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Characteristic Polynomial of Linear Hexagonal Spiders*

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Abstract: In this paper, we give the explicit expressions of characteristic polynomials of linear hexagonal spiders, which are representation of certain branched catacondensed benzenoid molecules. From our result, the number of perfect matchings of these graphs are easily obtained. Our new method can also be used to calculate the characteristic polynomial of any graph having threefold symmetry.

Key words: linear hexagonal spiders; recurrence relation; characteristic polynomial

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线性蜘蛛链的特征多项式

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摘　要： 六角系统图是苯型烃类物质的分子模型. 这类图的特征值与它们所对应的化学物质的性质有密切关系. 线性蜘蛛链是一种有支链的苯分子的结构模型. 为了计算线性蜘蛛链的特征多项式, 首先给出了一个递推关系的显式表达式, 然后将特征矩阵合理分块, 最后将它们对角化. 从而利用给出的递推关系式得到线性蜘蛛链的特征多项式. 由表达式可以计算出线性蜘蛛链的零度是0, 以及完美匹配数为$(n+2)(n^2+n+1)$. 给出的递推关系式以及组合数学与线性代数相结合的方法还可以用于计算其它具有三对称性的图的特征多项式.

关键词： 线性蜘蛛链；递推关系式；特征多项式

0 Introduction

Let G be a graph with n vertices, and $A(G)$ be its adjacency matrix. $\phi_G(\lambda)=|\lambda I_n - A(G)|$ is the characteristic polynomial of G, and the spectrum of G is the n roots of $\phi_G(\lambda)$. Even though these are classical algebraic concepts, it is amazing that they have close relation with the structure of graphs. Especially, the number of some basic subgraph of G is closely linked to the coefficients of $\phi_G(\lambda)$. This makes it possible to study the structure of graphs by algebraic methods. Obviously, it is extremely hard to give the spectrum or characteristic polynomial for an arbitrary graph with large n. But there are many results showed the spectra or characteristic polynomials for some special classes of graphs, see [1-3] for example.

A chemical structure can be conveniently represented by a graph. As an important example, benzenoid hydrocarbons can be represented by hexagonal systems naturally. The center graph, denoted by G_C, of a hexagonal system is defined to classify hexagonal systems. Each vertex of G_C is placed in the center of a hexagon of G, and two vertices are adjacent if

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the two hexagons are adjacent. A hexagonal system G is called a hexagonal chain if its center graph G_C is a path, and it is called a hexagonal spider if G_C is a tree with exactly one vertex of degree 3 and other vertices of degree 1 or degree 2. Hexagonal chains are graph representations of unbranched catacondensed benzenoid molecules, while hexagonal spiders are graph representation of branched catacondensed benzenoid molecules.

Denote by $m(G)$ the number of matchings of G, and $i(G)$ the number of independent sets of G. In chemical terminology, $m(G)$ and $i(G)$ are called the Hosoya index and Merrifield-Simmons index, respectively. Details of chemical applications of these two indices can be found in [4].

Chen and Zhao[5] computed the Hosoya index and Merrifield-Simmons index of hexagonal chains. Gutman[6] proved that the extremal graph among hexagonal chains of $m(G)$ and $i(G)$ is linear chain L_n, and Shiu[7] proved that the extremal graph among hexagonal spiders of $m(G)$ and $i(G)$ is linear hexagonal spider G_n shown in Fig 1. These works motivated us to find the spectral or characteristic polynomials of linear hexagonal spiders.

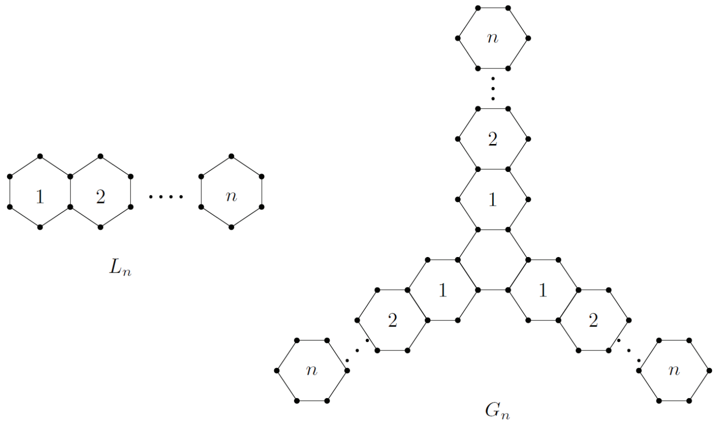

Fig 1 L_n and G_n

The spectrum of L_n can be found in [2], and Gutman determined it in a new way in [3]. This paper aim to give the characteristic polynomial of G_n. In very early years, there are several papers introduced some methods which may be used to calculate the characteristic polynomials of linear hexagonal spiders[8]. However, none of them gives the explicit expression. We develop a method to calculate the characteristic polynomials of linear hexagonal spiders by using the combinatorial techniques. Namely, the recurrence relation shown in Lemma 1. The proof of our main result involves a new technique. An iterative result is used to obtain the characteristic polynomial of the adjacency matrix of the resultant graph. A special case of Lemma 1 has been used to give the spectra of graphs under some operations[9]. This method can also be used to calculate the characteristic polynomial of any graph having threefold symmetry.

Theorem 1 Let G_n be the linear hexagonal spider. Then

$$|\lambda I - A(G_n)| = \frac{1}{4}(s-a)(t+b)(2st-sb-2ab+at)^2,$$

where

$$\begin{aligned} a &= \sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda(\lambda-1))^{n-i}+(-1)^n, \\ b &= \sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda(\lambda+1))^{n-i}+(-1)^n, \\ c &= \sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}(\lambda-1)^{n-i}, \\ d &= \sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}(\lambda+1)^{n-i}, \end{aligned}$$

$s=(\lambda-1)a-c$ and $t=(\lambda+1)b-d$.

In the next section, we will see that when $n = 1$, $s-a = \lambda^3-3\lambda^2+3$, $t+b = \lambda^3+3\lambda^2-3$ and $2st-sb-2ab+at = \lambda^6-6\lambda^4+9\lambda^2-3$, it is easy to see from Eisenstein's Irreducibility Criterion that all of them are irreducible in the rational polynomial ring $Q[x]$. So the expression given in Theorem 1 is best possible in some sense.

We will see from Theorem 1 that for linear hexagonal spider G_n, 0 is not an eigenvalue of G_n. In Hückel molecular orbital theory used in chemistry, this means that the chemical compound whose skeleton is represented by G_n is stable. Also, by Theorem 1, we obtain the number of perfect matchings in G_n is $K(G_n) = (n+2)(n^2+n+1)$.

1 Proof of Theorem 1

In this section, we give the proof of Theorem 1. First, we prove Lemma 1, which is the key of our proof.

Lemma 1 If $a_{2n} = a_{2n-1}D - a_{2n-2}$ and $a_{2n+1} = \lambda a_{2n} - a_{2n-1}$, for $a_0 = C$ and $a_1 = \lambda C - I$, where C and D are square matrices with the same order. Then

$$a_{2n} = C[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda D)^{n-i}+(-1)^nI]-[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}D^{n-i}],$$

and

$$a_{2n+1} = C[\sum_{i=0}^{n}(-1)^i\binom{2n-i+1}{i}\lambda^{n-i+1}D^{n-i}]-[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda D)^{n-i}+(-1)^nI]$$

for $n \geq 1$.

Proof We prove this lemma by induction on n. Note that $a_2 = a_1D - a_0 = C(\lambda D - I) - D$ and $a_3 = \lambda a_2 - a_1 = C(\lambda^2 D - 2\lambda I) - (\lambda D - I)$. We have that Lemma 1 is true for $n = 1$.

Suppose the Lemma 1 is true for n. We have

$$\begin{aligned}
a_{2n+2} &= a_{2n+1}D - a_{2n}\\
&= C[\sum_{i=0}^{n}(-1)^i\tbinom{2n-i+1}{i}(\lambda D)^{n-i+1}]-[\sum_{i=0}^{n-1}(-1)^i\tbinom{2n-i}{i}\lambda^{n-i}D^{n-i+1}+(-1)^nD]\\
&\quad -C[\sum_{i=0}^{n-1}(-1)^i\tbinom{2n-i}{i}(\lambda D)^{n-i}+(-1)^nI]+[\sum_{i=0}^{n-1}(-1)^i\tbinom{2n-i-1}{i}\lambda^{n-i-1}D^{n-i}]\\
&= C[(\lambda D)^{n+1}+\sum_{i=1}^{n}(-1)^i(\tbinom{2n-i+1}{i}+\tbinom{2n-i+1}{i-1})(\lambda D)^{n-i+1}+(-1)^{n+1}I]-\\
&\quad [\lambda^nD^{n+1}+\sum_{i=1}^{n-1}(-1)^i(\tbinom{2n-i}{i}+\tbinom{2n-i}{i-1})\lambda^{n-i}D^{n-i+1}+(-1)^nD+(-1)^nnD]\\
&= C[\sum_{i=0}^{n}(-1)^i\tbinom{2n-i+2}{i}(\lambda D)^{n-i+1}+(-1)^{n+1}I]-[\sum_{i=0}^{n}(-1)^i\tbinom{2n-i+1}{i}\lambda^{n-i}D^{n-i+1}].
\end{aligned}$$

By the same method, we have

$$a_{2n+3} = C[\sum_{i=0}^{n+1}(-1)^i\tbinom{2n-i+3}{i}\lambda^{n-i+2}D^{n-i+1}]-[\sum_{i=0}^{n}(-1)^i\tbinom{2n-i+2}{i}(\lambda D)^{n-i+1}+(-1)^{n+1}I].$$

This completes the proof.

Let G_n be the linear hexagonal spider shown in Fig 1. To calculate the characteristic polynomial of G_n, we first use the recurrence relation in Lemma 1 to drop the order of determinant $|\lambda I - A(G_n)|$. In the following, we always assume that $D = \begin{pmatrix} \lambda I_3 & -I_3 \\ -I_3 & \lambda I_3 \end{pmatrix}$ and $C = \lambda I_6 - A(C_6)$, where C_6 is the cycle of 6 vertices. We give the following lemma.

Lemma 2 Let G_n be the spider hexagonal system graph. Then

$$|\lambda I - A(G_n)| = |C[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda D)^{n-i}+(-1)^nI]-[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}D^{n-i}]| \qquad (1)$$

where $D = \begin{pmatrix} \lambda I_3 & -I_3 \\ -I_3 & \lambda I_3 \end{pmatrix}$, $C = \lambda I_6 - A(C_6)$ and C_6 is the cycle of 6 vertices.

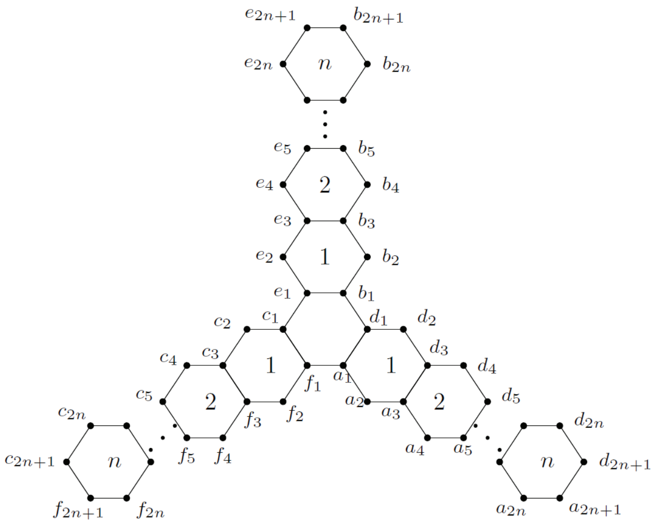

Fig 2 The label

Proof Let $X_i = \{a_i, b_i, c_i, d_i, e_i, f_i\}$ for $i = 1, 2, \cdots, 2n+1$, see Fig 2. We have

$$A = \begin{pmatrix} A(X_1,X_1) & A(X_1,X_2) & A(X_1,X_3) & \cdots & A(X_1,X_{2n}) & A(X_1,X_{2n+1}) \\ A(X_2,X_1) & A(X_2,X_2) & A(X_2,X_3) & \cdots & A(X_2,X_{2n}) & A(X_2,X_{2n+1}) \\ A(X_3,X_1) & A(X_3,X_2) & A(X_3,X_3) & \cdots & A(X_3,X_{2n}) & A(X_3,X_{2n+1}) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ A(X_{2n},X_1) & A(X_{2n},X_2) & A(X_{2n},X_3) & \cdots & A(X_{2n},X_{2n}) & A(X_{2n},X_{2n+1}) \\ A(X_{2n+1},X_1) & A(X_{2n+1},X_2) & A(X_{2n+1},X_3) & \cdots & A(X_{2n+1},X_{2n}) & A(X_{2n+1},X_{2n+1}) \end{pmatrix},$$

where the submatrix $A(X_s, X_t)$ corresponds the row-X_s and column-X_t, say

$$A(X_1,X_1) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \end{pmatrix} \text{ and } A(X_3,X_3) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

Note that $A(X_1, X_1) = A(C_6)$, the adjacency matrix of C_6. Now set $C = \lambda I_6 - A(C_6)$ and $D = \begin{pmatrix} \lambda I_3 & -I_3 \\ -I_3 & \lambda I_3 \end{pmatrix}$. It is easy to verify that $|\lambda I - A(G_n)|$ can be written as

$$|\lambda I - A(G_n)| \quad = \quad \begin{vmatrix} C & -I_6 & 0 & 0 & \cdots & \cdots & 0 \\ -I_6 & \lambda I_6 & -I_6 & 0 & \cdots & \cdots & 0 \\ 0 & -I_6 & D & -I_6 & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & 0 & -I_6 & \lambda I_6 & -I_6 \\ 0 & \cdots & \cdots & 0 & 0 & -I_6 & D \end{vmatrix} \tag{2}$$

For this block matrix, switch the first row with the others one by one, we get

$$|\lambda I - A(G_n)| \quad = \quad \begin{vmatrix} -I_6 & \lambda I_6 & -I_6 & 0 & \cdots & \cdots & 0 \\ 0 & -I_6 & D & -I_6 & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & 0 & -I_6 & \lambda I_6 & -I_6 \\ 0 & \cdots & \cdots & 0 & 0 & -I_6 & D \\ C & -I_6 & 0 & 0 & \cdots & \cdots & 0 \end{vmatrix} \tag{3}$$

Assume $a_0 = C$, $a_1 = \lambda C - I$, $a_2 = a_1 D - a_0$, $a_3 = \lambda a_2 - a_1$, $\cdots$, $a_{2k} = a_{2k-1}D - a_{2k-2}$, $a_{2k+1} = \lambda a_{2k} - a_{2k-1}$, $\cdots$. For block matrix (3), multiply its ith row by a_{i-1} from the left and then add to the last row successively for $i = 1, \cdots, 2n$, we obtain

$$|\lambda I - A(G_n)| = \begin{vmatrix} -I_6 & \lambda I_6 & -I_6 & 0 & \cdots & \cdots & 0 \\ 0 & -I_6 & D & -I_6 & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & \cdots & \cdots & 0 & -I_6 & \lambda I_6 & -I_6 \\ 0 & \cdots & \cdots & 0 & 0 & -I_6 & D \\ 0 & 0 & 0 & 0 & \cdots & \cdots & h_{2n} \end{vmatrix} \tag{4}$$

So $|\lambda I - A(G_n)| = |a_{2n}|$. By Lemma 1, we complete the proof.

The determinant on the right of equation (1) in Lemma 2 is a determinant of a matrix polynomial with respect to D and C, both of them have order six. To compute this determinant we need to diagonalize D.

Lemma 3 Let $D = \begin{pmatrix} \lambda I_3 & -I_3 \\ -I_3 & \lambda I_3 \end{pmatrix}$. Then $D = T\Lambda T^{-1}$, where

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 \end{pmatrix},$$

$$\Lambda = \begin{pmatrix} \lambda-1 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda-1 & 0 & 0 & 0 & 0 \\ 0 & 0 & \lambda-1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \lambda+1 & 0 & 0 \\ 0 & 0 & 0 & 0 & \lambda+1 & 0 \\ 0 & 0 & 0 & 0 & 0 & \lambda+1 \end{pmatrix}$$

and $T = T^T = T^{-1}$.

Proof One can easily verify Lemma 3 by hand.

For the preparation work to calculate the characteristic polynomial of G_n, we firstly define four polynomials with respect to λ bellow.

$$a = \sum_{i=0}^{n-1} (-1)^i \binom{2n-i}{i} (\lambda(\lambda-1))^{n-i} + (-1)^n \tag{5}$$

$$b = \sum_{i=0}^{n-1} (-1)^i \binom{2n-i}{i} (\lambda(\lambda+1))^{n-i} + (-1)^n \tag{6}$$

$$c = \sum_{i=0}^{n-1} (-1)^i \binom{2n-i-1}{i} \lambda^{n-i-1} (\lambda-1)^{n-i} \tag{7}$$

$$d = \sum_{i=0}^{n-1} (-1)^i \binom{2n-i-1}{i} \lambda^{n-i-1} (\lambda+1)^{n-i} \tag{8}$$

Lemma 4 Let G_n be the spider hexagonal system graph shown in Fig 1. Then

$$|\lambda I - A(G_n)| = \frac{1}{4}(\lambda a - 2a - c)(\lambda b + 2b - d)(ad + 2cd - 2\lambda bc - 2\lambda ad + 2\lambda^2 ab - 2ab - bc)^2.$$

Proof By Lemma 2,

$$|\lambda I-A(G_n)| \;=\; |C[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}(\lambda D)^{n-i}+(-1)^n I]-[\sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}D^{n-i}]|.$$

Set $f_1(x)=\sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}\lambda^{n-i}x^{n-i}+(-1)^n$ and $f_2(x)=\sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}x^{n-i}$, then we have $|\lambda I-A(G_n)|=|Cf_1(D)-f_2(D)|$. By Lemma 3, $D=T\Lambda T^{-1}$ and so $f_i(D)=Tf_i(\Lambda)T^{-1}$ for $i=1,2$. Thus, $|\lambda I-A(G_n)|=|CTf_1(\Lambda)T^{-1}-Tf_2(\Lambda)T^{-1}|$. Clearly, $f_1(\Lambda)$ and $f_2(\Lambda)$ are also diagonal matrices, where

$$f_1(\Lambda)=diag(f_1(\lambda-1),f_1(\lambda-1),f_1(\lambda-1),f_1(\lambda+1),f_1(\lambda+1),f_1(\lambda+1)),$$

and

$$f_2(\Lambda)=diag(f_2(\lambda-1),f_2(\lambda-1),f_2(\lambda-1),f_2(\lambda+1),f_2(\lambda+1),f_2(\lambda+1)).$$

From the definition of a,b,c and d, we can see that $a=f_1(\lambda-1)$, $b=f_1(\lambda+1)$, $c=f_2(\lambda-1)$ and $d=f_2(\lambda+1)$. Then let $\Lambda_1=f_1(\Lambda)=diag(a,a,a,b,b,b)$ and $\Lambda_2=f_2(\Lambda)=diag(c,c,c,d,d,d)$. We have $|\lambda I-A(G_n)|=|CT\Lambda_1T^{-1}-T\Lambda_2T^{-1}|$, which is a matrix of order six. So the result is easily given by Maple.

If we define $s=(\lambda-1)a-c$, then

$$\begin{aligned}
s &= (\lambda-1)a-c\\
&= \sum_{i=0}^{n-1}(-1)^i\binom{2n-i}{i}\lambda^{n-i}(\lambda-1)^{n-i+1}+(-1)^n(\lambda-1)-\sum_{i=0}^{n-1}(-1)^i\binom{2n-i-1}{i}\lambda^{n-i-1}(\lambda-1)^{n-i}\\
&= \lambda^n(\lambda-1)^{n+1}+\sum_{i=1}^{n-1}(-1)^i(\binom{2n-i}{i}+\binom{2n-i}{i-1})\lambda^{n-i}(\lambda-1)^{n-i+1}+(-1)^n(n+1)(\lambda-1)\\
&= \sum_{i=0}^{n}(-1)^i\binom{2n-i+1}{i}\lambda^{n-i}(\lambda-1)^{n-i+1} \qquad (9)
\end{aligned}$$

Similarly, if we define $t=(\lambda+1)b-d$, then

$$t=\sum_{i=0}^{n}(-1)^i\binom{2n-i+1}{i}\lambda^{n-i}(\lambda+1)^{n-i+1} \qquad (10)$$

By the definition of s and t, we get Theorem 1 immediately from Lemma 4.

2 Further Discussions

Since each of a, b, s and t in Theorem 1 is a polynomial in λ, they can be written in standard form. For (5), (6), (9) and (10), expanding $(\lambda-1)^{n-i}$ and $(\lambda+1)^{n-i}$ by Newton's binomial theorem gives the coefficients of λ^k. Define $\binom{n}{m}=0$ if $m<0$, we obtain the polynomials

$$a \;=\; \sum_{k=0}^{2n}[\sum_{i=n-k}^{n-\lceil\frac{k}{2}\rceil}(-1)^{i+k}\binom{2n-i}{i}\binom{n-i}{2(n-i)-k}]\lambda^k \qquad (11)$$

$$b \;=\; \sum_{k=0}^{2n}[\sum_{i=n-k}^{n-\lceil\frac{k}{2}\rceil}(-1)^{i}\binom{2n-i}{i}\binom{n-i}{2(n-i)-k}]\lambda^k \qquad (12)$$

$$s \;=\; \sum_{k=0}^{2n+1}[\sum_{i=n-k}^{n-\lfloor\frac{k}{2}\rfloor}(-1)^{i+k+1}\binom{2n-i+1}{i}\binom{n-i+1}{2(n-i)-k+1}]\lambda^k \qquad (13)$$

and

$$t \;=\; \sum_{k=0}^{2n+1}[\sum_{i=n-k}^{n-\lfloor\frac{k}{2}\rfloor}(-1)^{i}\binom{2n-i+1}{i}\binom{n-i+1}{2(n-i)-k+1}]\lambda^k \qquad (14)$$

So the coefficient of λ^k in $s-a$ is

$$\sum_{i=n-k}^{n-\lfloor \frac{k}{2} \rfloor}(-1)^{i+k+1}\binom{2n-i+1}{i}\binom{n-i+1}{2(n-i)-k+1}-\sum_{i=n-k}^{n-\lceil \frac{k}{2} \rceil}(-1)^{i+k}\binom{2n-i}{i}\binom{n-i}{2(n-i)-k},$$

and the coefficient of λ^k in $t+b$ is

$$\sum_{i=n-k}^{n-\lfloor \frac{k}{2} \rfloor}(-1)^{i}\binom{2n-i+1}{i}\binom{n-i+1}{2(n-i)-k+1}+\sum_{i=n-k}^{n-\lceil \frac{k}{2} \rceil}(-1)^{i}\binom{2n-i}{i}\binom{n-i}{2(n-i)-k}.$$

We can see from above that the coefficient of λ^k in $s-a$ is equal to the coefficient of λ^k in $t+b$ when k is odd and they are opposite when k is even. So if λ_i is a root of $s-a$ then $-\lambda_i$ is a root of $t+b$, i.e., the roots of $s-a$ and the roots of $t+b$ are symmetric about the origin. Meanwhile, from (11)~(14) we can see that $a_k(a) = -a_k(b)$, $a_k(s) = a_k(t)$ when k is odd and $a_k(a) = a_k(b)$, $a_k(s) = -a_k(t)$ when k is even, where $a_k(f)$ is the coefficient of λ^k in f. So the coefficient of λ^k in $(2st-sb-2ab+at)$ is zero when k is odd. It means that the roots of $(2st-sb-2ab+at)$ are symmetric about the origin either.

From (11)~(14) we can see that the coefficient of λ^0 in $\phi_{G_n}(\lambda)$ is equal to $-(n+2)^2(n^2+n+1)^2$. Thus, we have the following result.

Corollary 1 Let G_n be the linear hexagonal spider G_n. Then 0 is not the eigenvalue of G_n.

From Theorem 1, we can get the number of perfect matchings of linear hexagonal spider. In fact, a perfect matching (1-factor) is a Kekulé structure of a benzenoid hydrocarbon system. Kekulé structures are used in resonance theory and *ab initio* valence bond theory. The number of Kekulé structures is denoted by K. So, we denote by $K(G)$, the number of perfect matchings in graph G. The remarkable Dewar-Longuet-Higgins formula states that $\det A(G) = (-1)^{\frac{|V(G)|}{2}} K(G)^2$[10]. So we have the following corollary.

Corollary 2 Let G_n be the linear hexagonal spider G_n. Then the number of perfect matchings in G_n is $K(G_n) = (n+2)(n^2+n+1)$.

Proof By Dewar-Longuet-Higgins formula, $\det A(G) = (-1)^{|V(G_n)|}(-(n+2)^2(n^2+n+1)^2) = (-1)^{\frac{|V(G_n)|}{2}} K(G)^2$. The result follows from the fact that $|V(G_n)| = 12n+6$.

Theorem 1 gives an explicit expression for the characteristic polynomial of linear hexagonal spider G_n. Using this theorem, one can easily calculate the characteristic polynomial of G_n by computer for each given n. For examples, we give the expressions of $\phi_{G_n}(\lambda)$ for $n = 1,2,3,4$ with the help of Maple.

$$\phi_{G_1}(\lambda) = \left(\lambda^3-3\lambda^2+3\right)\left(\lambda^3+3\lambda^2-3\right)\left(\lambda^6-6\lambda^4+9\lambda^2-3\right)^2,$$

$$\begin{aligned}\phi_{G_2}(\lambda) &= (\lambda-2)(\lambda+2)\left(\lambda^4-2\lambda^3-3\lambda^2+3\lambda+2\right)\left(\lambda^4+2\lambda^3-3\lambda^2-3\lambda+2\right)\\ &\quad (\lambda-1)^2(\lambda+1)^2\left(\lambda^8-10\lambda^6+31\lambda^4-33\lambda^2+7\right)^2,\end{aligned}$$

$$\begin{aligned}\phi_{G_3}(\lambda) &= \left(\lambda^7+5\lambda^6+3\lambda^5-16\lambda^4-16\lambda^3+15\lambda^2+12\lambda-5\right)\\ &\quad \left(\lambda^7-5\lambda^6+3\lambda^5+16\lambda^4-16\lambda^3-15\lambda^2+12\lambda+5\right)\\ &\quad \left(\lambda^{14}-16\lambda^{12}+98\lambda^{10}-295\lambda^8+465\lambda^6-373\lambda^4+132\lambda^2-13\right)^2,\end{aligned}$$

$$\begin{aligned}\phi_{G_4}(\lambda) &= (\lambda-2)(\lambda+2)(\lambda^8+4\lambda^7-2\lambda^6-19\lambda^5-\lambda^4+29\lambda^3-14\lambda+3)\\ &\quad (\lambda^8-4\lambda^7-2\lambda^6+19\lambda^5-\lambda^4-29\lambda^3+14\lambda+3)(\lambda-1)^2(\lambda+1)^2\\ &\quad (\lambda^{16}-20\lambda^{14}+160\lambda^{12}-661\lambda^{10}+1518\lambda^8-1931\lambda^6+1259\lambda^4-340\lambda^2+21)^2.\end{aligned}$$

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