\sqrt{2}}{32\left(x+1+\sqrt{2}\right)}$$

and the coefficient of x^{2n-2} in $\frac{(x+3)^2}{4(x^2+2x-1)^2}$ is

$$\left(3+2\sqrt{2}\right)^{n-1}\left[\frac{2n-1}{16}\left(17+12\sqrt{2}\right)+\frac{2+\sqrt{2}}{32}\right]+\left(3-2\sqrt{2}\right)^{n-1}\left[\frac{2n-1}{16}\left(17-12\sqrt{2}\right)+\frac{2-\sqrt{2}}{32}\right]. \tag{10}$$

Because

$$\frac{x^2+4x+3}{2(x^4-6x^2+1)}=\frac{4+\sqrt{2}}{16\left(x-1-\sqrt{2}\right)}+\frac{4-\sqrt{2}}{16\left(x-1+\sqrt{2}\right)}-\frac{4+3\sqrt{2}}{16\left(x+1-\sqrt{2}\right)}+\frac{3\sqrt{2}-4}{16\left(x+1+\sqrt{2}\right)},$$

the coefficient of x^{2n-2} in $\frac{x^2+4x+3}{2(x^4-6x^2+1)}$ is

$$\frac{6-5\sqrt{2}}{8}\left(3-2\sqrt{2}\right)^{n-1}+\frac{6+5\sqrt{2}}{8}\left(3+2\sqrt{2}\right)^{n-1}. \tag{11}$$

Summarize (9), (10), and (11), we obtain the results. □

G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$
HR_3	75.57	HR_{10}	1754.26	HR_{17}	7771.12	HR_{24}	20867.88
HR_4	152.00	HR_{11}	2284.36	HR_{18}	9144.62	HR_{25}	23476.7
HR_5	271.10	HR_{12}	2910.94	HR_{19}	10670.60	HR_{26}	26294.00
HR_6	438.74	HR_{13}	3642.01	HR_{20}	12357.10	HR_{27}	29327.90
HR_7	662.89	HR_{14}	4485.56	HR_{21}	14212.00	HR_{28}	32586.20
HR_8	951.53	HR_{15}	5449.59	HR_{22}	16243.40	HR_{29}	36077.10
HR_9	1312.65	HR_{16}	6542.12	HR_{23}	18459.40	HR_{30}	39808.40

Table 1. Kirchhoff indices of HR_n for $3 \leq n \leq 30$.

Briefly, we denote $A_{2n-3} - A_{2n-5} + A_{2n-7} - \cdots - A_5 + A_3 - A_1$ as $\bar{A}$, the coefficient of x in $\bar{A}$ as Y and the constant of $\bar{A}$ as X. For the upcoming computation, we give a result from Calculus.

Lemma 3.6.

$$(2n-3)y^{2n-4} - (2n-5)y^{2n-6} + \cdots + 3y^2 - 1 = \left(\int \left((2n-3)y^{2n-4} - (2n-5)y^{2n-6} + \cdots + 3y^2 - 1\right) \mathrm{d}y\right)' = \frac{(2n-3)y^{2n} + (2n-1)y^{2n-2} + y^2 - 1}{(1+y^2)^2}.$$

By a similar computation as that in Lemma 3.5 and the result of Lemma 3.6, one can get

$$Y = \frac{1}{16}\left[(9\sqrt{2}-10)\left((3-2\sqrt{2})^{n-2} - (3-2\sqrt{2})^{n-3} + \cdots + (3-2\sqrt{2}) - 1\right)\right] - \frac{1}{16}\left[(9\sqrt{2}+10)\left((3+2\sqrt{2})^{n-2} - (3+2\sqrt{2})^{n-3} + \cdots + (3+2\sqrt{2}) - 1\right)\right] + \frac{1}{8}\left[(9-6\sqrt{2}) \cdot \left((2n-3)(3-2\sqrt{2})^{n-2} - (2n-5)(3-2\sqrt{2})^{n-3} + \cdots + 3(3-2\sqrt{2}) - 1\right)\right] + \frac{1}{8}\left[(9+6\sqrt{2})\left((2n-3)(3+2\sqrt{2})^{n-2} - (2n-5)(3+2\sqrt{2})^{n-3} + \cdots + 3(3+2\sqrt{2}) - 1\right)\right] = \frac{1}{32}\left[(3-2\sqrt{2})^{n-1}\left((12-6\sqrt{2})n - 16 + 13\sqrt{2}\right) + (3+2\sqrt{2})^{n-1}\left((12+6\sqrt{2})n - 16 - 13\sqrt{2}\right)\right] + \frac{1}{4}.$$

Lemma 3.7.

$$\alpha_{2n-1} = -\frac{(9\sqrt{2}+12)n}{4}(3+2\sqrt{2})^{n-1} + \frac{(9\sqrt{2}-12)n}{4}(3-2\sqrt{2})^{n-1}.$$

Proof: Because $\det(xI - L_S) = -2 + (x-2)A_{2n-1} - 2B_{2n-2}$. So, $\alpha_{2n-1} = c_{2n-1} - 2\beta_{2n-2} + 4Y - 2X$. □

By a similar computation, the result when $n \geq 4$ and even is the same as the odd case.

Theorem 3.8.

$$Kf(HR_n) = \frac{4n^3 - n}{3} - n^2\left[((3-2\sqrt{2})^{n-1}(9\sqrt{2}-12) - (3+2\sqrt{2})^{n-1}(9\sqrt{2}+12)\right] \cdot \left[(3+2\sqrt{2})^n + (3-2\sqrt{2})^n - 2\right]^{-1}.$$

Proof: Combining (4), (8), and (12) one can get the value of $Kf(HR_n)$. □

The Kirchhoff indices of Cyclopolyacenes from HR_3 to HR_{30} are listed in Table 1. Comparing the Kirchhoff index of HR_n with its Wiener index, we have Theorem 3.9.

Theorem 3.9.

$$\lim_{n \to \infty} \frac{Kf(HR_n)}{W(HR_n)} = \frac{1}{3}.$$

Proof: Consider the distance between two vertices, one from V_1 and another from V_2. The sum of distances between Vertex 1 and each vertex in V_2 is

$$1 + 2 + 3 + \cdots + n + (n+1) + n + \cdots + 3 + 2 = n^2 + 2n.$$

Note that the sum of distances between each vertex in V_1 labeled by an odd number and each vertex in V_2 is equal.

The sum of distances between Vertex 2 and each vertex in V_2 is

$$2 + 3 + 2 + \cdots + n + (n+1) + n + \cdots + 3 = n^2 + 2n + 2.$$

Likewise, the sum of distances between each vertice in V_1 labeled by even and each vertex in V_2 is equal. So the sum of distances between V_1 and V_2 is

$$(n^2 + 2n) \times n + (n^2 + 2n + 2) \times n = 2n^3 + 4n^2 + 2n.$$

The sum of distance between vertices in V_1 (also in V_2)

is n^3. So $W(HR_n) = 4n^3 + 4n^2 + 2n$. By Theorem 3.8, the result follows. □

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