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On the Characteristic Polynomial of a Hexagonal System and Its Application

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Abstract Let L_n be the hexagonal chain graph, F_n be the hexacyclic system graph and M_n be the Möbius hexacyclic system graph. Derflinger and Sofer gave the spectra of L_n and F_n by using group theoretical method. Later, Gutman gave the spectra of them using a polynomial result due to Godsil and McKay. In this paper, we give a simple and direct method to determine the characteristic polynomial and spectra of F_n and L_n. By the method, we give the characteristic polynomial and spectrum of M_n that is new. Additionally, the exact values of total π-electron energy and the nullities of L_n, F_n and M_n are obtained, and the bounds for the energy of L_n and M_n are also considered.

Keywords characteristic polynomial; spectrum; hexagonal system; circulant matrix; energy; nullity.

MR(2010) Subject Classification 05C50; 05C78

1. Introduction

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. Hexagonal systems are very important in theoretical chemistry because they are natural graph representations of benzenoid hydrocarbon [3]. Hexagonal chain graph shown in Fig.1 (a) is the graph representations of an important subclass of benzenoid molecules, namely the so-called unbranched catacondensed benzenoids, which play a distinguished role in the theoretical chemistry of benzenoid hydrocarbon. A great deal of mathematical and mathematico-chemical results on hexagonal chains were obtained (see [3–6] for examples). The hexacyclic system graph F_n is obtained from hexagonal chain L_n by identifying two pairs of ends of L_n which is shown in Fig.1 (b). The Möbius hexacyclic system graph M_n is shown in Fig.1 (c).

It is well-known that the theory of graph spectra is related to the Chemistry through the HMO (Hückel Molecular Orbital) Theory (see [7] for an extensive review on the topic), in which there are two problems to attract our attentions. One is posed by Günthad in [8] 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 [9, 10].

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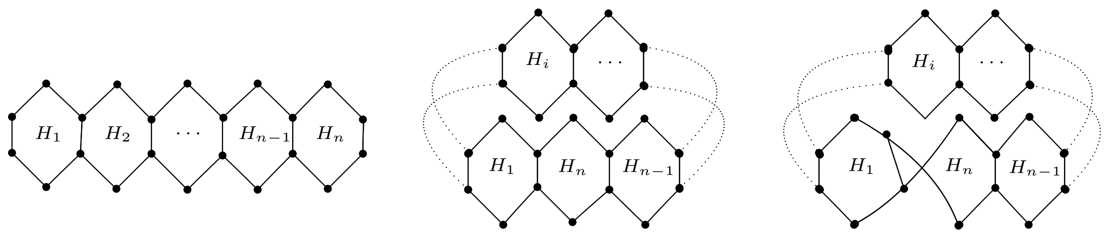
To our knowledge, the spectra of hexagonal chain graph L_n and hexacyclic system graph F_n were found in [1, 2]. However, the spectrum of Möbius hexacyclic system graph has not yet been found, to say nothing of the spectra of the general hexagonal graphs.

Another is originated from Hückel theory to determine the energies of (molecular) graph, the so called total π-electron energy E_π, by spectrum of the corresponding graph. For the researches on the energies of graphs one can refer to [11–15]. From a chemical point of view, it is of great interest to find the accurate values of energy $E_\pi(G) = \sum_{1\le i\le n} |\lambda_i|$ for graph G, where λ_i $(i = 1, 2, \ldots, n)$ are the eigenvalues of G. Additionally, L. Collatz and U. Sinogowitz in [16] posed the problem of characterizing all graphs which have zero eigenvalue. As it has been shown in [17], the occurrence of a zero eigenvalue in the spectrum of a bipartite graph (corresponding to an alternant hydrocarbon) indicates chemical instability of the molecule which such a graph represents. 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.

All the above mentioned problems are related to the spectrum of the corresponding molecular graph. Derflinger and Sofer in [1] gave the spectra of L_n and F_n by using group theoretical method. Later, Gutman in [2] gave the spectra of them using a polynomial result due to Godsil and McKay in [21]. In this paper we give the characteristic polynomials and spectra of L_n, F_n and M_n by a direct method and, by the way, the nullities of them are also determined. Furthermore the accurate values of total π-electron energies of L_n, F_n and M_n are obtained. At last, the bond for the energy of L_n and M_n are also considered.



(a) L_n (b) F_n (c) M_n

Figure 1 Hexagonal system graphs

2. Elementary

All graphs considered in this paper are simple, undirected and without loops. Let G be a graph with adjacency matrix $A(G)$, its vertices are labeled by $V(G) = \{1, 2, \ldots, n\}$ and d_i denotes the degree of vertex i. We denote by $\phi_G(\lambda) = |\lambda I_n - A(G)|$ the characteristic polynomial of G, where I_n is the identity matrix of order n. The multiset of eigenvalues of $A(G)$ is called the adjacency spectrum (or simply the spectrum) of G. Denote by $D(G)$ the diagonal matrix $\mathrm{diag}(d_1, \ldots, d_n)$, and $Q(G) = D(G)+A(G)$ 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 of G. A circulant matrix is a square matrix in which every row beginning with the second can be obtained from the preceding row by moving each of its elements one column to the right, with the last element circling to become the first. In this section, we will cite and establish some results for the later use.

Lemma 2.1 *Let A be a matrix of size $m \times n$ and A^{T} be the transpose of A. If $\left|A^{\mathrm{T}}A\right| \neq 0$, then the matrix*

$$\Delta = \begin{pmatrix} 0 & I_n & A^{\mathrm{T}} & 0 \\ I_n & 0 & 0 & A^{\mathrm{T}} \\ A & 0 & 0 & 0 \\ 0 & A & 0 & 0 \end{pmatrix}$$

has the characteristic polynomial:

$$\phi_{\Delta}(\lambda) = \lambda^{2(m-n)} \left|\lambda(\lambda+1)I_n - A^{\mathrm{T}}A\right| \cdot \left|\lambda(\lambda-1)I_n - A^{\mathrm{T}}A\right|. \tag{1}$$

Proof Suppose $\lambda = 0$. Then

$$\phi_{\Delta}(\lambda) = |-\Delta| = \begin{vmatrix} 0 & -I_n & -A^{\mathrm{T}} & 0 \\ -I_n & 0 & 0 & -A^{\mathrm{T}} \\ -A & 0 & 0 & 0 \\ 0 & -A & 0 & 0 \end{vmatrix} = \left|A^{\mathrm{T}}A\right|^2 = 0.$$

Thus $\left|A^{\mathrm{T}}A\right| = 0$, a contradiction. From the above we know that $\lambda \neq 0$. By the property of determinant we have

$$\begin{aligned}
\phi_{\Delta}(\lambda) &= |\lambda I - \Delta| \\
&= \begin{vmatrix} \lambda I_n & -I_n & -A^{\mathrm{T}} & 0 \\ -I_n & \lambda I_n & 0 & -A^{\mathrm{T}} \\ -A & 0 & \lambda I_m & 0 \\ 0 & -A & 0 & \lambda I_m \end{vmatrix} = \begin{vmatrix} \lambda I_n - \frac{A^{\mathrm{T}}A}{\lambda} & -I_n & 0 & 0 \\ -I_n & \lambda I_n - \frac{A^{\mathrm{T}}A}{\lambda} & 0 & 0 \\ -A & 0 & \lambda I_m & 0 \\ 0 & -A & 0 & \lambda I_m \end{vmatrix} \\
&= \lambda^{2m} \begin{vmatrix} \lambda I_n - \frac{A^{\mathrm{T}}A}{\lambda} & -I_n \\ -I_n & \lambda I_n - \frac{A^{\mathrm{T}}A}{\lambda} \end{vmatrix} \\
&= \lambda^{2m} \left| (\lambda+1)I_n - \frac{A^{\mathrm{T}}A}{\lambda} \right| \cdot \left| (\lambda-1)I_n - \frac{A^{\mathrm{T}}A}{\lambda} \right| \\
&= \lambda^{2(m-n)} \left|\lambda(\lambda+1)I_n - A^{\mathrm{T}}A\right| \cdot \left|\lambda(\lambda-1)I_n - A^{\mathrm{T}}A\right|.
\end{aligned}$$

The proof is completed. □

The following five results are familiar to us.

Lemma 2.2 ([18]) *The signless Laplacian matrix of a graph G is $Q(G) = D(G) + A(G)$. If M is the incidence matrix of G with n vertices and m edges, then*

$$MM^{\mathrm{T}} = D(G) + A(G) = Q(G). \tag{2}$$

Lemma 2.3 ([19]) *Let C_n be the cycle on n vertices and P_{n+1} be the path on $n+1$ vertices respectively. Then the Q-polynomials of C_n* and *P_{n+1}* are

$$Q_{C_n}(\lambda) = \prod_{j=1}^{n}(\lambda - 2 - 2\cos\frac{2\pi j}{n}), \tag{3}$$

$$Q_{P_{n+1}}(\lambda) = \prod_{j=1}^{n+1}(\lambda - 2 - 2\cos\frac{\pi j}{n+1}). \tag{4}$$

Lemma 2.4 ([20]) *If A, B are two circulant matrices of the same order and a and b are any two scalars, then $aA + bB$ is also a circulant matrix.*

Lemma 2.5 ([20]) *An $n \times n$ circulant matrix S takes the form*

$$S = \begin{pmatrix} s_0 & s_1 & \dots & s_{n-2} & s_{n-1} \\ s_{n-1} & s_0 & \dots & s_{n-3} & s_{n-2} \\ \vdots & s_{n-1} & s_0 & \ddots & \vdots \\ s_2 & & \ddots & \ddots & s_1 \\ s_1 & s_2 & \dots & s_{n-1} & s_0 \end{pmatrix}.$$

Then we have $S = s_0W^0 + s_1W^1 + s_2W^2 + \cdots + s_{n-1}W^{n-1}$, where W is the 'cyclic permutation' matrix given by $W = \begin{pmatrix} 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & \ddots & \ddots & \vdots & \vdots \\ \vdots & \ddots & \ddots & 0 & 0 \\ 0 & \cdots & 0 & 1 & 0 \end{pmatrix}$.

Lemma 2.6 ([20]) *Let S be an $n \times n$ circulant matrix. Then the eigenvalues of S are $\lambda_j = s_0 + s_1\omega_j + s_2\omega_j^2 + \cdots + s_{n-1}\omega_j^{n-1}$ where $j = 0, 1, \dots, n-1$ and the determinant of S can be computed as:*

$$\det(S) = \prod_{j=0}^{n-1}(s_0 + s_1\omega_j + s_2\omega_j^2 + \cdots + s_{n-1}\omega_j^{n-1}), \tag{5}$$

where $\omega_j = e^{\frac{2\pi j}{n}i}$ are the n-th roots of unity and $i = \sqrt{-1}$ is the imaginary unit.

3. The characteristic polynomial of hexacyclic system graph

Here we use a simple and direct method to give an explicit expression for the characteristic polynomials of hexagonal system graph L_n and F_n. Now we label L_n as in Fig.2, and it will be exactly the F_n if the vertices 1 and x_1 are coincided and simultaneously $1'$ and x_2 are coincided.

In this section we prefer to consider the characteristic polynomial and spectrum of F_n in details, and, as the same, that of L_n follows immediately.

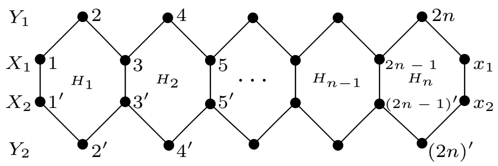


Figure 2 A prescribed hexagonal system graph L_n or F_n

Lemma 3.1 *Let F_n be a hexacyclic system graph with n hexagons. Then the characteristic* *polynomial of F_n is given by*

$$\phi_{F_n}(\lambda) = \prod_{j=1}^{n} (\lambda^2 + \lambda - 2 - 2\cos\frac{2\pi j}{n})(\lambda^2 - \lambda - 2 - 2\cos\frac{2\pi j}{n}). \tag{6}$$

Proof We partition the vertex set $V(F_n)$ into four parts: $V(F_n) = X_1 \cup X_2 \cup Y_1 \cup Y_2$, where the vertices are ordered as below (to see Fig.2):

$$\begin{cases} X_1 = \{1, 3, 5, \ldots, 2n-1\}, \\ X_2 = \{1', 3', 5', \ldots, (2n-1)'\}, \\ Y_1 = \{2, 4, 6, \ldots, 2n-2, 2n\}, \\ Y_2 = \{2', 4', 6', \ldots, (2n-2)', (2n)'\}, \end{cases}$$

where $1 = x_1$ and $1' = x_2$.

Let $A(F_n)$ be the adjacency matrix of F_n. For $i = 1, 2$, let $A(X_i, Y_i) = (a_{uv})_{n\times n}$ denote the block matrix of $A(F_n)$ corresponding to X_i, the row-set, and Y_i, the column set. To be exact, $a_{uv} = 1$ if $u \in X_i$ is adjacent with $v \in Y_i$ in F_n, and $a_{uv} = 0$ otherwise. Thus, in accordance with the labeling of vertices in Fig.2, we see that

$$\begin{cases} A(X_1, X_2) = A(X_2, X_1) = I_n, \\ A(Y_1, X_1) = A(Y_2, X_2) = C, \\ A(X_1, Y_1) = A(X_2, Y_2) = C^{\mathrm{T}}, \end{cases}$$

where C will be labeled as $C = A(Y_1, X_1) = \begin{pmatrix} 1 & 1 & & & & \\ & 1 & 1 & & & \\ & & 1 & 1 & & \\ & & & \ddots & \ddots & \\ & & & & 1 & 1 \\ 1 & & & & & 1 \end{pmatrix}_{n\times n}$. Now we can represent the adjacency matrix of F_n as follows:

$$A(F_n) = \begin{pmatrix} 0 & A(X_1, X_2) & A(X_1, Y_1) & 0 \\ A(X_2, X_1) & 0 & 0 & A(X_2, Y_2) \\ A(Y_1, X_1) & 0 & 0 & 0 \\ 0 & A(Y_2, X_2) & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & I_n & C^{\mathrm{T}} & 0 \\ I_n & 0 & 0 & C^{\mathrm{T}} \\ C & 0 & 0 & 0 \\ 0 & C & 0 & 0 \end{pmatrix}. \tag{7}$$

It is easy to see that C^{T} is just the incidence matrix of the n-cycle C_n and by Lemma 2.2, we have

$$C^{\mathrm{T}}C = D(C_n) + A(C_n) = Q(C_n), \tag{8}$$

where $Q(C_n)$ is the signless Laplacian matrix of C_n. Obviously, $\left|C^{\mathrm{T}}C\right| \neq 0$.

By Lemma 2.1 and Eq. (8), we obtain

$$\phi_{F_n}(\lambda) = \begin{vmatrix} \lambda I_n & -I_n & -C^{\mathrm{T}} & 0 \\ -I_n & \lambda I_n & 0 & -C^{\mathrm{T}} \\ -C & 0 & \lambda I_n & 0 \\ 0 & -C & 0 & \lambda I_n \end{vmatrix}$$

$$= \lambda^{2n} \cdot |(\lambda+1)I_n - \frac{C^{\mathrm{T}}C}{\lambda}| \times |(\lambda-1)I_n - \frac{C^{\mathrm{T}}C}{\lambda}|$$
$$= |(\lambda^2+\lambda)I_n - C^{\mathrm{T}}C| \times |(\lambda^2-\lambda)I_n - C^{\mathrm{T}}C|$$

$$= |(\lambda^2+\lambda)I_n - Q(C_n)| \times |(\lambda^2-\lambda)I_n - Q(C_n)|$$
$$= Q_{C_n}(\lambda^2+\lambda)\cdot Q_{C_n}(\lambda^2-\lambda).$$

Using Lemma 2.3, we have

$$\phi_{F_n}(\lambda) = \prod_{j=1}^{n}(\lambda^2+\lambda-2-2\cos\frac{2\pi j}{n})\cdot\prod_{j=1}^{n}(\lambda^2-\lambda-2-2\cos\frac{2\pi j}{n}).$$

The proof is completed. □

The result below immediately follows from Lemma 3.1.

Theorem 3.1 ([1, 2]) *The characteristic eigenvalues of F_n are*

$$\begin{cases} \frac{1}{2}\left(1 \pm \sqrt{9+8\cos\frac{2\pi j}{n}}\right), & j=1,2,\ldots,n; \\ \frac{1}{2}\left(-1 \pm \sqrt{9+8\cos\frac{2\pi j}{n}}\right), & j=1,2,\ldots,n. \end{cases}$$

If F_n is replaced with L_n in the proof of Lemma 3.1, then the adjacency matrix of F_n in Eq. (7) will be changed as:

$$A(L_n) = \begin{pmatrix} 0 & I_{n+1} & B^{\mathrm{T}} & 0 \\ I_{n+1} & 0 & 0 & B^{\mathrm{T}} \\ B & 0 & 0 & 0 \\ 0 & B & 0 & 0 \end{pmatrix}$$

where C^{T} is replaced with B^{T}, the incidence matrix of the P_{n+1}, and the corresponding $Q(C_n)$ in Eq. (8) will be changed as $B^{\mathrm{T}}B = D(P_{n+1}) + A(P_{n+1}) = Q(P_{n+1})$. Consequently, $\phi_{L_n}(\lambda) = \lambda^{-2}Q_{P_{n+1}}(\lambda^2+\lambda)\cdot Q_{P_{n+1}}(\lambda^2-\lambda)$, which leads to the characteristic polynomial of hexagonal system graph L_n,

$$\phi_{L_n}(\lambda) = \lambda^{-2}\prod_{j=1}^{n+1}(\lambda^2+\lambda-2-2\cos\frac{\pi j}{n+1})(\lambda^2-\lambda-2-2\cos\frac{\pi j}{n+1}). \tag{9}$$

The result below immediately follows from Eq. (9).

Theorem 3.2 ([1, 2]) *The eigenvalues of hexagonal chain graph L_n are*

$$\begin{cases} \pm 1; & \\ \frac{1}{2}\left(1 \pm \sqrt{9+8\cos\frac{\pi j}{n+1}}\right), & j=1,2,\ldots,n; \\ \frac{1}{2}\left(-1 \pm \sqrt{9+8\cos\frac{\pi j}{n+1}}\right), & j=1,2,\ldots,n. \end{cases}$$

From Theorem 3.2 we know that the eigenvalue multiplicity of L_n: (i) if n is even, then every eigenvalue of L_n has multiplicity 1; (ii) if n is odd, then $1, -1$ have multiplicity 2 and other eigenvalues are simple. From Theorem 3.2 we claim that the spectral radius: $\rho_{L_n} = \frac{1}{2}(1+\sqrt{9+8\cos\frac{\pi}{n+1}})$ and $\eta(L_n)=0$, which is known in [11]. Since $\lim_{n\to\infty}\frac{1}{2}(1+\sqrt{9+8\cos\frac{\pi}{n+1}}) = \frac{1+\sqrt{17}}{2}$, we have the corollaries below.

Corollary 3.1 *Let $\lambda(L_n)$ and $\rho(L_n)$ be the eigenvalue and spectral radius of L_n, respectively. Then $\rho_{L_n} = \frac{1}{2}(1+\sqrt{9+8\cos\frac{\pi}{n+1}})$ and $-\frac{1+\sqrt{17}}{2} < \lambda(L_n) < \frac{1+\sqrt{17}}{2}$.*

From Theorem 3.1 we know that the eigenvalue multiplicity of F_n:

(i) If n is even, then eigenvalues $\pm 1, \frac{1\pm\sqrt{17}}{2}, \frac{-1\pm\sqrt{17}}{2}$ have multiplicity equal to 1, and other eigenvalues have multiplicity equal to 2; (ii) if n is odd, then eigenvalues $\frac{1\pm\sqrt{17}}{2}, \frac{-1\pm\sqrt{17}}{2}$ have multiplicity equal to 1, and other eigenvalues have multiplicity equal to 2.

From Theorem 3.1 we see that the spectral radius of F_n is $\rho(F_n) = \frac{1+\sqrt{17}}{2}$ that achieves at $\frac{1}{2}(1+\sqrt{9+8\cos\frac{2\pi j}{n}})$ for $j = n$, and is independent for any n. Thus $-\frac{1+\sqrt{17}}{2} \leq \lambda(F_n) \leq \frac{1+\sqrt{17}}{2}$. We also get the nullity of F_n as follows.

Corollary 3.2 *Let F_n be a hexacyclic system graph with n hexagons. The nullity of F_n is $\eta(F_n) = 1 + (-1)^n$, and so $\eta(F_n) \leq 2$.*

4. The characteristic polynomial of Möbius hexacyclic system graph

In this section, we will give a theorem to explicitly express the characteristic polynomial of Möbius hexacyclic system graph M_n that is new, from which the spectrum is also determined. Now we label M_n as in Fig.3.

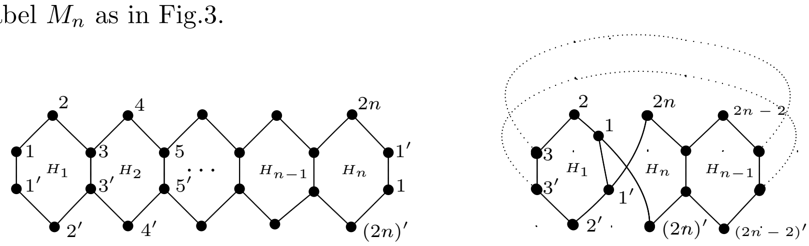


Figure 3 A prescribed Möbius hexacyclic system graph M_n

Theorem 4.1 *Let M_n be a Möbius hexacyclic system graph with n hexagons. Then the characteristic polynomial of M_n is given below:*

$$\phi_{M_n}(\lambda) = \prod_{j=0}^{2n-1}\left(\lambda^2 - (-1)^j\lambda - 2 - 2\cos\frac{\pi j}{n}\right). \tag{10}$$

Proof We partition the vertices set $V(M_n)$ into four parts: $V(M_n) = \widetilde{X}_1 \cup \widetilde{X}_2 \cup \widetilde{Y}_1 \cup \widetilde{Y}_2$, where the vertices are ordered as below (to see Fig.3):

$$\begin{cases} \widetilde{X}_1 = \{1, 3, 5, \ldots, 2n-1\}, \\ \widetilde{X}_2 = \{1', 3', 5', \ldots, (2n-1)'\}, \\ \widetilde{Y}_1 = \{2, 4, 6, \ldots, 2n-2, 2n\}, \\ \widetilde{Y}_2 = \{2', 4', 6', \ldots, (2n-2)', (2n)'\}. \end{cases}$$

According to the representation method of F_n, we represent the adjacency matrix of M_n as:

$$A(M_n)=\begin{array}{c} \\ \widetilde{X}_1 \\ \widetilde{X}_2 \\ \widetilde{Y}_1 \\ \widetilde{Y}_2 \end{array}\!\!\begin{array}{c} \begin{array}{cccc} \widetilde{X}_1 & \widetilde{X}_2 & \widetilde{Y}_1 & \widetilde{Y}_2 \end{array} \\ \left(\begin{array}{cc:c} 0 & I_n & \multirow{2}{*}{$\widetilde{C}$} \\ I_n & 0 & \\ \hdashline \multicolumn{2}{c:}{\widetilde{C}^{\mathrm{T}}} & 0 \end{array}\right)_{4n\times 4n} \end{array}$$

where $\widetilde{C}=\begin{pmatrix} 1 & & & & & 1 \\ 1 & 1 & & & & \\ & 1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & & 1 & \\ & & & & 1 & 1 \end{pmatrix}_{2n\times 2n}$ and $\widetilde{C}\widetilde{C}^{\mathrm{T}}=\begin{pmatrix} 2 & 1 & & & & & 1 \\ 1 & 2 & 1 & & & & \\ & 1 & 2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & 2 & 1 & \\ & & & & 1 & 2 & 1 \\ 1 & & & & & 1 & 2 \end{pmatrix}_{2n\times 2n}$.

In fact, $\widetilde{C}$ and $\widetilde{C}\widetilde{C}^{\mathrm{T}}$ are circulant matrices of order $2n$. Let

$$M^*=\lambda\cdot\begin{pmatrix} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{pmatrix}-\widetilde{C}\cdot\widetilde{C}^{\mathrm{T}}.$$

By Lemma 2.4 M^* is also a circulant matrix of order $2n$. Using Lemma 2.5, we obtain

$$\begin{aligned} M^*&=\begin{pmatrix} \lambda^2-2 & -1 & \dots & 0 & 0 & -\lambda & 0 & \dots & 0 & -1 \\ -1 & \lambda^2-2 & \dots & 0 & 0 & 0 & -\lambda & \dots & 0 & 0 \\ & \vdots & \ddots & & & \vdots & & \ddots & & \\ 0 & 0 & \dots & \lambda^2-2 & -1 & 0 & 0 & \dots & -\lambda & 0 \\ 0 & 0 & \dots & -1 & \lambda^2-2 & -1 & 0 & \dots & 0 & -\lambda \\ -\lambda & 0 & \dots & 0 & -1 & \lambda^2-2 & -1 & \dots & 0 & 0 \\ 0 & -\lambda & \dots & 0 & 0 & -1 & \lambda^2-2 & \dots & 0 & 0 \\ & \vdots & \ddots & & & \vdots & & \ddots & & \\ 0 & 0 & \dots & -\lambda & 0 & 0 & 0 & \dots & \lambda^2-2 & -1 \\ -1 & 0 & \dots & 0 & -\lambda & 0 & 0 & \dots & -1 & \lambda^2-2 \end{pmatrix}_{2n\times 2n} \\ &=(\lambda^2-2)W^0+(-1)W^1+(-\lambda)W^n+(-1)W^{2n-1}. \end{aligned}$$

Then the characteristic polynomial of M_n is

$$\begin{aligned} \phi_{M_n}(\lambda)=|\lambda I_{4n}-A(M_n)|&=\begin{vmatrix} \begin{pmatrix} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{pmatrix} & -\widetilde{C} \\ -\widetilde{C}^{\mathrm{T}} & \lambda I_{2n} \end{vmatrix} \\ &=\begin{vmatrix} \begin{pmatrix} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{pmatrix}-\frac{\widetilde{C}\widetilde{C}^{\mathrm{T}}}{\lambda} & 0 \\ -\widetilde{C}^{\mathrm{T}} & \lambda I_{2n} \end{vmatrix}=\lambda^{2n}\cdot\left|\begin{pmatrix} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{pmatrix}-\frac{\widetilde{C}\widetilde{C}^{\mathrm{T}}}{\lambda}\right| \\ &=\left|\lambda\cdot\begin{pmatrix} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{pmatrix}-\widetilde{C}\cdot\widetilde{C}^{\mathrm{T}}\right|=\det(M^*). \end{aligned}$$

It is not difficult to calculate the determinant of M^*. Applying Lemma 2.6, we have

$$\det(M^*)=\prod_{j=0}^{2n-1}\left((\lambda^2-2)+(-1)\omega_j^1+(-\lambda)\omega_j^n+(-1)\omega_j^{2n-1}\right) \tag{11}$$

where $\omega_j=e^{\frac{2\pi j}{2n}i}=e^{\frac{\pi j}{n}i}$ and $i=\sqrt{-1}$. By direct computation $\omega_j=e^{\frac{\pi j}{n}i}$ also has the following relations: (i) $\omega_j^n=(-1)^j$; (ii) $\omega_j+\omega_j^{2n-1}=2\cos\frac{\pi j}{n}$. Thus, by Eq. (11) we have

$$\det(M^*)=\prod_{j=0}^{2n-1}\left(\lambda^2-(-1)^j\lambda-2-2\cos\frac{\pi j}{n}\right).$$

So the characteristic polynomial of M_n is

$$\phi_{M_n}(\lambda) = |\lambda I_{4n} - A(M_n)| = \det(M^*) = \prod_{j=0}^{2n-1} \left(\lambda^2 - (-1)^j\lambda - 2 - 2\cos\frac{\pi j}{n}\right).$$

The proof is completed. $\square$

The characteristic eigenvalues of Möbius hexacyclic system graph M_n immediately follow from Theorem 4.1.

Theorem 4.2 *The characteristic eigenvalues of M_n are*

$$\begin{cases} \frac{1}{2}\left(1 \pm \sqrt{9+8\cos\frac{\pi j}{n}}\right), & j = 2k \\ \frac{1}{2}\left(-1 \pm \sqrt{9+8\cos\frac{\pi j}{n}}\right), & j = 2k+1 \end{cases} \quad \text{where } k = 0, 1, \ldots, n-1.$$

Consequently, we get the spectrum of Möbius hexacyclic system graph M_n from Theorem 4.2.

Corollary 4.1 *The characteristic eigenvalues of M_n are*

$$\begin{cases} \frac{1}{2}\left(1 \pm \sqrt{9+8\cos\frac{2k\pi}{n}}\right), & k = 1, 2, \ldots, n \\ \frac{1}{2}\left(-1 \pm \sqrt{9+8\cos\frac{(2k-1)\pi}{n}}\right), & k = 1, 2, \ldots, n \end{cases}$$

and furthermore

(i) If n is even, then eigenvalues $1, 0, \frac{1\pm\sqrt{17}}{2}$, have multiplicity equal to 1, and other eigenvalues have multiplicity equal to 2.

(ii) If n is odd, then eigenvalues $-1, 0, \frac{1\pm\sqrt{17}}{2}$ have multiplicity equal to 1, and other eigenvalues have multiplicity equal to 2.

From Corollary 4.1 we claim that the spectral radius of M_n is $\rho_{M_n} = \frac{1+\sqrt{17}}{2}$ that achieves at $\frac{1}{2}(1+\sqrt{9+8\cos\frac{2k\pi}{n}})$ for $k = n$ and the minimum eigenvalue is $\lambda_{4n}(M_n) = \frac{1}{2}(-1-\sqrt{9+8\cos\frac{\pi}{n}})$ that achieves at $\frac{1}{2}\left(-1-\sqrt{9+8\cos\frac{(2k+1)\pi}{n}}\right)$ for $k = n$. Since $\lim_{n\to\infty}\frac{1}{2}(-1-\sqrt{9+8\cos\frac{\pi}{n}}) = \frac{-1-\sqrt{17}}{2}$, we have the following corollaries.

Corollary 4.2 *Let $\lambda(M_n)$ be the eigenvalue of M_n. Then $-\frac{1+\sqrt{17}}{2} < \lambda(M_n) \leq \frac{1+\sqrt{17}}{2}$.*

From Corollary 4.1, the nullity of M_n immediately follows.

Corollary 4.3 *Let M_n be a Möbius hexacyclic system graph with n hexagons. Then the nullity of M_n is $\eta(M_n) = 1$.*

5. The energies of L_n, F_n and M_n

In this section, we will give the exact values of the energies of L_n, F_n and M_n. From Theorems 3.1, 3.2 and 4.2, we can obtain the accurate values of the energies of L_n, F_n and M_n, and give an upper bound for the energies of L_n and M_n.

Theorem 5.1 *Let $E(L_n)$ be the energy of hexagonal chain graph L_n. Then*

$$E(L_n) = 2 + 2\sum_{j=1}^{n} \sqrt{9 + 8\cos\frac{\pi j}{n+1}} \le 6n + 2$$

and the energy value $E(L_n)$ is always no more than $6n+2$.

Proof By Theorem 3.2, we have the energy of hexagonal chain graph L_n

$$\begin{aligned}
E(L_n) =& \sum_{i=1}^{4n+2} |\lambda_i| \\
=& |1| + |-1| + \sum_{j=1}^{n} \left| \frac{1}{2}\left(1 + \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)\right| + \sum_{j=1}^{n} \left| \frac{1}{2}\left(1 - \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)\right| \\
&+ \sum_{j=1}^{n} \left| \frac{1}{2}\left(-1 + \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)\right| + \sum_{j=1}^{n} \left| \frac{1}{2}\left(-1 - \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)\right| \\
=& 2 + 2\sum_{j=1}^{n} \frac{1}{2}\left(\left|1 + \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right| + \left|-1 + \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right|\right) \\
=& 2 + 2\sum_{j=1}^{n} \frac{1}{2}\left(1 + \sqrt{9 + 8\cos\frac{\pi j}{n+1}} + \sqrt{9 + 8\cos\frac{\pi j}{n+1}} - 1\right) \\
=& 2 + 2\sum_{j=1}^{n} \sqrt{9 + 8\cos\frac{\pi j}{n+1}}.
\end{aligned}$$

Applying Cauchy-Schwartz inequality to $(1, 1, \ldots, 1)$ and $(\sqrt{9 + 8\cos\frac{\pi}{n+1}}, \ldots, \sqrt{9 + 8\cos\frac{n\pi}{n+1}})$, we have

$$\begin{aligned}
\left(\sum_{j=1}^{n} \sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)^2 &\le \sum_{j=1}^{n} 1^2 \times \sum_{j=1}^{n} \left(\sqrt{9 + 8\cos\frac{\pi j}{n+1}}\right)^2 \\
&= n \cdot \sum_{j=1}^{n} (9 + 8\cos\frac{\pi j}{n+1}) \\
&= n \cdot \left(9n + 8\sum_{j=1}^{n} \cos\frac{\pi j}{n+1}\right) \\
&= 9n^2.
\end{aligned}$$

It is easy to get

$$E(L_n) = 2 + 2\sum_{j=1}^{n} \sqrt{9 + 8\cos\frac{\pi j}{n+1}} \le 6n + 2. \tag{12}$$

If $n = 1$, then the equality in (12) holds. So the proof of Theorem 5.1 is completed. $\square$

In addition, we obtain the accurate value of the energy of F_n by Theorem 3.1.

Theorem 5.2 *If the energy of F_n is denoted by $E(F_n)$, then*

$$E(F_n) = 2\sum_{j=1}^{n}\sqrt{9+8\cos\frac{2\pi j}{n}}.$$

Proof By Theorem 3.1 we have

$$\begin{aligned}
E(F_n) =& \sum_{i=1}^{4n}|\lambda_i| \\
=& \sum_{j=1}^{n}\left|\frac{1+\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right| + \sum_{j=1}^{n}\left|\frac{1-\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right| + \\
& \sum_{j=1}^{n}\left|\frac{-1+\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right| + \sum_{j=1}^{n}\left|\frac{-1-\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right| \\
=& 2\sum_{j=1}^{n}\left(\left|\frac{1+\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right| + \left|\frac{1-\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right|\right) \\
=& 2\sum_{j=1}^{n}\left(\frac{1+\sqrt{9+8\cos\frac{2\pi j}{n}}}{2} + \frac{-1+\sqrt{9+8\cos\frac{2\pi j}{n}}}{2}\right) \\
=& 2\sum_{j=1}^{n}\sqrt{9+8\cos\frac{2\pi j}{n}}.
\end{aligned}$$

The proof is completed. □

We obtain the accurate value of the energy of M_n by Theorem 4.2 and give an upper bound for the energy of M_n.

Theorem 5.3 *If the energy of M_n is denoted by $E(M_n)$, then*

$$E(M_n) = \sum_{j=1}^{2n}\sqrt{9+8\cos\frac{\pi j}{n}} < 6n$$

and the energy value $E(M_n)$ is always less than $6n$.

Proof By Corollary 4.1 we have

$$\begin{aligned}
E(M_n) =& \sum_{i=1}^{4n}|\lambda_i| \\
=& \sum_{j=1}^{n}\left|\frac{1}{2}\left(1+\sqrt{9+8\cos\frac{2\pi j}{n}}\right)\right| + \sum_{j=1}^{n}\left|\frac{1}{2}\left(1-\sqrt{9+8\cos\frac{2\pi j}{n}}\right)\right| + \\
& \sum_{j=1}^{n}\left|\frac{1}{2}\left(-1+\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}\right)\right| + \sum_{j=1}^{n}\left|\frac{1}{2}\left(-1-\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}\right)\right| \\
=& \frac{1}{2}\sum_{j=1}^{n}\left(1+\sqrt{9+8\cos\frac{2\pi j}{n}}+\sqrt{9+8\cos\frac{2\pi j}{n}}-1\right) +
\end{aligned}$$

$$
\begin{aligned}
&\frac{1}{2}\sum_{j=1}^{n}\left(\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}-1+\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}+1\right)\\
&=\sum_{j=1}^{n}\sqrt{9+8\cos\frac{2\pi j}{n}}+\sum_{j=1}^{n}\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}\\
&=\sum_{j=1}^{n}\left(\sqrt{9+8\cos\frac{2\pi j}{n}}+\sqrt{9+8\cos\frac{(2j+1)\pi}{n}}\right)\\
&=\sum_{j=1}^{2n}\sqrt{9+8\cos\frac{\pi j}{n}}.
\end{aligned}
$$

Applying Cauchy-Schwartz inequality to $(1,1,\ldots,1)$ and $\left(\sqrt{9+8\cos\frac{\pi}{n}},\ldots,\sqrt{9+8\cos\frac{2n\pi}{n}}\right)$, we have

$$
\begin{aligned}
\left(\sum_{j=1}^{2n}\sqrt{9+8\cos\frac{\pi j}{n}}\right)^2 &< \sum_{j=1}^{2n}1^2\times\sum_{j=1}^{2n}\left(\sqrt{9+8\cos\frac{\pi j}{n}}\right)^2\\
&=2n\cdot\sum_{j=1}^{2n}(9+8\cos\frac{\pi j}{n})\\
&=2n\cdot\left(18n+8\sum_{j=1}^{2n}\cos\frac{\pi j}{n}\right)\\
&=36n^2
\end{aligned}
$$

It is easy to get

$$E(M_n)=\sum_{j=1}^{2n}\sqrt{9+8\cos\frac{\pi j}{n}}<6n.$$

The proof is completed. □

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References

[1] G. DERFLINGER, H. SOFER. *Die HMO-Koeffizienten der linearen Polyacene in geschlossener Form.* Chem., 1968, **99**:1866–1875.

[2] I. GUTMAN. *Spectral properties of some graphs derived from bipartite graphs.* MATCH-Commun. Math. Comput. Chem., 1980, **8**: 291–314.

[3] I. GUTMAN, S. J. CYVIN. *Introduction to the Theory of Benzenoid Hydrocarbons.* Springer-Verlag Berlin Heidelberg, 1989.

[4] I. GUTMAN. *Advances in the Theory of Benzenoid Hydrocarbons 2.* Topics in Current Chemistry, Vol. 162, Springer-Verlag Berlin Heidelberg, 1992.

[5] I. GUTMAN, S. J. CYVIN. *Advances in the Theory of Benzenoid Hydrocarbons.* Topics in Current Chemistry, Vol. 153, Springer-Verlag Berlin Heidelberg, 1990.

[6] P. E. JOHN. *Calculating the characteristic polynomial and the eigenvectors of a weighted hexagonal system (benzenoid hydrocarbons with heteroatoms).* MATCH-Commun. Math. Comput. Chem., 1994, **30**: 153–169.

[7] M. RANDIĆ. *Aromaticity of polycyclic conjugated hydrocarbons.* Chem, Rev., 2003, **103**(9): 3449–3606.

[8] H. H. GÜNTHAD, H. PRIBAS. *Zusammenhang von Graphentherie und Mo-Theorie von Molekeln mit Systemen konjugierter Bindungen*. Helv. Chem. Acta, 1956, **39**: 1645–1653.
[9] D. M. CVETKOVIĆ, M. DOOB, H. SACHS. *Spectra of Graphs-Theory and Applications (III)*. Revised and Enlarged Edition, Johan Ambrosius Bart. Verlag, Heidilberg-Leipzig, 1995.
[10] E. R. VAN DAM, W. H. HAEMERS. *Developments on spectral characterizations of graphs*. Discrete Math., 2009, **309**(3): 576–586.
[11] D. M. CVETKOVIĆ, M. DOOB, H. SACHS. *Spectra of Graphs Theory and Applications*. Academic Press, New York, SanFrancisco, London, 1980.
[12] I. GUTMAN. *The energy of a graph*. Ber. Math.-Statist. Sekt. Forsch. Graz., 1978, **103**: 1–22.
[13] I. GUTMAN. *The energy of a graph: old and new results*. Algebraic Combinatorics and Applications, Springer-Verlag, Berlin, 2001.
[14] Haizhen REN, Fuji ZHANG. *Double hexagonal chains with minimal total ϕ-electron energy*. J. Math. Chem., 2007, **42**(4): 1041–1056.
[15] Fuji ZHANG, Huaien LI. *On maximal energy ordering of acyclic conjugated molecules*. DIMACS Ser. Discrete Math. Theoret. Comput. Sci., 51, Amer. Math. Soc., Providence, RI, 2000.
[16] L. COLLATZ, U. SINOGOWITZ. *Spektron endlicher Grafen*. Abh. Math. Sem. Univ. Hamburg, 1957, **21**: 63–77.
[17] H. C. LONGUET-HIGGINS. *Resonance structures and MO in unsaturated hydrocarbons*. J. Chem. Phys., 1950, **18**: 265–274.
[18] D. M. CVETKOVIĆ, P. ROWLINSON, S. SIMIĆ. *An Introduction to the Theory of Graph Spectra*. Cambridge University Press, Cambridge, 2010.
[19] D. M. CVETKOVIĆ, S. K. SIMIĆ. *Towards a spectral theory of graphs based on the signless Laplacian (III)*. Appl. Anal. Discrete Math., 2010, **4**(1): 156–166.
[20] P. J. DAVIS. *Circulant Matrices*. Wiley-Interscience, NY, 1979.
[21] C. D. GODSIL, B. D. MCKAY. *A new graph product and its spectrum*. Bull. Austral. Math. Soc., 1978, **18**(1): 21–28.
[22] C. GODSIL, G. ROYLE. *Algebraic Graph Theory*. Springer-Verlag, New York, 2004.
[23] Lianzhu ZHANG, Feng TIAN. *Extremal hexagonal chains concerning largest eigenvalue*. Sci. China Ser. A, 2001, **44**(9): 1089–1097.
[24] J. RADA, I. GUTMAN, R. CRUZ. *The energy of directed hexagonal systems*. Linear Algebra Appl., 2013, **439**(7): 1825–1833.