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On the Characteristic Polynomial and the Spectrum of a Hexagonal System[1]

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Abstract

The hexagonal system considered here is the graph, denoted by H_3^n, which is formed by $3n-1$ ($n \geq 2$) hexagons and usually called prolate rectangle of benzenoid system in theoretical chemistry. In this paper, we give the explicit expressions of characteristic polynomial $\phi(H_3^n)$. Additionally, the spectral radius and the multiplicity of eigenvalues ± 1 of H_3^n are determined. By the way, we obtain the number of Kekulé structures and nullity of H_3^n which agree with the known result.

1. INTRODUCTION

Generally, a *hexagonal system* (benzenoid hydrocarbon) is 2-connected plan graph such that each of its interior face is bonded by a regular hexagon of unit length 1. The mathematical theory of hexagonal systems and its relevance to chemistry are presented in [1–3].

It is well-known that the theory of graph spectra is related to the Chemistry through the HMO (Hückel Molecular Orbital) Theory (see [2] for an extensive review on the topic),

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in which there are some problems to attract our attentions. One is posed by Günthad in [4] that if the (molecular) graph is determined by the spectrum of the corresponding graph? For the researches of the spectral determined problem one can refer to [5, 6]. As our knowledge, the spectrum of hexagonal systems L_n and F_n shown in Fig.1 are found in [7, 8]. Zhang and Zhou give the explicit expressions of characteristic polynomials of an homologous series of benzenoid systems in [9], however, the spectra of other hexagonal systems are not known. Denote by $\eta(G)$ the algebraic multiplicity of eigenvalue 0 in the spectrum of the (bipartite) graph G, which is normally called the *nullity* of G. A *Kekulé structure* K of a hexagonal system H corresponds to a perfect matching (1-factor) of H. The remarkable Dewar-Longuet-Higgins formula states that $\det A(G) = (-1)^{\frac{n}{2}} K^2$. The nullity and the number of Kekulé structures of a graph are two indexes related to chemical properties of hexagonal systems. For the corresponding researches, one can refer to [1, 6, 10, 11] for references.

Let H_3^n be a hexagonal system shown in Fig.2. In this paper, we focus to determine characteristic polynomials of H_3^n, which can be represented by the Q-spectrum of the path in section 3. Furthermore, we give the spectral radius of H_3^n and determine the multiplicity of eigenvalues ± 1 of H_3^n. By the way, we get the number of Kekulé structures and nullity of H_3^n which agree with a result obtained by T.F.Yen in [12].

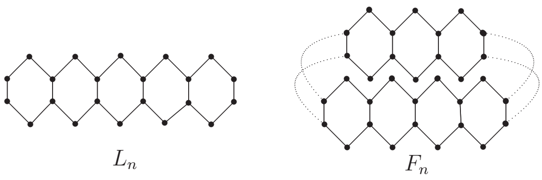

Figure 1: Hexagonal systems L_n and F_n

2. ELEMENTARY

All graphs considered in the paper are simple and undirected. Let G be a graph with adjacency matrix $A(G)$. Its vertices are labeled by $V(G) = \{1, 2, \ldots\}$ and d_i denotes the degree of vertex i. Denote by $\phi_G(\lambda) = |\lambda I_n - A(G)|$ the *characteristic polynomial* of G. The multiset of eigenvalues of $A(G)$ is called the *adjacency spectrum*, or simply the *spectrum*. The largest eigenvalue $\rho(G)$ is called the *spectral radius* of G. Denote by D the diagonal matrix $diag(d_1, \ldots, d_n)$, and $Q(G) = A(G) + D$ the *signless Laplacian matrix* of G. The characteristic polynomial $Q_G(\lambda) = |\lambda I_n - Q(G)|$ is called the *Q-polynomial* of G and the multiset of eigenvalues of $Q(G)$ is called the *Q-spectrum*.

Let P_{n+1} be a path on $n+1$ vertices. Throughout this paper, we will denote the signless Laplacian matrix of P_{n+1} by $\mathbf{Q}$, i.e., $\mathbf{Q} = Q(P_{n+1})$, and B_n^{T} is the incidence matrix of P_{n+1}. It is clear that

$$B_n^{\mathrm{T}} B_n = \begin{pmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & \ddots & \\ & & \ddots & 1 \\ & & & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \end{pmatrix} = A(P_{n+1}) + D(P_{n+1}) = \mathbf{Q}.$$

In the rest of this section, we will cite some known results for the later use.

Lemma 2.1. [13] Let P_n be the path on n vertices. Then the *Q-polynomial* of P_n is

$$Q_{P_n}(q) = \prod_{j=1}^{n} (q - 2 - 2\cos\frac{\pi j}{n}).$$

It is immediately follows the result from Lemma 2.1.

Corollary 2.1. The eigenvalues of $\mathbf{Q} = Q(P_{n+1})$ are $q_j = 2+2\cos\frac{\pi j}{n+1}, \quad j = 1, 2, \ldots, n+1.$

The following result is well known.

Lemma 2.2. Let A and B be $n \times n$ matrices. Then $\begin{vmatrix} A & B \\ B & A \end{vmatrix} = |A+B||A-B|$.

Lemma 2.3. [6] For a connected graph G and $H \subset G$, we have $\rho(G) < \rho(H)$.

Denote by $r_0(f(x))$ the largest root of polynomial $f(x)$.

Lemma 2.4. [14] If $f_i(x) < f_j(x)$ for any $x \geq r_0(f_j(x))$, then $r_0(f_i(x)) > r_0(f_j(x))$.

Lemma 2.5. [6] Let $\mu_j(G)$ be the j-th largest Laplacian eigenvalue of G, and $\mu_1(G) \geq \ldots \geq \mu_{n-1}(G) \geq \mu_n(G) = 0$. Then $\tau(G) = \frac{1}{n}\prod_{j=1}^{n-1}\mu_j(G)$, where $\tau(G)$ is the number of spanning tree.

Lemma 2.6. Let q_j be the j-th largest Q-eigenvalue of the path P_{n+1}. Then $\prod_{j=1}^{n} q_j = n+1$.

Proof. Let μ_j be the Laplacian eigenvalues of P_{n+1}, where $j = 1, 2, \ldots, n+1$. By Lemma 2.5, we have $\frac{1}{n+1}\prod_{j=1}^{n}\mu_j = \tau(P_{n+1}) = 1$, and so $\prod_{j=1}^{n}\mu_j = n+1$. Since P_{n+1} is a bipartite graph, $q_j = \mu_j (j = 1, 2, \ldots, n+1)$. Thus we have $\prod_{j=1}^{n} q_j = \prod_{j=1}^{n}\mu_j = n+1$. ■

Lemma 2.7. [1] Let graph G has n vertices and K be the number of Kekulé structures of G. Then $\det A(G) = (-1)^{\frac{n}{2}} K^2$.

3. THE CHARACTERISTIC POLYNOMIAL OF H_3^n

In this section, we will give an explicit expression for the characteristic polynomial of hexagonal system H_3^n which is labeled in Fig.2, where $n \geq 2$.

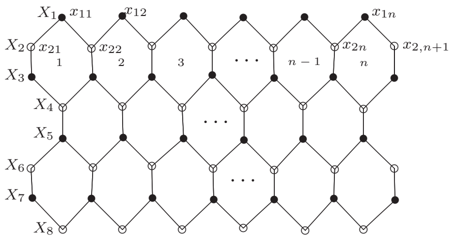

Figure 2: A coordinate label for vertices of H_3^n

The vertex set $V(H_3^n)$ is partitioned into eight parts: $V(H_3^n) = X_1 \cup X_2 \cup \cdots \cup X_8$, where $X_1 = \{x_{11}, x_{12}, ..., x_{1n}\}$, $X_2 = \{x_{21}, x_{22}, ..., x_{2,n+1}\}$ and so on (see Fig.2).

It is easy to see that H_3^n has $3n-1$ hexagons and $|V(H_3^n)| = 8n+4$. Let $A(H_3^n)$ be the adjacency matrix of H_3^n. For $1 \leq i, j \leq 8$, let $A(X_i, X_j) = (a_{kl})$ denote the block matrix of $A(H_3^n)$ corresponding X_i (the row-set) and X_j (the column-set). Clearly, $A(X_j, X_i)$ is the transpose of $A(X_i, X_j)$. To exactly $a_{kl} = 1$ if $x_{ik} \in X_i$ is adjacent with $x_{jl} \in X_j$ in H_3^n, and $a_{kl} = 0$ otherwise. For instance,

$$A(X_1, X_2) = \begin{array}{c} \\ x_{11} \\ x_{12} \\ x_{13} \\ \vdots \\ x_{1n} \end{array} \begin{array}{c} x_{21} \; x_{22} \; \cdots \; x_{2n} \; x_{2,n+1} \\ \begin{pmatrix} 1 & 1 & & & \\ & 1 & 1 & & \\ & & 1 & & \\ & & \ddots & \ddots & \\ & & & 1 & 1 \end{pmatrix}_{n \times (n+1)} \end{array} = B_n.$$

Thus, in accordance with the partition of vertices in Fig.2, we see that

$$\begin{cases} A(X_1, X_2) = A(X_5, X_6) = B_n, \\ A(X_2, X_3) = A(X_6, X_7) = I_{n+1}, \\ A(X_3, X_4) = A(X_7, X_8) = B_n^{\mathrm{T}}, \\ A(X_4, X_5) = I_n. \end{cases}$$

and the other block matrix $A(X_i, X_j)$ equals 0. Thus the adjacency matrix of H_3^n can be represented in the form of block-matrix according to the ordering of $X_1, X_2, ..., X_8$ as following.

$$A(H_3^n) = \left(\begin{array}{cccccccc} 0 & B_n & & & & & & \\ B_n^{\mathrm{T}} & 0 & I_{n+1} & & & & & \\ & I_{n+1} & 0 & B_n^{\mathrm{T}} & & & & \\ & & B_n & 0 & I_n & & & \\ & & & I_n & 0 & B_n & & \\ & & & & B_n^{\mathrm{T}} & 0 & I_{n+1} & \\ & & & & & I_{n+1} & 0 & B_n^{\mathrm{T}} \\ & & & & & & B_n & 0 \end{array}\right) \begin{array}{c} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \end{array} \tag{1}$$

Now we give our main result bellow.

Theorem 3.1. Let H_3^n be a hexagonal system with $3n-1$ hexagons shown in Fig.2. Then the characteristic polynomial of H_3^n is given bellow:

$$\phi_{H_3^n}(\lambda) = (\lambda^2-1)^2 \prod_{j=1}^{n} \varphi_j(\lambda)\psi_j(\lambda), \tag{2}$$

where $\begin{cases} \varphi_j(\lambda) & = \lambda^4+\lambda^3-(2q_j+1)\lambda^2-(q_j+1)\lambda+q_j^2 \\ \psi_j(\lambda) & = \lambda^4-\lambda^3-(2q_j+1)\lambda^2+(q_j+1)\lambda+q_j^2 \end{cases}$
and $\quad q_j = 2+2\cos\frac{\pi j}{n+1}$.

Proof. First we express $\phi_{H_3^n}(\lambda)$ in the form of determinant according to Eq. (1)

$$\phi_{H_3^n}(\lambda) = \left|\lambda I_{8n+4} - A(H_3^n)\right| = \det M_0 \tag{3}$$

where

$$M_0 = \lambda I_{8n+4} - A(H_3^n) = \begin{pmatrix} \lambda I_n & -B_n & & & & & & \\ -B_n^{\mathrm{T}} & \lambda I_{n+1} & -I_{n+1} & & & & & \\ & -I_{n+1} & \lambda I_{n+1} & -B_n^{\mathrm{T}} & & & & \\ & & -B_n & \lambda I_n & -I_n & & & \\ & & & -I_n & \lambda I_n & -B_n & & \\ & & & & -B_n^{\mathrm{T}} & \lambda I_{n+1} & -I_{n+1} & \\ & & & & & -I_{n+1} & \lambda I_{n+1} & -B_n^{\mathrm{T}} \\ & & & & & & -B_n & \lambda I_n \end{pmatrix}_{8\times 8}.$$

Denote by P_1, P_2, P_3, P_4 the elementary block matrices bellow,

$$P_1 = \begin{pmatrix} I_n & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{B_n^{\mathrm{T}}}{\lambda} & I_{n+1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{n+1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_n & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{n+1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{n+1} & \frac{B_n^{\mathrm{T}}}{\lambda} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & I_n \end{pmatrix}, \quad P_2 = \begin{pmatrix} I_n & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I_{n+1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{n+1} & \frac{B_n^{\mathrm{T}}}{\lambda} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & I_n & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{I_n}{\lambda} & I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & I_{n+1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I_{n+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & I_n \end{pmatrix},$$

$$P_3 = \begin{pmatrix} I_n & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & I_{n+1} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & I_{n+1} & 0 & \frac{B_n^{\mathrm{T}}}{\lambda^2-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & I_n & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{\lambda B_n^{\mathrm{T}}}{\lambda^2-1} & I_{n+1} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & I_{n+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & I_n \end{pmatrix}, \quad P_4 = \begin{pmatrix} I_{n+1} & \lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda} & 0 & 0 \\ 0 & I_{n+1} & 0 & 0 \\ 0 & 0 & I_{n+1} & 0 \\ 0 & 0 & \lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda} & I_{n+1} \end{pmatrix}.$$

Clearly, $\det P_1 = \det P_2 = \det P_3 = \det P_4 = 1$.

By multiplying $\frac{B_n^{\mathrm{T}}}{\lambda}$ to the first block row of M_0, and then add it to the second block row of M_0; afterwards, by multiplying $\frac{B_n^{\mathrm{T}}}{\lambda}$ to the last block row of M_0, and then add it next to last block row of M_0. Thus we obtain

$$P_1 \cdot M_0 = M_1 \tag{4}$$

where

$$M_1 = \begin{pmatrix} \lambda I_n & -B_n & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & -I_{n+1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -I_{n+1} & \lambda I_{n+1} & -B_n^{\mathrm{T}} & 0 & 0 & 0 & 0 \\ 0 & 0 & -B_n & \lambda I_n & -I_n & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_n & \lambda I_n & -B_n & 0 & 0 \\ 0 & 0 & 0 & 0 & -B_n^{\mathrm{T}} & \lambda I_{n+1} & -I_{n+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & -I_{n+1} & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -B_n & \lambda I_n \end{pmatrix}.$$

By multiplying $\frac{B_n^{\mathrm{T}}}{\lambda}$ to the 4th-block row of M_1, and then add it to the 3th-block row of M_1; afterwards, by multiplying $\frac{1}{\lambda}$ to the 4th-block row of M_1, and then add it to the 5th-block row of M_1. Now we obtain

$$P_2 \cdot M_1 = M_2 \tag{5}$$

where

$$M_2 = \begin{pmatrix} \lambda I_n & -B_n & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & -I_{n+1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -I_{n+1} & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & 0 & \frac{-B_n^{\mathrm{T}}}{\lambda} & 0 & 0 & 0 \\ 0 & 0 & -B_n & \lambda I_n & -I_n & 0 & 0 & 0 \\ 0 & 0 & \frac{-B_n}{\lambda} & 0 & (\lambda - \frac{1}{\lambda}) I_n & -B_n & 0 & 0 \\ 0 & 0 & 0 & 0 & -B_n^{\mathrm{T}} & \lambda I_{n+1} & -I_{n+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & -I_{n+1} & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -B_n & \lambda I_n \end{pmatrix}.$$

By multiplying $\frac{B_n^{\mathrm{T}}}{\lambda^2 - 1}$ to the 5th-block row of M_2, and then add it to the 3th-block row of M_2; afterwards, by multiplying $\frac{\lambda B_n^{\mathrm{T}}}{\lambda^2 - 1}$ to the 5th-block row of M_2, and then add it to the 6th-block row of M_2, we obtain

$$P_3 \cdot M_2 = M_3 \tag{6}$$

where

$$M_3 = \begin{pmatrix} \lambda I_n & -B_n & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & -I_{n+1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -I_{n+1} & \lambda I_{n+1} - \frac{\lambda B_n^{\mathrm{T}} B_n}{\lambda^2 - 1} & 0 & 0 & -\frac{B_n^{\mathrm{T}} B_n}{\lambda^2 - 1} & 0 & 0 \\ 0 & 0 & -B_n & \lambda I_n & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{B_n^{\mathrm{T}}}{\lambda} & 0 & (\lambda - \frac{1}{\lambda}) I_n & -B_n & 0 & 0 \\ 0 & 0 & -\frac{\lambda B_n^{\mathrm{T}} B_n}{\lambda^2 - 1} & 0 & 0 & \lambda I_{n+1} - \frac{\lambda B_n^{\mathrm{T}} B_n}{\lambda^2 - 1} & -I_{n+1} & 0 \\ 0 & 0 & 0 & 0 & 0 & -I_{n+1} & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -B_n & \lambda I_n \end{pmatrix}.$$

Now we expand the determinant M_3 according to its 1th-, 4th-, 5th- and 8th-columns and obtain

$$\det M_3 = \lambda^{2n}(\lambda^2-1)^n \det M_4 \tag{7}$$

where

$$M_4 = \begin{pmatrix} \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} & -I_{n+1} & & \\ -I_{n+1} & \lambda I_{n+1} - \frac{\lambda B_n^{\mathrm{T}} B_n}{\lambda^2-1} & -\frac{B_n^{\mathrm{T}} B_n}{\lambda^2-1} & \\ & -\frac{B_n^{\mathrm{T}} B_n}{\lambda^2-1} & \lambda I_{n+1} - \frac{\lambda B_n^{\mathrm{T}} B_n}{\lambda^2-1} & -I_{n+1} \\ & & -I_{n+1} & \lambda I_{n+1} - \frac{B_n^{\mathrm{T}} B_n}{\lambda} \end{pmatrix}.$$

Recall that $B_n^{\mathrm{T}} B_n = \mathbf{Q}$. By multiplying $(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})$ to the 2th-block row of M_4, and then add it to the first row of M_4; afterwards, by multiplying $(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})$ to the 3th-block row of M_4, and then add it to the 4th-block row of M_4, we obtain

$$P_4 \cdot M_4 = M_5. \tag{8}$$

$$M_5 = \begin{pmatrix} 0 & (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} & -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) & 0 \\ -I_{n+1} & \lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1} & -\frac{\mathbf{Q}}{\lambda^2-1} & 0 \\ 0 & -\frac{\mathbf{Q}}{\lambda^2-1} & \lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1} & -I_{n+1} \\ 0 & -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) & (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} & 0 \end{pmatrix}.$$

Now we expand the determinant M_5 spread determinant of according to its 1th- and 4th-columns and obtain

$$\det M_5 = \det M_6 \tag{9}$$

where

$$M_6 = \begin{pmatrix} (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} & -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) \\ -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) & (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} \end{pmatrix}.$$

By Lemma 2.2, we have

$$\begin{aligned} \det M_6 &= \begin{vmatrix} (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} & -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) \\ -\frac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda}) & (\lambda I_{n+1} - \frac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \frac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} \end{vmatrix} \\ &= \left| (\lambda I_{n+1} - \tfrac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \tfrac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} + \tfrac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \tfrac{\mathbf{Q}}{\lambda}) \right| \\ &\quad \times \left| (\lambda I_{n+1} - \tfrac{\mathbf{Q}}{\lambda})(\lambda I_{n+1} - \tfrac{\lambda \mathbf{Q}}{\lambda^2-1}) - I_{n+1} - \tfrac{\mathbf{Q}}{\lambda^2-1}(\lambda I_{n+1} - \tfrac{\mathbf{Q}}{\lambda}) \right| \\ &= \left| \frac{\mathbf{Q}^2}{\lambda(\lambda+1)} + \frac{(-2\lambda-1)\mathbf{Q}}{\lambda+1} + (\lambda^2-1) I_{n+1} \right| \left| \frac{\mathbf{Q}^2}{\lambda(\lambda-1)} + \frac{(-2\lambda+1)\mathbf{Q}}{\lambda-1} + (\lambda^2-1) I_{n+1} \right|. \end{aligned}$$

Combining the above terms of Eqs. (3)-(9), we have

$$\begin{aligned} \phi_{H_3^n}(\lambda) &= \det M_0 = \lambda^{2n}(\lambda^2-1)^n \det M_6 \\ &= \lambda^{2n}(\lambda^2-1)^n \left| \tfrac{\mathbf{Q}^2}{\lambda(\lambda+1)} + \tfrac{(-2\lambda-1)\mathbf{Q}}{\lambda+1} + (\lambda^2-1) I_{n+1} \right| \left| \tfrac{\mathbf{Q}^2}{\lambda(\lambda-1)} + \tfrac{(-2\lambda+1)\mathbf{Q}}{\lambda-1} + (\lambda^2-1) I_{n+1} \right| \\ &= \frac{1}{\lambda^2(\lambda^2-1)} \left| \mathbf{Q}^2 + \lambda(-2\lambda-1)\mathbf{Q} + \lambda(\lambda+1)(\lambda^2-1) I_{n+1} \right| \left| \mathbf{Q}^2 + \lambda(-2\lambda+1)\mathbf{Q} + \lambda(\lambda-1)(\lambda^2-1) I_{n+1} \right| \end{aligned} \tag{10}$$

Set $F(\mathbf{Q}) = \mathbf{Q}^2 + \lambda(-2\lambda - 1)\mathbf{Q} + \lambda(\lambda + 1)(\lambda^2 - 1)I_{n+1}$ and $G(\mathbf{Q}) = \mathbf{Q}^2 + \lambda(-2\lambda + 1)\mathbf{Q} + \lambda(\lambda - 1)(\lambda^2 - 1)I_{n+1}$. From Corollary 2.1, $\mathbf{Q}$ has eigenvalues: $q_j = 2 + 2\cos\frac{\pi j}{n+1}$, $j = 1, 2, \ldots, n+1$ (especially, $q_j = 0$ if $j = n+1$). It follows that the determinant of $F(\mathbf{Q})$ can be explicitly presented by

$$\begin{aligned} |F(\mathbf{Q})| &= \prod_{j=1}^{n+1}[q_j^2 + \lambda(-2\lambda - 1)q_j + \lambda(\lambda+1)(\lambda^2 - 1)] \\ &= \lambda(\lambda+1)(\lambda^2-1)\prod_{j=1}^{n}[q_j^2 + (-2\lambda^2 - \lambda)q_j + \lambda(\lambda+1)(\lambda^2-1)] \\ &= \lambda(\lambda+1)(\lambda^2-1)\prod_{j=1}^{n}\varphi_j(\lambda), \end{aligned}$$

where $\varphi_j(\lambda) = \lambda^4 + \lambda^3 - (2q_j + 1)\lambda^2 - (q_j + 1)\lambda + q_j^2$. Similarly, we obtain

$$|G(\mathbf{Q})| = \lambda(\lambda - 1)(\lambda^2 - 1)\prod_{j=1}^{n}\psi_j(\lambda),$$

where $\psi_j(\lambda) = \lambda^4 - \lambda^3 - (2q_j + 1)\lambda^2 + (q_j + 1)\lambda + q_j^2$. Finally, from Eq. (10) we get

$$\phi_{H_3^n}(\lambda) = \frac{1}{\lambda^2(\lambda^2 - 1)}|F(\mathbf{Q})||G(\mathbf{Q})| = (\lambda^2 - 1)^2\prod_{j=1}^{n}\varphi_j(\lambda)\psi_j(\lambda).$$

At last we mention that the above discussions are true whenever $\lambda \neq 0$. It implies that our formula (2) is also valid for $\lambda = 0$ since $\phi_{H_3^n}(\lambda)$ is a polynomial of $8n+4$ degree which is uniquely determined by its $8n + 4$ roots. It completes the proof. ■

By using Theorem 3.1 we give an example to find the characteristic polynomial and spectrum of H_3^n for $n = 2$.

Example 1. *For $n = 2$, H_3^n has 5 hexagons and 20 vertices. By Theorem 3.1, $q_1 = 3$, $q_2 = 1$, the corresponding $\varphi_i(\lambda)$ and $\psi_i(\lambda)$ are*

$$\begin{aligned} \varphi_1(\lambda) &= \lambda^4 + \lambda^3 - 7\lambda^2 - 4\lambda + 9, \quad \varphi_2(\lambda) = \lambda^4 + \lambda^3 - 3\lambda^2 - 2\lambda + 1, \\ \psi_1(\lambda) &= \lambda^4 - \lambda^3 - 7\lambda^2 + 4\lambda + 9, \quad \psi_2(\lambda) = \lambda^4 - \lambda^3 - 3\lambda^2 + 2\lambda + 1. \end{aligned}$$

By simple calculation, we obtain the characteristic polynomial of H_3^2 from Eq. (2):

$$\begin{aligned} \phi(H_3^2) &= (\lambda^2 - 1)^2\prod_{i=1}^{2}\varphi_i(\lambda)\psi_i(\lambda) \\ &= \lambda^{20} - 24\lambda^{18} + 240\lambda^{16} - 1314\lambda^{14} + 4350\lambda^{12} - 9066\lambda^{10} + 11985\lambda^8 \\ &\quad -9834\lambda^6 + 4695\lambda^4 - 1114\lambda^2 + 81. \end{aligned}$$

The spectrum of H_3^2 is given in Table 1.

Table 1 The spectrum of H_3^2

polynomial	*eigenvalues*			
$\varphi_1(\lambda)$	−2.5884	−1.5936	1.0000	2.1819
$\varphi_2(\lambda)$	−1.8794	−1.0000	0.3473	1.5231
$\psi_1(\lambda)$	2.5884	1.5936	−1.0000	−2.1819
$\psi_2(\lambda)$	1.8794	1.0000	−0.3473	−1.5231
$(\lambda^2 - 1)^2$	−1	−1	1	1

Eq. (2) indicates that $\psi_j(x_0) = 0$ if and only if $\varphi_j(-x_0) = 0$. By Theorem 3.1, the spectral radius of H_3^n must be the largest root of $\varphi_j(\lambda)$ or $\psi_j(\lambda)$ for some $j \in \{1, 2, \ldots, n\}$. Recall that $r_0(f(\lambda))$ is the largest root of $f(\lambda)$, by applying Lemma 2.4 and Theorem 3.1 we will show that $r_0(\psi_1(\lambda))$ is the spectral radius of H_3^n.

Lemma 3.1. For any positive integers $n \geq 2$, the spectral radius of H_3^n is the largest root of $\varphi_1(\lambda)$ or $\psi_1(\lambda)$.

Proof. Clearly, L_2 is a subgraph of H_3^n. By Lemma 2.3, $\rho(H_3^n) > \rho(L_2) = \frac{1}{2}(1 + \sqrt{13})$.

First we suppose that $\rho(H_3^n)$ achieves at the largest roots of $\varphi_i(\lambda)$ for $i = 1, 2, ..., n$, and will show that $r_0(\varphi_1(\lambda)) > r_0(\varphi_i(\lambda))$ for $i = 2, \ldots, n$. By assumption, there exists $\rho(H_3^n) = r_0(\varphi_j(\lambda))$ for some $1 \leq j \leq n$. Then $r_0(\varphi_j(\lambda)) > \frac{1}{2}(1 + \sqrt{13})$. It is all right if $j = 1$. Otherwise, there exists $\varphi_i(\lambda)$ such that $i < j$. By Theorem 3.1,

$$\varphi_i(\lambda) - \varphi_j(\lambda) = (q_j - q_i)(2\lambda^2 + \lambda - (q_i + q_j)).$$

Note that $\frac{1}{4}(-1 + \sqrt{1 + 8(q_i + q_j)})$ is the large root of $2\lambda^2 + \lambda - (q_i + q_j)$, and $4 > q_i = 2 + 2\cos\frac{\pi i}{n+1} > q_j = 2 + 2\cos\frac{\pi j}{n+1}$ if $i < j$. We see that $\varphi_i(\lambda) < \varphi_j(\lambda)$ if $\lambda > \frac{1}{4}(-1 + \sqrt{1 + 8(q_i + q_j)})$. Also note that

$$\frac{1}{4}(-1 + \sqrt{1 + 8(q_i + q_j)}) < \frac{1}{4}(-1 + \sqrt{65}) < \frac{1}{2}(1 + \sqrt{13}) < r_0(\varphi_j(\lambda)).$$

We have $\varphi_i(\lambda) < \varphi_j(\lambda)$ for $\lambda > r_0(\varphi_j(\lambda))$. It follows that $r_0(\varphi_i(\lambda)) > r_0(\varphi_j(\lambda)) = \rho(H_3^n)$ by Lemma 2.4, a contradiction.

Next we suppose that $\rho(H_3^n)$ achieves at the largest roots of $\psi_i(\lambda)$ for $i = 1, 2, ..., n$, and will show that $r_0(\psi_1(\lambda)) > r_0(\psi_i(\lambda))$ for $i = 2, \ldots, n$. By assumption, there exists $\rho(H_3^n) = r_0(\psi_j(\lambda))$ for some $1 \leq j \leq n$. Then $r_0(\psi_j(\lambda)) > \frac{1}{2}(1 + \sqrt{13})$. It is all right if $j = 1$. Otherwise, there exists $\psi_i(\lambda)$ such that $i < j$. By Theorem 3.1,

$$\psi_i(\lambda) - \psi_j(\lambda) = (q_j - q_i)(2\lambda^2 - \lambda - (q_i + q_j)).$$

Note that $\frac{1}{4}(1 + \sqrt{1 + 8(q_i + q_j)})$ is the large root of $2\lambda^2 - \lambda - (q_i + q_j)$, and $4 > q_i = 2 + 2\cos\frac{\pi i}{n+1} > q_j = 2 + 2\cos\frac{\pi j}{n+1}$ if $i < j$. We see that $\psi_i(\lambda) < \psi_j(\lambda)$ if $\lambda > \frac{1}{4}(1 + \sqrt{1 + 8(q_i + q_j)})$. Also note that

$$\frac{1}{4}(1 + \sqrt{1 + 8(q_i + q_j)}) < \frac{1}{4}(1 + \sqrt{65}) < \frac{1}{2}(1 + \sqrt{13}) < r_0(\psi_j(\lambda)).$$

We have $\psi_i(\lambda) < \psi_j(\lambda)$ for $\lambda > r_0(\psi_j(\lambda))$. It follows that $r_0(\psi_i(\lambda)) > r_0(\psi_j(\lambda)) = \rho(H_3^n)$ by Lemma 2.4, a contradiction. ■

Lemma 3.2. $r_0(\psi_1(\lambda))$ is always greater than $\sqrt{5}$.

Proof. By Theorem 3.1, $\psi_1(\lambda) = \lambda^4 - \lambda^3 - (2q_1+1)\lambda^2 + (q_1+1)\lambda + q_1^2$. Note that $q_1 = 2 + 2\cos\frac{\pi}{n+1}$. Regarding $\cos\frac{\pi}{n+1}$ as x, we have

$$\psi_1(\frac{5}{2}) = 4x^2 - 12x + \frac{59}{16} \text{ and } \psi_1(3) = 4x^2 - 22x + 22.$$

Since $n \geq 2$, $\frac{1}{2} \leq x = \cos\frac{\pi}{n+1} < 1$. It is routine to verify that $\psi_1(\frac{5}{2}) < 0 < \psi_1(3)$. Then $\psi_1(\lambda)$ has a root $r_1 \in (\frac{5}{2}, 3)$, and so $r_0(\psi_1(\lambda)) \geq r_1 > \frac{5}{2} > \sqrt{5}$.

It follows our result. ■

Theorem 3.2 For any positive integers $n \geq 2$, the largest root of $\psi_1(\lambda)$ is the spectral radius of H_3^n.

Proof. By Lemma 3.1, it suffices to show that $r_0(\varphi_1(\lambda)) < r_0(\psi_1(\lambda))$. By Lemma 3.2, we may assume that $r_0(\varphi_1(\lambda)) > \sqrt{5}$. Now consider

$$\psi_1(\lambda) - \varphi_1(\lambda) = -2\lambda(\lambda^2 - (q_1+1)).$$

We see that $\psi_1(\lambda) < \varphi_1(\lambda)$ if $\lambda > \sqrt{q_1+1}$. Note that $\sqrt{q_1+1} < \sqrt{5} < r_0(\varphi_1(\lambda))$. We claim that $\psi_1(\lambda) < \varphi_1(\lambda)$ for $\lambda > r_0(\varphi_1(\lambda))$. It follows that $r_0(\psi_1(\lambda)) > r_0(\varphi_1(\lambda))$ by Lemma 2.4. It completes the proof. ■

It is well know that biquadratic equation has formula solution, by Theorem 3.2 one can give the spectral radius of H_3^n in explicit formulation. In the following corollary, we give the multiplicities of eigenvalues 1 and -1 of H_3^n.

Corollary 3.1. Hexagonal system H_3^n always has eigenvalues ± 1. Eigenvalues ± 1 have multiplicity equal to 4 if and only if $n + 1 \equiv 0 (\text{mod} 3)$. Otherwise, eigenvalues ± 1 have multiplicity equal to 2.

Proof. Let $\prod_{j=1}^{n} \varphi_j(\lambda)\psi_j(\lambda) = f(\lambda)$, where $\varphi_j(\lambda) = \lambda^4 + \lambda^3 - (2q_j+1)\lambda^2 - (q_j+1)\lambda + q_j^2$, $\psi_j(\lambda) = \lambda^4 - \lambda^3 - (2q_j+1)\lambda^2 + (q_j+1)\lambda + q_j^2$ and $q_j = 2 + 2\cos\frac{\pi j}{n+1}$, where $j = 1, 2, \ldots, n$. By Theorem 3.1, $\phi_{H_3^n}(\lambda) = (\lambda^2-1)^2 f(\lambda)$. Clearly, $(\lambda^2-1)^2$ contains the eigenvalues ± 1 with multiplicity 2.

Suppose that ± 1 are the roots of $f(\lambda)$, then $f(\pm 1) = 0$, that is, $\prod_{j=1}^{n} q_j^4 (q_j - 3)^2 (q_j - 1)^2 = 0$. It follows $q_j = 0, 1$ or 3. Clearly, $q_j = 2 + 2\cos\frac{\pi j}{n+1} \neq 0$ since $1 \leq j \leq n$. $q_j = 2 + 2\cos\frac{\pi j}{n+1} = 1$ if and only if $j = \frac{2(n+1)}{3} \in \{1, 2, \ldots, n\}$; similarly, $q_j = 2 + 2\cos\frac{\pi j}{n+1} = 3$

if and only if $j = \frac{n+1}{3} \in \{1, 2, \ldots, n\}$. Thus ± 1 are the roots of $f(\lambda)$ with multiplicity 2 if and only if $n + 1 \equiv 0(\bmod 3)$. Otherwise, $f(\pm 1) \neq 0$. It follows our results by the above arguments. ■

By the way, we give the number of Kekulé structures of the graph H_3^n in terms of the spectrum, which agrees with the result obtained by T.F.Yen [12].

Corollary 3.2. Let $K(H_3^n)$ be the number of Kekulé structures for hexagonal system H_3^n. Then $K(H_3^n) = (n+1)^2$.

Proof. By Theorem 3.1, we have $\det A(H_3^n) = \phi_{H_3^n}(0) = \prod_{j=1}^{n} q_j^4$, where $q_j = 2+2\cos\frac{\pi j}{n+1}$. Using Lemma 2.6 and Lemma 2.7, $[K(H_3^n)]^2 = \det A(H_3^n) = \prod_{j=1}^{n} q_j^4 = (n+1)^4$. The results follows. ■

It immediately follows the result from Corollary 3.2.

Corollary 3.3 The nullity of H_3^n is $\eta(H_3^n) = 0$.

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