Journal of Mathematical Research with Applications
May, 2023, Vol. 43, No. 3, pp. 266–276
DOI:10.3770/j.issn:2095-2651.2023.03.002
Http://jmre.dlut.edu.cn

On the A_α-Characteristic Polynomials and the A_α-Spectra of Two Classes of Hexagonal Systems

Mengyue YUAN, Fei WEN*, Ranran WANG
Institute of Applied Mathematics, Lanzhou Jiaotong University, Gansu 730070*, P. R. China*

Abstract The A_α-matrix of a graph G is defined as $A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G)$ ($\alpha \in [0,1]$), given by Nikiforov in 2017, where $A(G)$ and $D(G)$ are, respectively, the adjacency matrix and the degree matrix of graph G. Let F_n and M_n be hexacyclic system graph and Möbius hexacyclic system graph, respectively. In this paper, according to the determinant and the eigenvalues of a circulant matrix, we firstly present A_α-characteristic polynomial and A_α-spectrum of F_n (resp., M_n). Furthermore, we obtain the upper bound of the A_α-energy of F_n (resp., M_n).

Keywords A_α-characteristic polynomial; A_α-spectrum; hexagonal system

MR(2020) Subject Classification 05C50

1. Introduction

All graphs considered here are simple finite undirected graph. Let $G = (V(G), E(G))$ be a connected graph with vertex set $V(G)$ and edge set $E(G)$. $|V(G)|$ and $|E(G)|$ are often called the order and the size of the graph G, respectively. Let $A(G)$ denote the adjacency matrix, and $D(G)$ denote the diagonal matrix of the degrees of G. For any real $\alpha \in [0,1]$, Nikiforov [1] defined the matrix $A_\alpha(G)$ as

$$A_\alpha(G) = \alpha D(G) + (1-\alpha)A(G).$$

It is clear that $A_0(G) = A(G)$, $A_1(G) = D(G)$ and $2A_{1/2}(G) = Q(G)$, where $Q(G)$ is the signless Laplacian matrix. Moreover, $L(G) = \frac{A_\alpha - A_\beta}{\alpha-\beta}$ if $\alpha \neq \beta$ for any $\alpha, \beta \in [0,1]$, where $L(G)$ is the Laplacian matrix. We denote by $\Phi(A_\alpha(G);\lambda) = \det(\lambda I_n - A_\alpha(G))$ the A_α-characteristic polynomial of graph G, where I_n is the identity matrix. For convenience, we assume that the A_α-eigenvalues of G are $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \lambda_n(G)$. Then the A_α-spectrum of G is a multiset of distinct eigenvalues together with their multiplicities. The largest A_α-eigenvalue of $A_\alpha(G)$ is called the A_α-spectral radius of G, denoted by $\rho(A_\alpha(G))$. For more properties on $A_\alpha(G)$, we refer the reader to [2–7].

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. Let F_n and M_n be respectively

Received April 28, 2022; Accepted August 22, 2022
Supported by the National Natural Science Foundation of China (Grant No. 11961041), the Natural Science Foundation of Gansu Province (Grant No. 21JR11RA065) and the Excellent Postgraduates of Gansu Provincial Department of Education "Star of Innovation" Foundation (Grant No. 2021CXZX-594).
* Corresponding author
E-mail address: wenfei@lzjtu.edu.cn (Fei WEN)

hexacyclic system graph and Möbius hexacyclic system graph with n hexagons, shown in Figure 1. For undefined terminologies and notations here, we refer to [8].

It is well-known that Hexagonal systems are very important in theoretical chemistry because they are natural graph representations of benzenoid hydrocarbon. Up to now, the adjacency spectra of hexagonal systems L_n and F_n are investigated in [9,10]. The adjacency characteristic polynomial of H_3^n called prolate rectangle of benzenoid system in theoretical chemistry is determined by Lou et al. [11]. In addition, the normalized Laplacian polynomials and spectra of F_n and M_n were given by Shi et al. [12].

In this paper, we consider the A_α-characteristic polynomials and A_α-spectra of F_n and M_n. From a chemical point of view, it is of great interest to find the values of energy for a graph. Therefore, as an application, we obtain the upper bounds of the A_α-energy of F_n and M_n, respectively.

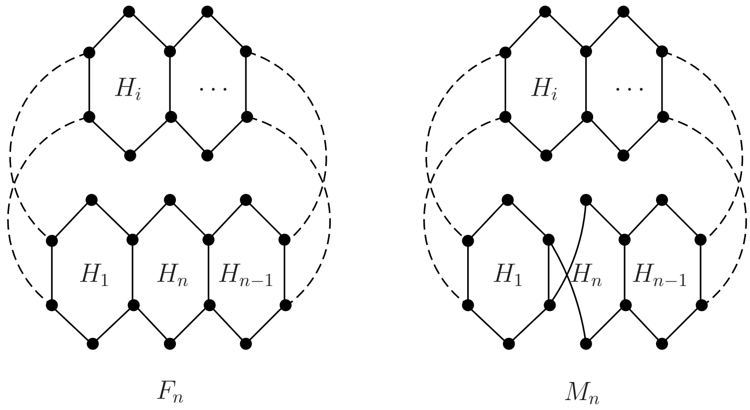

Figure 1 Graphs F_n and M_n

2. Preliminaries

In this section, we recall some basic lemmas which will be useful for the proof of main results.

Lemma 2.1 ([13]) *Let C_n be the cycle on n vertices. Then the Q-polynomial of C_n is*

$$Q(C_n;\lambda)=\prod_{j=1}^{n}(\lambda-2-2\cos\frac{2\pi j}{n}).$$

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

Lemma 2.3 ([14]) *Let $(0,1,0,\dots,0)$ and $(s_1,s_2,\dots,s_n)$ be the elements of the first row of circulant matrices W and S, respectively. Then*

$$S=\sum_{j=1}^{n}s_j\omega^{j-1},$$

where the eigenvalues of W *are* $1,\omega,\omega^2,\dots,\omega^{n-1}$, $\omega=e^{\frac{2\pi i}{n}}$.

Lemma 2.4 ([14,15]) *Let* S *be an* $n\times n$ *circulant matrix. Then the eigenvalues of* S *are*

$$\lambda_r=\sum_{j=1}^{n}s_jw^{(j-1)r}=s_1+s_2\omega^r+\cdots+s_n\omega^{(n-1)r},\quad r=0,1,\dots,n-1,$$

and $\det(S)=\prod_{r=0}^{n-1}(s_1+s_2\omega^r+\cdots+s_n\omega^{(n-1)r})$.

Lemma 2.5 ([16]) *Let* M, N, P *and* Q *be matrices of order* $p\times p$, $p\times q$, $q\times p$ *and* $q\times q$, *respectively, and* M *and* Q *are non-singular square matrices. Then*

$$\begin{vmatrix} M & N\\ P & Q\end{vmatrix}=|M||Q-PM^{-1}N|=|Q||M-NQ^{-1}P|.$$

3. Main results

The main results of this section are that the A_α-spectra of F_n and M_n are, respectively, determined.

3.1 The A_α-spectrum of F_n

At first, we give a partition of the vertex set of F_n, denoted by $V(F_n)=V_1\cup V_2\cup V_3\cup V_4$, where $V_i=\{v_{i1},v_{i2},\dots,v_{in}\}$ $(i=1,2,3,4)$, as shown in the Figure 2. Clearly, $|V(F_n)|=4n$. Let $A(V_i,V_j)=(a_{kl})$ denote the block matrix of $A(F_n)$ corresponding to the V_i block row and the V_j block column. If $v_{ik}\in V_i$ is adjacent with $v_{jl}\in V_j$, then $a_{kl}=1$, otherwise $a_{kl}=0$. Then we have

$$R=A(V_2,V_1)=A(V_3,V_4)=\begin{pmatrix}1 & & & & & 1\\ 1 & 1 & & & & \\ & 1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 1 & \\ & & & & 1 & 1\end{pmatrix}_{n\times n}.$$

Observe that the matrix R is the incidence matrix of C_n and $RR^{\mathrm T}=D(C_n)+A(C_n)=Q(C_n)$.

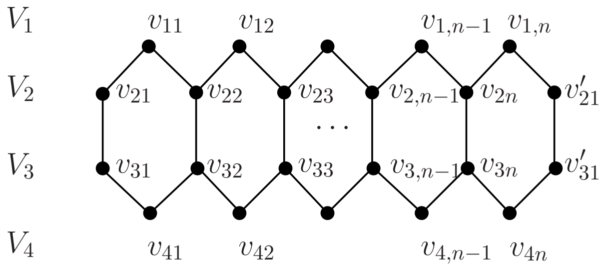

Figure 2 Labeling of graphs F_n

Based on the above, we obtain the following theorem.

Theorem 3.1 *Let F_n be a hexagonal system with n hexagons. Then the A_α-characteristic polynomial of F_n is*

$$\Phi(A_\alpha(F_n);\lambda) = \prod_{j=1}^{n}\big((\lambda-2\alpha)(\lambda-2\alpha-1)-(1-\alpha)^2(2+2\cos\frac{2\pi j}{n})\big)\times \prod_{j=1}^{n}\big((\lambda-2\alpha)(\lambda-4\alpha+1)-(1-\alpha)^2(2+2\cos\frac{2\pi j}{n})\big).$$

Proof In accordance with the vertex partition above, we can express the adjacency matrix and the degree matrix of F_n in the form of block matrix below:

$$A(F_n) = \begin{array}{c} \\ V_1 \\ V_2 \\ V_3 \\ V_4 \end{array}\begin{array}{c} \begin{array}{cccc} V_1 & V_2 & V_3 & V_4 \end{array} \\ \begin{pmatrix} \mathbf{0}_n & R^{\mathrm{T}} & \mathbf{0}_n & \mathbf{0}_n \\ R & \mathbf{0}_n & I_n & \mathbf{0}_n \\ \mathbf{0}_n & I_n & \mathbf{0}_n & R \\ \mathbf{0}_n & \mathbf{0}_n & R^{\mathrm{T}} & \mathbf{0}_n \end{pmatrix}\end{array}, \qquad D(F_n) = \begin{array}{c} \\ V_1 \\ V_2 \\ V_3 \\ V_4 \end{array}\begin{array}{c} \begin{array}{cccc} V_1 & V_2 & V_3 & V_4 \end{array} \\ \begin{pmatrix} 2I_n & & & \\ & 3I_n & & \\ & & 3I_n & \\ & & & 2I_n \end{pmatrix}\end{array}.$$

It then follows from the definition of A_α-matrix that

$$A_\alpha(F_n) = \alpha D(F_n) + (1-\alpha)A(F_n) = \begin{array}{c} \\ V_1 \\ V_2 \\ V_3 \\ V_4 \end{array}\begin{array}{c} \begin{array}{cccc} V_1 & V_2 & V_3 & V_4 \end{array} \\ \begin{pmatrix} 2\alpha I_n & (1-\alpha)R^{\mathrm{T}} & \mathbf{0}_n & \mathbf{0}_n \\ (1-\alpha)R & 3\alpha I_n & (1-\alpha)I_n & \mathbf{0}_n \\ \mathbf{0}_n & (1-\alpha)I_n & 3\alpha I_n & (1-\alpha)R \\ \mathbf{0}_n & \mathbf{0}_n & (1-\alpha)R^{\mathrm{T}} & 2\alpha I_n \end{pmatrix}\end{array}.$$

Thus, $\Phi(A_\alpha(F_n);\lambda)$ can be represented in the form of determinant as follows:

$$\Phi(A_\alpha(F_n);\lambda) = |\lambda I_{4n} - A_\alpha(F_n)| = \det B_0,$$

where

$$B_0 = \lambda I_{4n} - A_\alpha(F_n) = \begin{pmatrix} (\lambda-2\alpha)I_n & -(1-\alpha)R^{\mathrm{T}} & \mathbf{0}_n & \mathbf{0}_n \\ -(1-\alpha)R & (\lambda-3\alpha)I_n & -(1-\alpha)I_n & \mathbf{0}_n \\ \mathbf{0}_n & -(1-\alpha)I_n & (\lambda-3\alpha)I_n & -(1-\alpha)R \\ \mathbf{0}_n & \mathbf{0}_n & -(1-\alpha)R^{\mathrm{T}} & (\lambda-2\alpha)I_n \end{pmatrix}.$$

By multiplying the first block row by $\frac{1-\alpha}{\lambda-2\alpha}R$ and then adding it to the second block row, and multiplying the fourth row by $\frac{1-\alpha}{\lambda-2\alpha}R$ and then adding it to the third block row, we get the matrix B_1 shown as follows:

$$B_1 = \begin{pmatrix} (\lambda-2\alpha)I_n & -(1-\alpha)R^{\mathrm{T}} & \mathbf{0}_n & \mathbf{0}_n \\ \mathbf{0}_n & (\lambda-3\alpha)I_n - \frac{(1-\alpha)^2RR^{\mathrm{T}}}{\lambda-2\alpha} & -(1-\alpha)I_n & \mathbf{0}_n \\ \mathbf{0}_n & -(1-\alpha)I_n & (\lambda-3\alpha)I_n - \frac{(1-\alpha)^2RR^{\mathrm{T}}}{\lambda-2\alpha} & \mathbf{0}_n \\ \mathbf{0}_n & \mathbf{0}_n & -(1-\alpha)R^{\mathrm{T}} & (\lambda-2\alpha)I_n \end{pmatrix}.$$

After that, applying the Laplace's Extension Theorem in the first and fourth block columns of

B_1, we get

$$\det B_1 = (\lambda - 2\alpha)^{2n} \cdot \det B_2,$$

where

$$\det B_2 = \begin{vmatrix} (\lambda-3\alpha)I_n - \frac{(1-\alpha)^2RR^{\mathrm{T}}}{\lambda-2\alpha} & -(1-\alpha)I_n \\ -(1-\alpha)I_n & (\lambda-3\alpha)I_n - \frac{(1-\alpha)^2RR^{\mathrm{T}}}{\lambda-2\alpha} \end{vmatrix}.$$

Note that $RR^{\mathrm{T}} = Q(C_n)$. It follows from Lemmas 2.1 and 2.2 that

$$\begin{aligned} \det B_1 =& (\lambda-2\alpha)^{2n}|(\lambda-3\alpha)I_n - \frac{(1-\alpha)^2Q(C_n)}{\lambda-2\alpha} - (1-\alpha)I_n||(\lambda-3\alpha)I_n - \\ & \frac{(1-\alpha)^2Q(C_n)}{\lambda-2\alpha} + (1-\alpha)I_n| \\ =& (\lambda-2\alpha)^{2n}|(\lambda-2\alpha-1)I_n - \frac{(1-\alpha)^2Q(C_n)}{\lambda-2\alpha}||(\lambda-4\alpha+1)I_n - \frac{(1-\alpha)^2Q(C_n)}{\lambda-2\alpha}| \\ =& |(\lambda-2\alpha)(\lambda-2\alpha-1)I_n - (1-\alpha)^2Q(C_n)||(\lambda-2\alpha)(\lambda-4\alpha+1)I_n - (1-\alpha)^2Q(C_n)|. \end{aligned}$$

Therefore, we have

$$\begin{aligned} \Phi(A_\alpha(F_n);\lambda) &= \det B_0 = \det B_1 \\ &= \prod_{j=1}^{n}\big((\lambda-2\alpha)(\lambda-2\alpha-1) - (1-\alpha)^2(2+2\cos\frac{2\pi j}{n})\big)\times \\ & \prod_{j=1}^{n}\big((\lambda-2\alpha)(\lambda-4\alpha+1) - (1-\alpha)^2(2+2\cos\frac{2\pi j}{n})\big). \quad \square \end{aligned}$$

Through Theorem 3.1, we get the following corollary.

Corollary 3.2 *Let F_n be a hexagonal system with n hexagons. Then the A_α-eigenvalues of graph F_n are*

$$\begin{cases} \lambda_{1,2}^{j} = \dfrac{(4\alpha+1) \pm \sqrt{8(1+\cos\frac{2\pi j}{n})(\alpha-1)^2+1}}{2}, & j=1,2,\ldots,n; \\ \lambda_{3,4}^{j} = \dfrac{(6\alpha-1) \pm 2\sqrt{(2+2\cos\frac{2\pi j}{n})(\alpha-1)^2+(\alpha^2-\alpha+1)}}{2}, & j=1,2,\ldots,n. \end{cases}$$

3.2 The A_α-spectrum of M_n

We give a vertex partition $V(M_n) = V \cup U$ of M_n, where $V = \{v_1, v_2, \ldots, v_n, v_1', v_2', \ldots, v_n'\}$ and $U = \{u_1, u_2, \ldots, u_n, u_1', u_2', \ldots, u_n'\}$ (shown in Figure 3). According to the label of $V(M_n)$, the adjacency matrix of M_n can be expressed in the form of block matrix:

$$A(M_n) = \begin{matrix} & V & U \\ V & Y & R \\ U & R^{\mathrm{T}} & \mathbf{0} \end{matrix}$$

where $Y = A(V,V) = \begin{pmatrix} \mathbf{0}_n & I_n \\ I_n & \mathbf{0}_n \end{pmatrix}$ and $R = A(V,U) = \begin{pmatrix} 1 & & & & & 1 \\ 1 & 1 & & & & \\ & 1 & 1 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 1 & \\ & & & & 1 & 1 \end{pmatrix}_{2n\times 2n}$.

Note that $D(M_n) = \begin{pmatrix} 3I_{2n} & \\ & 2I_{2n} \end{pmatrix}$. So, we get the following theorem.

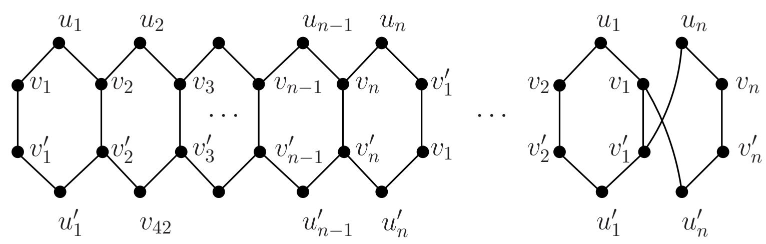

Figure 3 Labeling of graphs M_n

Theorem 3.3 *Let M_n be the Möbius hexacyclic system graph with n hexagons. Then the A_α-characteristic polynomial of M_n is*

$$\Phi(A_\alpha(M_n);\lambda) = \prod_{r=0}^{n-1}\big((\lambda^2 - 5\alpha\lambda + 4\alpha^2 + 4\alpha - 2) - 2(1-\alpha)^2\cos\frac{\pi r}{n} - (-1)^r(\lambda - 2\alpha)(1-\alpha)\big).$$

Proof Combining the above with the definition of A_α-matrix yields

$$A_\alpha(M_n) = \alpha D(M_n) + (1-\alpha)A(M_n) = \begin{pmatrix} 3\alpha I_{2n} + (1-\alpha)Y & (1-\alpha)R \\ (1-\alpha)R^{\mathrm{T}} & 2\alpha I_{2n} \end{pmatrix}.$$

The A_α-characteristic polynomial of M_n can be expressed as:

$$\Phi(A_\alpha(M_n);\lambda) = |\lambda I_{4n} - A_\alpha(M_n)| = \begin{vmatrix} (\lambda - 3\alpha)I_{2n} - (1-\alpha)Y & -(1-\alpha)R \\ -(1-\alpha)R^{\mathrm{T}} & (\lambda - 2\alpha)I_{2n} \end{vmatrix}.$$

According to Lemma 2.5, one can get

$$\begin{aligned}\Phi(A_\alpha(M_n);\lambda) &= (\lambda - 2\alpha)^{2n}\det((\lambda - 3\alpha)I_{2n} - (1-\alpha)Y - \frac{(1-\alpha)^2}{\lambda - 2\alpha}RR^{\mathrm{T}}) \\ &= \det((\lambda - 2\alpha)(\lambda - 3\alpha)I_{2n} - (\lambda - 2\alpha)(1-\alpha)Y - (1-\alpha)^2RR^{\mathrm{T}}) \\ &= \det(B_0).\end{aligned}$$

By direct calculation, we have

$$RR^{\mathrm{T}}=\begin{pmatrix}2&1&&&&&1\\1&2&1&&&&\\&1&2&1&&&\\&&\ddots&\ddots&\ddots&&\\&&&1&2&1&\\&&&&1&2&1\\1&&&&&1&2\end{pmatrix}.$$

Therefore,

$$\begin{aligned}B_0&=(\lambda-2\alpha)(\lambda-3\alpha)I_{2n}-(\lambda-2\alpha)(1-\alpha)Y-(1-\alpha)^2RR^{\mathrm{T}}\\&=(\lambda^2-5\alpha\lambda+6\alpha^2)I_{2n}-\begin{pmatrix}0&\cdots&0&(\lambda-2\alpha)(1-\alpha)&&\\\vdots&\ddots&\vdots&&\ddots&\\0&\cdots&0&&&(\lambda-2\alpha)(1-\alpha)\\(\lambda-2\alpha)(1-\alpha)&&&0&\cdots&0\\&\ddots&&\vdots&\ddots&\vdots\\&&(\lambda-2\alpha)(1-\alpha)&0&\cdots&0\end{pmatrix}-\\&\begin{pmatrix}2(1-\alpha)^2&(1-\alpha)^2&&&&(1-\alpha)^2\\(1-\alpha)^2&2(1-\alpha)^2&(1-\alpha)^2&&&\\&(1-\alpha)^2&2(1-\alpha)^2&(1-\alpha)^2&&\\&&\ddots&\ddots&\ddots&\\&&&(1-\alpha)^2&2(1-\alpha)^2&(1-\alpha)^2\\(1-\alpha)^2&&&&(1-\alpha)^2&2(1-\alpha)^2\end{pmatrix}\\&=\begin{pmatrix}B_{01}&B_{02}\\B_{02}&B_{01}\end{pmatrix},\end{aligned}$$

where

$$B_{01}=\begin{pmatrix}\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2&-(1-\alpha)^2&&\\-(1-\alpha)^2&\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2&-(1-\alpha)^2&\\&&\ddots&\\&&-(1-\alpha)^2&\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2\end{pmatrix}_{n\times n}$$

and

$$B_{02}=\begin{pmatrix}-(\lambda-2\alpha)(1-\alpha)&&&-(1-\alpha)^2\\&-(\lambda-2\alpha)(1-\alpha)&&\\&&\ddots&\\-(1-\alpha)^2&&&-(\lambda-2\alpha)(1-\alpha)\end{pmatrix}_{n\times n}.$$

It can be seen from above that the matrix is a circulant matrix, and the elements in the first row are

$$[\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2,-(1-\alpha)^2,0,\ldots,0,-(\lambda-2\alpha)(1-\alpha),0,\ldots,0,-(1-\alpha)^2]$$

i.e.,

$$s_1=\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2,\ s_2=-(1-\alpha)^2,$$
$$s_{n+1}=-(\lambda-2\alpha)(1-\alpha),\ s_{2n}=-(1-\alpha)^2$$

and $s_i=0$ otherwise. By Lemma 2.3, we can obtain

$$\begin{aligned}B_0&=s_1W^0+s_2W^1+s_{n+1}W^n+s_{2n}W^{2n-1}\\&=\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2W^0-(1-\alpha)^2W^1-(\lambda-2\alpha)(1-\alpha)W^n-(1-\alpha)^2W^{2n-1}.\end{aligned}$$

And then, it follows from Lemma 2.4 that

$$\det B_0=\prod_{r=0}^{n-1}\big(\lambda^2-5\alpha\lambda+6\alpha^2-2(1-\alpha)^2-(1-\alpha)^2\omega^r-(\lambda-2\alpha)(1-\alpha)\omega^{nr}-(1-\alpha)^2\omega^{(2n-1)r}\big),$$

where $\omega^r=e^{\frac{\pi r}{n}i}$, $i^2=-1$. By simple computation, we have

$$\omega^r=\cos\frac{\pi r}{n}+i\sin\frac{\pi r}{n},\ \omega^{nr}=\cos\pi r+i\sin\pi r=(-1)^r,\ \omega^{(2n-1)r}=\cos\frac{\pi r}{n}-i\sin\frac{\pi r}{n}.$$

Thus, one can obtain

$$\begin{aligned}\Phi(A_\alpha(M_n);\lambda)=\det B_0&=\prod_{r=0}^{n-1}\big((\lambda^2-5\alpha\lambda+4\alpha^2+4\alpha-2)-(1-\alpha)^2(\cos\frac{\pi r}{n}+i\sin\frac{\pi r}{n})-\\&\quad(\lambda-2\alpha)(1-\alpha)(-1)^r-(1-\alpha)^2(\cos\frac{\pi r}{n}-i\sin\frac{\pi r}{n})\big)\\&=\prod_{r=0}^{n-1}\big((\lambda^2-5\alpha\lambda+4\alpha^2+4\alpha-2)-2(1-\alpha)^2\cos\frac{\pi r}{n}-(-1)^r(\lambda-2\alpha)(1-\alpha)\big),\end{aligned}$$

as required. □

Corollary 3.4 *Let M_n be the Möbius hexacyclic system graph with n hexagons. Then the A_α-eigenvalues of graph M_n are*

$$\begin{cases}\lambda^r_{1,2}=\dfrac{(4\alpha+1)\pm\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2\cos\frac{\pi r}{n}}}{2}, \text{ when } r=2k,k=1,2,\ldots,n;\\ \lambda^r_{3,4}=\dfrac{(6\alpha-1)\pm\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2\cos\frac{\pi r}{n}}}{2}, \text{ when } r=2k-1,k=1,2,\ldots,n.\end{cases}$$

i.e.,

$$\begin{cases}\lambda^k_{1,2}=\dfrac{(4\alpha+1)\pm\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2\cos\frac{2k\pi}{n}}}{2}, & k=1,2,\ldots,n;\\ \lambda^k_{3,4}=\dfrac{(6\alpha-1)\pm\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2\cos\frac{(2k-1)\pi}{n}}}{2}, & k=1,2,\ldots,n.\end{cases}$$

Remark 3.5 It is noteworthy that $A_\alpha(G)$ is the convex combinations of $A(G)$ and $D(G)$, and it can underpin a unified theory of $A(G)$ and $Q(G)$. For the above conclusions, if α takes different values, one can get the A-spectrum, L-spectrum and Q-spectrum of graph F_n (resp., M_n).

4. Applications

The energy of the graph comes from theoretical chemistry. In [17], the graph energy of a simple graph G is defined by Gutman as the sum of the absolute values of the eigenvalues of the adjacency matrix $A(G)$, namely as $\mathbf{E(G)} = \sum_{j=1}^{n} |\mu_j|$, where $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of $A(G)$. Somewhere around the year 2006, the number of papers on graph energy began to increase significantly. In view of the above, a natural step in this direction was to investigate some graph energy variants, i.e., apply eigenvalues of various other graph matrix, generally having the similar definitions as the original energy definition. For example, the Laplacian energy [18], the distance energy [19], the signless Laplacian energy [20], the Seidel energy [21] as well as the Hermitian energy [22], etc.

Similarly, we now define the A_α-energy of G as $\mathbb{E}_\alpha(G) = \sum_{i=1}^{n} |\lambda_i|$, that is, the sum of the absolute values of all eigenvalues of $A_\alpha(G)$. As an application, we study the A_α-energy of F_n and M_n, and obtain the upper bounds of the A_α-energy of F_n and M_n, respectively.

Theorem 4.1 *Let F_n be a hexagonal system with n hexagons, and $\mathbb{E}_\alpha(F_n)$ be the A_α-energy of F_n. Then*

$$\mathbb{E}_\alpha(F_n) \le \frac{n}{2}(8\alpha + 1 + (\sqrt{16(\alpha-1)^2+1}) + |(6\alpha-1) + 2\sqrt{4(\alpha-1)^2 + (\alpha^2-\alpha+1)}| + |6\alpha - 1 - 2\sqrt{\alpha^2-\alpha+1}|).$$

Proof According to the definition of A_α-energy and Corollary 3.2, we have

$$\begin{aligned}\mathbb{E}_\alpha(F_n) =& \sum_{j=1}^{n} |\frac{(4\alpha+1) + \sqrt{8(1+\cos\frac{2\pi j}{n})(\alpha-1)^2+1}}{2}| + \\ & \sum_{j=1}^{n} |\frac{(4\alpha+1) - \sqrt{8(1+\cos\frac{2\pi j}{n})(\alpha-1)^2+1}}{2}| + \\ & \sum_{j=1}^{n} |\frac{(6\alpha-1) + 2\sqrt{(2+2\cos\frac{2\pi j}{n})(\alpha-1)^2 + (\alpha^2-\alpha+1)}}{2}| + \\ & \sum_{j=1}^{n} |\frac{(6\alpha-1) - 2\sqrt{(2+2\cos\frac{2\pi j}{n})(\alpha-1)^2 + (\alpha^2-\alpha+1)}}{2}| \\ \le & \sum_{j=1}^{n} (\frac{(4\alpha+1) + \sqrt{8(1+\cos\frac{2\pi j}{n})(\alpha-1)^2+1}}{2}) + \sum_{j=1}^{n} (\frac{(4\alpha+1)-1}{2}) + \\ & \sum_{j=1}^{n} |\frac{(6\alpha-1) + 2\sqrt{(2+2\cos\frac{2\pi j}{n})(\alpha-1)^2 + (\alpha^2-\alpha+1)}}{2}| + \\ & \sum_{j=1}^{n} |\frac{(6\alpha-1) - 2\sqrt{\alpha^2-\alpha+1}}{2}|\end{aligned}$$

$$\begin{aligned}&\le\frac{n}{2}(4\alpha+1)+\frac{n}{2}(\sqrt{16(\alpha-1)^2+1})+2\alpha n+\frac{n}{2}|(6\alpha-1)+\\&2\sqrt{4(\alpha-1)^2+(\alpha^2-\alpha+1)}|+\frac{n}{2}|6\alpha-1-2\sqrt{\alpha^2-\alpha+1}|\\&=\frac{n}{2}(8\alpha+1+(\sqrt{16(\alpha-1)^2+1})+|(6\alpha-1)+\\&2\sqrt{4(\alpha-1)^2+(\alpha^2-\alpha+1)}|+|6\alpha-1-2\sqrt{\alpha^2-\alpha+1}|)\end{aligned}$$

Thus, the result follows. □

Theorem 4.2 *Let M_n be the Möbius hexacyclic system graph with n hexagons, and $\mathbb{E}_\alpha(M_n)$ be the A_α-energy of M_n. Then*

$$\begin{aligned}\mathbb{E}_\alpha(M_n)\le&\frac{n}{2}(14\alpha+1+\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2}+\\&|(6\alpha-1)+\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2}|).\end{aligned}$$

Proof According to the definition of A_α-energy and Corollary 3.4, we can obtain

$$\begin{aligned}\mathbb{E}_\alpha(M_n)=&\sum_{k=1}^{n}|\frac{(4\alpha+1)+\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2\cos\frac{2k\pi}{n}}}{2}|+\\&\sum_{k=1}^{n}|\frac{(4\alpha+1)-\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2\cos\frac{2k\pi}{n}}}{2}|+\\&\sum_{k=1}^{n}|\frac{(6\alpha-1)+\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2\cos\frac{(2k-1)\pi}{n}}}{2}|+\\&\sum_{k=1}^{n}|\frac{(6\alpha-1)-\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2\cos\frac{(2k-1)\pi}{n}}}{2}|\\\le&\frac{n}{2}|(4\alpha+1)+\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2}|+\frac{n}{2}(4\alpha+1)+\\&\frac{n}{2}|(6\alpha-1)+\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2}|+\frac{n}{2}(6\alpha-1)\\=&\frac{n}{2}\big(14\alpha+1+\sqrt{(4\alpha+1)^2-4(\alpha^2+6\alpha-2)+8(1-\alpha)^2}+\\&|(6\alpha-1)+\sqrt{(6\alpha-1)^2-4(6\alpha^2-2\alpha-2)+8(1-\alpha)^2}|\big).\end{aligned}$$

Hence, we complete the proof. □

Acknowledgements We sincerely thank the referees for their time and comments.

References

[1] V. NIKIFOROV. *Merging the A- and Q-spectral theories*. Appl. Anal. Discrete Math., 2017, **11**: 81–107.

[2] V. NIKIFOROV, G. PASTÉN, O. ROJO, et al. *On the A_α-spectra of trees*. Linear Algebra Appl., 2017, **520**: 286–305.

[3] Huiqing LIN, Jie XUE, Jinlong SHU. *On the A_α-spectra of graphs*. Linear Algebra Appl., 2018, **556**: 210–219.

[4] V. NIKIFOROV, O. ROJO. *A note on the positive semidefiniteness of $A_\alpha(G)$*. Linear Algebra Appl., 2017, **519**: 156–163.

[5] V. NIKIFOROV, O. ROJO. *On the α-index of graphs with pendent paths*. Linear Algebra Appl., 2018, **550**: 87–104.

[6] Huiqiu LIN, Xiaogang LIU, Jie XUE. *Graphs determined by their A_α-spectra*. Discrete Math., 2019, **342**(2): 441–450.

[7] Xiaogang LIU, Shunyi LIU. *On the A_α-characteristic polynomial of a graph*. Linear Algebra Appl., 2018, **546**: 274–288.

[8] D. CVETKOVIĆ, P. ROWLINSON, S. K. SIMIĆ. *An Introduction to the Theory of Graph Spectra*. Cambridge University Press, Cambridge, 2010.

[9] G. DERFLINGER, H. SOFER. *Die HMO-Koeffizienten der linearen Polyacene in geschlossener form*. Monatshefte Für Chemie, 1968, **99**(5): 1866–1875.

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

[11] Zhenzhen LOU, Qiongxiang HUANG, Daijun YIN. *On the characteristic polynomial and the spectrum of a Hexagonal system*. MATCH Commun. Math. Comput. Chem., 2014, **72**(1): 153–164.

[12] Yinfang SHI, You ZHANG, Fei WEN. *Normalized Laplacian spectrum of two classes of Hexagonal systems and the applications*. J. Jilin University (Science Edition), 2019, **57**(4): 824–832.

[13] D. CVETKOVIĆ. *Towards a Spectral Theory of Graphs Based on the Signless Laplacian. III*. Appl. Anal. Discrete Math., 2010, **4**(1): 156–166.

[14] N. BIGGS. *Algebraic Graph Theory. II*. Cambridge University Press, Cambridge, 1993.

[15] P. J. DAVIS. *Circulant Matrices*. John Wiley & Sons, New York, 1979.

[16] Fuzhen ZHANG. *The Schur Complement and Its Application*. Springer-Verlag, New York, 2005.

[17] I. GUTMAN. *The energy of a graph*. Ber Math-Statist Sekt Forsch Graz, 1978, **103**: 2177–2187.

[18] I. GUTMAN, Bo ZHOU. *Laplacian energy of a graph*. Linear Algebra Appl., 2006, **414**(1): 29–37.

[19] G. INDULAL, I. GUTMAN, A. VIJAYAKUMAR. *On distance energy of graphs*. MATCH Commun. Math. Comput. Chem., 2008, **60**(2): 461–472.

[20] N. ABREU, D. M. CARDOSO, I. GUTMAN, et al. *Bounds for the signless Laplacian energy*. Linear Algebra Appl., 2011, **435**(10): 2365–2374.

[21] W. H. HAEMERS. *Seidel switching and graph energy*. MATCH Commun. Math. Comput. Chem., 2012, **68**(3): 653–659.

[22] Jianxi LIU, Xueliang LI. *Hermitian-adjacency matrices and Hermitian energies of mixed graphs*. Linear Algebra Appl., 2015, **466**: 182–207.