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 \( \pi \)-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.

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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 $E_\pi$, 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 $E_\pi(G) = \sum_{1 \leq i \leq n} |\lambda_i|$ for graph $G$, where $\lambda_i$ ($i = 1, 2, \ldots, n$) 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.

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 $\text{diag}(d_1, \ldots, d_n)$, 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 $|A^T A| \neq 0$, then the matrix

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

has the characteristic polynomial:

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

(1)

**Proof** Suppose $\lambda = 0$. Then

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

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

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

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

$$
MM^T = D(G) + A(G) = Q(G).
$$

(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

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

(3)
\[
Q_{p_{n+1}}(\lambda) = \prod_{j=1}^{n+1} (\lambda - 2 - 2 \cos \frac{\pi j}{n+1}).
\] (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

\[
S = \begin{pmatrix}
  s_0 & s_1 & \cdots & s_{n-2} & s_{n-1} \\
  s_{n-1} & s_0 & \cdots & s_{n-3} & s_{n-2} \\
  \vdots & s_{n-1} & s_0 & \cdots & \vdots \\
  s_2 & \cdots & \cdots & s_1 \\
  s_1 & s_2 & \cdots & s_{n-1} & s_0
\end{pmatrix}.
\]

Then we have \(S = s_0 W^0 + s_1 W^1 + s_2 W^2 + \cdots + s_{n-1} W^{n-1}\), where \(W\) is the ‘cyclic permutation’ matrix given by

\[
W = \begin{pmatrix}
  0 & 0 & \cdots & 0 & 1 \\
  1 & 0 & \cdots & 0 & 0 \\
  \vdots & \ddots & \ddots & \ddots & \vdots \\
  \vdots & \ddots & \ddots & \ddots & 0 \\
  0 & \cdots & 0 & 0 & 1
\end{pmatrix}.
\]

**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 \(j = 0, 1, \ldots, n-1\) and the determinant of \(S\) can be computed as:

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

where \(\omega_j = e^{\frac{2\pi j}{n}}\) 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.

![A prescribed hexagonal system graph L_n or F_n](image)

**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

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

(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):

\[
\begin{align*}
X_1 &= \{1, 3, 5, \ldots, 2n - 1\}, \\
X_2 &= \{1', 3', 5', \ldots, (2n - 1)\}', \\
Y_1 &= \{2, 4, 6, \ldots, 2n - 2, 2n\}, \\
Y_2 &= \{2', 4', 6', \ldots, (2n - 2)', (2n)'\},
\end{align*}
\]

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

$$
\begin{align*}
A(X_1, X_2) &= A(X_2, X_1) = I_n, \\
A(Y_1, X_1) &= A(Y_2, X_2) = C, \\
A(X_1, Y_1) &= A(X_2, Y_2) = C^T,
\end{align*}
$$

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

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

(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

$$
C^TC = D(C_n) + A(C_n) = Q(C_n),
$$

(8)

where $Q(C_n)$ is the signless Laplacian matrix of $C_n$. Obviously, $|C^TC| \neq 0$.

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

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

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

$$
= |(\lambda^2 + \lambda)I_n - C^TC| \times |(\lambda^2 - \lambda)I_n - C^TC|
$$
= |(\lambda^2 + \lambda)I_n - Q(C_n)| \times |(\lambda^2 - \lambda)I_n - Q(C_n)|
= QC_n(\lambda^2 + \lambda) \cdot QC_n(\lambda^2 - \lambda).

Using Lemma 2.3, we have
\phi Fn(\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:
\[
A(L_n) = \begin{pmatrix}
0 & I_{n+1} & B^T & 0 \\
I_{n+1} & 0 & 0 & B^T \\
B & 0 & 0 & 0 \\
0 & B & 0 & 0
\end{pmatrix}
\]

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 \(B^T B = D(P_{n+1}) + A(P_{n+1}) = Q(P_{n+1})\). 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 $\pm 1, \frac{1+\sqrt{17}}{2}, -\frac{1+\sqrt{17}}{2}$ have multiplicity equal to 1, and other eigenvalues have multiplicity equal to 2; (ii) if $n$ is odd, then eigenvalues $\frac{1+\sqrt{17}}{2}, -\frac{1+\sqrt{17}}{2}$ 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 M"obius hexacyclic system graph

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

Theorem 4.1 Let $M_n$ be a M"obius hexacyclic system graph with $n$ hexagons. Then the characteristic polynomial of $M_n$ is given below:

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

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

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

According to the representation method of $F_n$, we represent the adjacency matrix of $M_n$ as:
It is not difficult to calculate the determinant of $M$. By Lemma 2.4 $e$ is also a circulant matrix of order 2. Let

$$M^* = \lambda \cdot \left( \begin{array}{cc} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{array} \right) - \tilde{C} \cdot \tilde{C}^T.$$ 

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

$$M^* = \left( \begin{array}{cccc} \lambda^2 - 2 & -1 & \ldots & 0 \\ -1 & \lambda^2 - 2 & \ldots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & -1 & \lambda^2 - 2 \\ -\lambda & 0 & \ldots & 0 \\ 0 & -\lambda & \ldots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \ldots & -\lambda & 0 \\ 0 & \ldots & 0 & -\lambda \end{array} \right)_{2n \times 2n} = (\lambda^2 - 2)W^0 + (-1)W^1 + (-\lambda)W^n + (-1)W^{2n-1}.$$

Then the characteristic polynomial of $M_n$ is

$$\phi_{M_n}(\lambda) = |M_{4n} - A(M_n)| = \left| \begin{array}{cc} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{array} \right| - \tilde{C} \left| \begin{array}{cc} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{array} \right| - \tilde{C} \cdot \tilde{C}^T = |\lambda^2 \cdot \left( \begin{array}{cc} \lambda I_n & -I_n \\ -I_n & \lambda I_n \end{array} \right) - \tilde{C} \cdot \tilde{C}^T| = \text{det}(M^*).$$

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

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

where $\omega_j = e^{\frac{2\pi j}{n}} = e^{\frac{\pi j}{n}}$ and $i = \sqrt{-1}$. By direct computation $\omega_j = e^{\frac{\pi j}{n}}$ 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

$$\text{det}(M^*) = \prod_{j=0}^{2n-1} \left( \lambda^2 - (-1)^j \lambda - 2 - 2 \cos \frac{\pi j}{n} \right).$$
So the characteristic polynomial of $M_n$ is
\[ \phi_{M_n}(\lambda) = |M_{4n} - A(M_n)| = \det(M^*) = \prod_{j=0}^{2n-1} \left( \lambda^2 - (-1)^j \lambda - 2 - 2 \cos \frac{\pi j}{n} \right). \]

The proof is completed. \(\square\)

The characteristic eigenvalues of M"obius hexacyclic system graph $M_n$ immediately follow from Theorem 4.1.

**Theorem 4.2** The characteristic eigenvalues of $M_n$ are
\[
\begin{cases}
\frac{1}{2} \left( 1 \pm \sqrt{9 + 8 \cos \frac{2k \pi}{n}} \right), & j = 2k \\
\frac{1}{2} \left( -1 \pm \sqrt{9 + 8 \cos \frac{2(2k - 1) \pi}{n}} \right), & j = 2k + 1
\end{cases}
\]
where $k = 0, 1, \ldots, n-1$.

Consequently, we get the spectrum of M"obius hexacyclic system graph $M_n$ from Theorem 4.2.

**Corollary 4.1** The characteristic eigenvalues of $M_n$ are
\[
\begin{cases}
\frac{1}{2} \left( 1 \pm \sqrt{9 + 8 \cos \frac{2k \pi}{n}} \right), & k = 1, 2, \ldots, n \\
\frac{1}{2} \left( -1 \pm \sqrt{9 + 8 \cos \frac{2(2k - 1) \pi}{n}} \right), & k = 1, 2, \ldots, n
\end{cases}
\]
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 $\lambda_{4n}(M_n) = \frac{1}{2}(-1 - \sqrt{9 + 8 \cos \frac{2k \pi}{n}})$ that achieves at $\frac{1}{2}(-1 - \sqrt{9 + 8 \cos \frac{2(2k + 1) \pi}{n}})$ for $k = n$. Since $\lim_{n \to \infty} \frac{1}{2}(-1 - \sqrt{9 + 8 \cos \frac{2k \pi}{n}}) = -\frac{1 - \sqrt{17}}{2}$, 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 M"obius 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

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

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 $L_n$

$$E(L_n) = \sum_{i=1}^{4n+2} |\lambda_i|$$

$$= |1| + |1| + \sum_{j=1}^{n} \left| \frac{1}{2} \left( 1 + \sqrt{9 + 8 \cos \frac{\pi j}{n + 1}} \right) + \sum_{j=1}^{n} \frac{1}{2} \left( 1 - \sqrt{9 + 8 \cos \frac{\pi j}{n + 1}} \right) \right|$$

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

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

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

$$\left( \sum_{j=1}^{n} \sqrt{9 + 8 \cos \frac{\pi j}{n + 1}} \right)^2 \leq \sum_{j=1}^{n} 1^2 \times \sum_{j=1}^{n} \left( \sqrt{9 + 8 \cos \frac{\pi j}{n + 1}} \right)^2$$

$$= n \sum_{j=1}^{n} \left( 9 + 8 \cos \frac{\pi j}{n + 1} \right)$$

$$= n \left( 9n + 8 \sum_{j=1}^{n} \cos \frac{\pi j}{n + 1} \right)$$

$$= 9n^2.$$

It is easy to get

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

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

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

$$E(F_n) = \sum_{i=1}^{4n} |\lambda_i|$$

$$= \sum_{j=1}^{n} \left| \frac{1 + \sqrt{9 + 8 \cos \frac{2\pi j}{n}}}{2} \right| + \sum_{j=1}^{n} \left| \frac{1 - \sqrt{9 + 8 \cos \frac{2\pi j}{n}}}{2} \right| +$$

$$\sum_{j=1}^{n} \left| \frac{-1 + \sqrt{9 + 8 \cos \frac{2\pi j}{n}}}{2} \right| + \sum_{j=1}^{n} \left| \frac{-1 - \sqrt{9 + 8 \cos \frac{2\pi j}{n}}}{2} \right|$$

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

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

The proof is completed. $\Box$

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

$$E(M_n) = \sum_{i=1}^{4n} |\lambda_i|$$

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

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

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

Applying Cauchy-Schwartz inequality to \((1, 1, \ldots, 1)\) and \(\left( \sqrt{9 + 8 \cos \frac{\pi j}{n}}, \ldots, \sqrt{9 + 8 \cos \frac{2n\pi j}{n}} \right)\), we have
\[
\left( \sum_{j=1}^{2n} \sqrt{9 + 8 \cos \frac{\pi j}{n}} \right)^2 < \sum_{j=1}^{2n} 1^2 \times \sum_{j=1}^{2n} \left( \sqrt{9 + 8 \cos \frac{\pi j}{n}} \right)^2 \\
= 2n \cdot \sum_{j=1}^{2n} \left( 9 + 8 \cos \frac{\pi j}{n} \right) \\
= 2n \cdot \left( 18n + 8 \sum_{j=1}^{2n} \cos \frac{\pi j}{n} \right) \\
= 36n^2.
\]

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. \(\square\)

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References

On the characteristic polynomial of a hexagonal system and its application


