On graphs with exactly one anti-adjacency eigenvalue and beyond

Jianfeng Wang\textsuperscript{a,1}, Xingyu Lei\textsuperscript{a}, Mei Lu\textsuperscript{b}, Sezer Sorgun\textsuperscript{c}, Hakan Küçük\textsuperscript{c}

\textsuperscript{a}School of Mathematics and Statistics, Shandong University of Technology, Zibo 255049, China
\textsuperscript{b}Department of Mathematical Sciences, TsingHua University, Beijing 100084, China
\textsuperscript{c}Department of Mathematics, Nevşehir Hacı Bektaş Veli University, Turkey

Abstract

The anti-adjacency matrix of a graph is constructed from the distance matrix of a graph by keeping each row and each column only the largest distances. This matrix can be interpreted as the opposite of the adjacency matrix, which is instead constructed from the distance matrix of a graph by keeping in each row and each column only the distances equal to 1. The (anti-)adjacency eigenvalues of a graph are those of its (anti-)adjacency matrix. Employing a novel technique introduced by Haemers [Spectral characterization of mixed extensions of small graphs, Discrete Math. 342 (2019) 2760–2764], we characterize all connected graphs with exactly one positive anti-adjacency eigenvalue, which is an analog of Smith’s classical result that a connected graph with exactly one positive adjacency eigenvalue iff it is a complete multipartite graph. On this basis, we identify the connected graphs with all but at most two anti-adjacency eigenvalues equal to $-2$ and 0. Moreover, for the anti-adjacency matrix we determine the HL-index of graphs with exactly one positive anti-adjacency eigenvalue, where the HL-index measures how large in absolute value may be the median eigenvalues of a graph. We finally propose some problems for further study.

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1 Introduction

To study the graphs determined by the spectrum of adjacency matrices, Haemers \cite{7} introduced a useful operation on a graph named as mixed extension. Consider a graph $G$ with vertex set \{1, \ldots, n\}. Let $V_1, \ldots, V_n$ be mutually disjoint nonempty finite sets. We define a graph $H$ with vertex set the union of $V_1, \ldots, V_n$ as follows. For each $i$, the vertices of $V_i$ are either all mutually adjacent ($V_i$ is a clique), or all mutually nonadjacent ($V_i$ is a coclique). When $i \neq j$, a vertex of $V_i$ is adjacent to a vertex of $V_j$ if and only if $i$ and $j$ are adjacent in $G$. We call $H$ a mixed extension of $G$. We represent a mixed extension by an $n$-tuple $(t_1, \ldots, t_n)$ of nonzero integers, where $t_i > 0$ indicates that $V_i$ is a clique of order $t_i$, and $t_i < 0$ means that $V_i$ is a coclique of order $-t_i$. Haemers’s definition is more convenient and powerful, which is motivated by a concrete question for which the pineapple graphs are determined by the adjacency spectra \cite{21}. We refer to \cite{7, 8} for basic results on mixed extensions and to \cite{1} for graph spectra.

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\textsuperscript{1}Corresponding author.

Email addresses: jfwang@sdut.edu.cn (J.F. Wang), xyleiyuki@aliyun.com (X. Lei), lumei@tsinghua.edu.cn (M. Lu), srgnrzs@gmail.com (S. Sorgun), hakankucuk1979@gmail.com (H. Küçük).
Along with other techniques, Haemers [7] determined all graphs with at most three eigenvalues unequal to 0 and –1, consisting of all mixed extensions of graphs on at most three vertices together with some particular mixed extensions of the paths $P_4$ and $P_5$. Subsequently, Haemers et al. [8] investigated the mixed extension of $P_3$ on being determined by the adjacency spectrum and presented several cospectral families. Comparatively, Cioabă et al. [2] provided another method for constructing graphs with all but two eigenvalues equal to ±1. Moreover, Cioabă et al. [8] identified the graphs with all but two eigenvalues equal to –2 or 0. For the distance matrices of graphs, an approach has been successful for the graphs with exactly two distance eigenvalues different from –1 and –2 [10] or –1 and –3 [11].

In this paper, one will see that the mixed extension of a graph has new applications to the so-called anti-adjacency matrix of graphs. We only consider finite, simple and connected graphs. Let $G = (V(G), E(G))$ be a graph with order $|V(G)| = n$. The distance $d_G(v, w)$ between two vertices $v$ and $w$ is the minimum length of the paths joining them. The diameter of $G$, denoted by $\dim(G)$, is the greatest distance between any two vertices in $G$. The eccentricity $\varepsilon_G(u)$ of the vertex $u \in V(G)$ is given by $\varepsilon_G(u) = \max\{d(u, v) \mid v \in V(G)\}$. Then the anti-adjacency matrix (or eccentricity matrix) $A(G) = (\varepsilon_{uv})$ of $G$ are defined as follows [23]:

$$
\varepsilon_{uv} = \begin{cases} 
    d_G(u, v) & \text{if } d_G(u, v) = \min\{\varepsilon_G(u), \varepsilon_G(v)\}, \\
    0 & \text{otherwise}.
\end{cases}
$$

(1)

By comparing the definitions, it turns out that $A(G)$ is equal to the $D_{\text{MAX}}$-matrix introduced by Randić in [17] as a tool for Chemical Graph Theory. Anyway, since the importance of vertex-eccentricity is not limited to applications to chemistry, the author asserted that such matrix might open new directions of exploration in other branches of graph theory as well.

The matrix $A(G)$ is constructed from the distance matrix by only keeping the largest distances for each row and each column, whereas the remaining entries become null. That is why $A(G)$ can be interpreted as the opposite of the adjacency matrix, which is instead constructed from the distance matrix by keeping only distances equal to 1 on each row and each column. From this point of view, $A(G)$ and $A(G)$ are extremal among all possible distance-like matrices. As a contrast with $A(G)$, the anti-adjacency matrix has some fantastic properties, one of which is that $A(G)$ of a connected graph is not necessarily irreducible. See the published papers [9] [12] [23] [25] [27] [28] and the arXiv preprints [13] [22] for more results about this newer matrix.

We next introduce some notations borrowed from spectral graph theory. The $A$-polynomial of $G$ is defined as $\phi(G, \lambda) = \det(\lambda I - A(G))$, where $I$ is the identity matrix. The roots of the $A$-polynomial are the $A$-eigenvalues and the $A$-spectrum, denoted also by $\text{Spec}_A(G)$, of $G$ is the multiset consisting of the $A$-eigenvalues. Since $A(G)$ is symmetric, the $A$-eigenvalues are real. Let $\xi_1 \geq \xi_2 \geq \ldots \geq \xi_n$ be the anti-adjacency eigenvalues of a graph with order $n$. If $\xi_1' > \xi_2' > \ldots > \xi_k'$ are all distinct $A$-eigenvalues, then the $A$-spectrum can be written as

$$
\text{Spec}_A(G) = \{\xi_1, \xi_2, \ldots, \xi_n\} = \left\{ \frac{\xi_1}{m_1}, \frac{\xi_2}{m_2}, \ldots, \frac{\xi_k}{m_k} \right\},
$$

where $m_i$ is the algebraic multiplicity of the eigenvalue $\xi_i' \ (1 \leq i \leq k)$.

For any graph matrix $M$, the $M$-cospectral graphs are non-isomorphic graphs with the same $M$-spectrum. We say that $G$ is determined by the $M$-spectrum if no $M$-cospectral graphs of $G$ exist. Usually, $M$ is the adjacency, or the Laplacian, or the anti-adjacency matrices and so on.

The most important reason why the authors [26] tended to build a spectral theory based on the anti-adjacency matrix is that they tried to detect the proportion of cospectral graphs relating to two famous conjectures: One is that almost all graphs are adjacency cospectral
posed by Schwenk \textsuperscript{[15]}; the other is that almost all graphs are determined by the adjacency (or Laplacian) spectrum formally proposed by Haemers \textsuperscript{[6]}. In their paper, the authors \textsuperscript{[20]} showed that, when \( n \to \infty \), the fractions of non-isomorphic cospectral graphs with respect to the adjacency and the anti-adjacency matrix behave like those only concerning the self-centered graphs with diameter two. Moreover, they also obtained that the connected graphs have exactly two distinct \( A \)-eigenvalues iff they are \( r \)-antipodal graphs, which could be used to construct much more \( A \)-cospectral graphs.

Recall, a classical result, due to Smith \textsuperscript{[4, Theorem 6.7]}, is that a connected graph has exactly one positive adjacency eigenvalue if and only if \( G \) is a complete multipartite graph \( K_{n_1,n_2,\ldots,n_t} \), which is just the mixed extension of complete graph \( K_t \) of type \((-n_1,-n_2,\ldots,-n_t)\). Contrastively, we will determine the graphs with exactly one positive anti-adjacency eigenvalue, which is the mixed extension of star \( K_{1,k+1} \) in Theorem \textsuperscript{1.1}. Based on this result, we classify the graphs with all but two anti-adjacency eigenvalues equal to \(-2\) and 0 in Theorem \textsuperscript{1.2}. Relatively, Cioab˘a et.al \textsuperscript{[3]} determined all connected graphs for which adjacency matrices have at most two eigenvalues not equal to \(-2\) and 0, which are different from the graphs in the above theorem. In their classification, there are thirteen families of such graphs. Additionally, for the adjacency matrix, the multiplicity of eigenvalue 0 is well-known as the \textit{nullity} of a graph that has been studied widely; while it was a hot topic to determined the graphs with the smallest eigenvalue at least \(-2\), which has been summarized in \textsuperscript{[5]}. For the anti-adjacency matrix, the graphs with the smallest \( A \)-eigenvalue at least \(-2\) was characterized in \textsuperscript{[23]}.

Fowler and Pisanski \textsuperscript{[16,17]} introduced the notion of the HL-index of a graph w.r.t. the adjacency matrix. It is related to the HOMO-LUMO separation studied in theoretical chemistry. Similarly, the HL-\textit{index} \( R_A(G) \) w.r.t. anti-adjacency matrix of a (molecular) graph \( G \) of order \( n \) is defined as

\[ R_A(G) = \max\{|\xi_H|,|\xi_L|\}, \]

where \( H = \lfloor \frac{n+1}{2} \rfloor \), \( L = \lceil \frac{n+1}{2} \rceil \). See \textsuperscript{[14,15,16, eg.]} for more details about the HL-index w.r.t. adjacency matrices of graphs. Actually, for the anti-adjacency matrix, by cumbersome calculations we can completely determine the HL-index of graphs with exactly one positive anti-adjacency eigenvalue.

In order to state the following main results in this paper, we describe the mixed extensions of a star. Let \( K_{1,k+1} \) be a star with the vertex \( v_0 \) of degree \( k+1 \) and the other vertices \( v_1, v_2, \ldots, v_{k+1} \). We represent by \( S(t_0,t_1,\ldots,t_{k}) \) the mixed extension of the star \( K_{1,k+1} \) of the type \( (t_0,t_1,\ldots,t_{k}) \). If \( t_1 \geq t_2 \geq \cdots \geq t_q \geq 2 > t_{q+1} = \cdots = t_k = 1 \), then \( S(t_0,t_1,\ldots,t_{k}) \cong S(t_0,-p,t_1,\ldots,t_q) \), where \( 0 \leq p,q \leq k \) \((p = k-q)\) and \( t_j \geq 2 \) \((1 \leq j \leq q)\). It is worth noting that each \( t_i \geq 2 \) \((i = 1,2,\ldots,k)\) if \( p = 0 \).

\textbf{Theorem 1.1.} A connected graph \( G \) has exactly one positive \( A \)-eigenvalue if and only if \( G \) is the mixed extension of star \( S_{1,q+1} \) of type \( (t_0,-p,t_1,\ldots,t_q) \) with \( p,q \geq 0 \) and \( t_j \geq 2 \) \((1 \leq j \leq q)\), where

\begin{itemize}
  \item[(i)] \( t_0 = 1, \ p + q \geq 1 \);
  \item[(ii)] \( t_0 = 2, \ p,q \geq 0 \);
  \item[(iii)] \( t_0 = 3, \ 0 \leq q \leq 4-p \) \((0 \leq p \leq 4)\);
  \item[(iv)] \( t_0 = 4, \ 0 \leq q \leq 3-p \) \((0 \leq p \leq 3)\);
  \item[(v)] \( t_0 \geq 5, \ 0 \leq q \leq 2-p \) \((0 \leq p \leq 2)\).
\end{itemize}
Theorem 1.2. Let $G$ be a connected graph. Then

(i) No graph has exactly one $A$-eigenvalue different from $0$ and $-2$.

(ii) The graph with all but two $A$-eigenvalues equal to $-2$ and $0$ if and only if $G$ is the mixed extension of star $S_{1,1}$ of type $(-t_0, -t_1)$, where $t_0, t_1 \geq 1$.

Write the set $\{t_1, t_2, \cdots, t_q\}$ as the multiset $\{k_1 \cdot t_1, \cdots, k_h \cdot t_h\}$, where $k_i$ is the number of $t_i's$ $(1 \leq i \leq h)$. Clearly, $S(t_0, -p, t_1, \cdots, t_q) \cong S(t_0, -p, k_1 \cdot t_1, \cdots, k_h \cdot t_h)$ and $\sum_{i=1}^{h} k_i = q$.

Theorem 1.3. Let $G = S(t_0, -p, k_1 \cdot t_1, \cdots, k_h \cdot t_h)$ be the mixed extension of star $K_{1,q+1}$ defined in Theorem 1.2. For $p + q \leq 1$, then $R_A(G) = 1$. For $p + q \geq 2$,

(i) if $p + q \leq \left\lceil \frac{n-2t_0}{2} \right\rceil$, then $R_A(G) = 0$.

(ii) if $p + q = \left\lceil \frac{n-2t_0+2}{2} \right\rceil$, for $t_0 = 1, q = 0$ or $t_0 = 3, p + q = 4$ or $t_0 = 4, p + q = 3$, $R_A(G) = 0$; for the other cases in conditions (i)-(v) of Theorem 1.2, $R_A(G) \in (0,1)$.

(iii) if $\left\lceil \frac{n-2t_0+4}{2} \right\rceil \leq p + q \leq \left\lceil \frac{n}{2} \right\rceil$, then $R_A(G) = 1$.

(iv) if $p + q \geq \left\lceil \frac{n+2}{2} \right\rceil$ and $q \leq \left\lceil \frac{n-2}{2} \right\rceil$, then $R_A(G) = 2$.

(v) if $p + q \geq \left\lceil \frac{n+2}{2} \right\rceil$ and

(a) for $q = \left\lceil \frac{n}{2} \right\rceil$, then $R_A(G) \in (-2, -2t_h)$;

(b) for $\left\lceil \frac{n+2}{2} \right\rceil \leq q \leq \left\lceil \frac{n+2k_h-2}{2} \right\rceil$, then $R_A(G) = -2t_h$;

(c) for $q = \left\lceil \frac{n + \sum_{a=0}^{h-1} 2k_{h-a}}{2} \right\rceil$, then $R_A(G) \in (-2t_{h-i}, -2t_{h-i-1})$ $(0 \leq i \leq h-1)$;

(d) for $\left\lceil \frac{n + \sum_{a=0}^{i} 2k_{h-a}+2}{2} \right\rceil \leq q \leq \left\lceil \frac{n + \sum_{a=0}^{i+1} 2k_{h-a}-2}{2} \right\rceil$, then $R_A(G) = -2t_{h-i-1}$ $(0 \leq i \leq h-2)$.

Here is the remainder of the paper. In Section 2 we mainly give the proof of Theorem 1.1 which is decomposed into a series of lemmas. Especially, we determine the spectral distribution in the graphs with exactly one positive $A$-eigenvalue. In Sections 3 and 4 we respectively provide the proofs for Theorems 1.2 and 1.3 based on the results in previous section. In Section 5 we give some remarks and put forward several problems for further study.

2 Graphs with exactly one positive $A$-eigenvalue

Throughout the paper, let $\mathcal{G}$ be the set of graphs with exactly one positive $A$-eigenvalue. For two graphs $G$ and $H$, let $G \cup H$ be their disjoint union, and $H \subseteq G$ (or $H \notin \mathcal{G}$) denote that $H$ is (or not) an induced subgraph of $G$. We denote by $G \vee H$ the join obtained from $G \cup H$ by joining each vertex of $G$ to each one of $H$.

Lemma 2.1 (Cauchy Interlace Theorem). Let $R$ be a real symmetric $n \times n$ matrix and let $S$ be a principal submatrix of $R$ with order $m \times m$. Then, for $i = 1, 2, \cdots, m$,

$$\lambda_{n-m+i}(R) \leq \lambda_i(S) \leq \lambda_i(R),$$

where $\lambda_1(R) \geq \lambda_2(R) \geq \cdots \geq \lambda_n(R)$ and $\lambda_1(S) \geq \lambda_2(S) \geq \cdots \geq \lambda_m(S)$ are respectively the eigenvalues of $R$ and $S$. 


Lemma 2.2. Let $G$ be a connected graph and $H \subseteq G$. For any vertices $u, v \in V(H)$, if $\varepsilon_H(u) = \varepsilon_G(u)$ and $d_H(u, v) = d_G(u, v)$, then $A(H)$ is a principal submatrix of $A(G)$.

Proof. For any two vertices $u, v \in V(H)$, we consider the $uv^{th}$ entry of $A(H)$ and $A(G)$, i.e., $\varepsilon_{uv}(H)$ and $\varepsilon_{uv}(G)$. If $\varepsilon_{uv}(G) \neq 0$, we get $\varepsilon_{uv}(G) = d_G(u, v)$ and then $d_H(u, v) = d_G(u, v) = \min\{\varepsilon_G(u), \varepsilon_G(v)\} = \min\{\varepsilon_H(u), \varepsilon_H(v)\}$. So $\varepsilon_{uv}(H) = d_H(u, v) = d_G(u, v) = \varepsilon_{uv}(G)$. If $\varepsilon_{uv}(G) = 0$, then $d_H(u, v) = d_G(u, v) < \min\{\varepsilon_G(u), \varepsilon_G(v)\} = \min\{\varepsilon_H(u), \varepsilon_H(v)\}$. So $\varepsilon_{uv}(H) = 0 = \varepsilon_{uv}(G)$. From the above discussion, $\varepsilon_{uv}(H) = \varepsilon_{uv}(G)$ and so $A(H)$ is a principal submatrix of $A(G)$. \qed

The following corollary obviously follows from Lemmas 2.1 and 2.2.

Corollary 2.3. Under the conditions in Lemma 2.2, for $i = 1, 2, \ldots, n'$,

$$\varepsilon_{n-n'+i}(G) \leq \varepsilon_i(H) \leq \varepsilon_i(G),$$

where $n' = |H|$ and $\varepsilon_i(G)$ $(i = 1, 2, \ldots, n)$ is the $A$-eigenvalue of $G$.

| Label | Graph | $\xi_2$ |
|-------|-------|---------|
| $F_1$ | $S(5, -3)$ | $4 - \sqrt{15}$ |
| $F_2$ | $S(5, -2, 2)$ | $0.138+$ |
| $F_3$ | $S(5, -1, 2, 2)$ | $0.152+$ |
| $F_4$ | $S(4, -4)$ | $\sqrt{12}(9 - \sqrt{73})$ |
| $F_5$ | $S(4, -3, 2)$ | $0.238+$ |
| $F_6$ | $S(4, -2, 2, 2)$ | $0.248+$ |
| $F_7$ | $S(4, -1, 2, 2, 2)$ | $0.259+$ |
| $F_8$ | $S(3, -5)$ | $5 - 2\sqrt{6}$ |
| $F_9$ | $S(3, -4, 2)$ | $0.103+$ |
| $F_{10}$ | $S(3, -3, 2, 2)$ | $0.105+$ |
| $F_{11}$ | $S(3, -2, 2, 2, 2)$ | $0.107+$ |
| $F_{12}$ | $S(3, -1, 2, 2, 2, 2)$ | $0.109+$ |

Table 1: The second largest $A$-eigenvalues of $F_1$–$F_{12}$.

The subsequent lemma follows from Corollary 2.3 and Table 1.

Lemma 2.4. Let $G = S(t_0, -p, t_1, \ldots, t_q)$ be a mixed extension with $p, q \geq 0$, $t_j \geq 2$ $(1 \leq j \leq q)$. If $G \in \mathcal{G}$, then the graphs $F_1$–$F_{12}$ in Table 1 are not the induced subgraphs of $G$.

As usual, let $C_n, P_n, K_n$ denote the cycle, path and complete graph of order $n$, respectively.

Lemma 2.5. For any $G \in \mathcal{G}$, $\text{diam}(G) \leq 2$.

Proof. Assume that $\text{diam}(G) \geq 3$. Let $P_{d+1} = v_0v_1 \ldots v_{d-1}v_d$ be a path with length $\text{diam}(G) = d$ of $G$. Then $\varepsilon_G(v_0) = \varepsilon_G(v_d) = d$ and $d-1 \leq \varepsilon_G(v_1), \varepsilon_G(v_{d-1}) \leq d$. Let us consider the following cases.

Case 1. $\varepsilon_G(v_1) = d$ and $\varepsilon_G(v_{d-1}) = d$, or $\varepsilon_G(v_1) \leq d$ and $\varepsilon_G(v_{d-1}) = d$. Without loss of generality, for some $u \in V(G)$ set $\varepsilon_G(v_1) = d_G(v_1, u) = d = \varepsilon_G(u)$. Then the principal submatrix of $A(G)$ indexed by $\{v_0, v_d, v_1, u\}$ is

$$W_1 = \begin{pmatrix} 0 & d & 0 & \varepsilon_{vu} \\ d & 0 & 0 & \varepsilon_{vu} \\ 0 & 0 & 0 & d \\ \varepsilon_{w_0} & \varepsilon_{w_d} & d & 0 \end{pmatrix}.$$
By $d_G(v_i, u) \leq d$ we have $\epsilon_{v_iu} \in \{0, d\}$ ($0 \leq i \leq d$). Thereby, the principal submatrix of $A(G)$ indexed by $\{v_0, v_d, v_1\}$ is one of the following matrices:

$$W_2 = \begin{pmatrix} 0 & d & 0 & 0 \\ d & 0 & 0 & 0 \\ 0 & 0 & 0 & d \\ 0 & 0 & d & 0 \end{pmatrix}, W_3 = \begin{pmatrix} 0 & d & 0 & 0 \\ d & 0 & 0 & d \\ 0 & 0 & 0 & d \\ 0 & d & 0 & 0 \end{pmatrix}, W_4 = \begin{pmatrix} 0 & d & 0 & d \\ d & 0 & 0 & 0 \\ 0 & 0 & 0 & d \\ d & 0 & 0 & 0 \end{pmatrix}, W_5 = \begin{pmatrix} 0 & d & 0 & d \\ d & 0 & 0 & d \\ 0 & 0 & 0 & d \\ d & d & d & 0 \end{pmatrix}.$$  

A direct calculation shows that the second largest eigenvalues of the first three matrices above are respectively $d > 0$, $\frac{1}{2} + \frac{\sqrt{5}}{2}d > 0$, $\frac{1}{2} + \frac{\sqrt{5}}{2}d > 0$, and that the characteristic polynomial of $W_5$ is

$$\phi_{W_5}(\lambda) = (\lambda + d)f(\lambda), \text{ where } f(\lambda) = \lambda^3 - d\lambda^2 - 3d^2\lambda + d^3.$$  

For $d \geq 3$ we get $f(-d^2) = d^3 + 3d^4 - d^5 - d^6 < 0$, $f(0) = d^3 > 0$, $f(d) = -2d^3 < 0$ and $f(d^2) = d^3 - 3d^4 - d^5 + d^6 > 0$. Hence, the second eigenvalue $\xi_2(W_5)$ of $W_5$ is greater than 0.

By Lemma 2.1 we get $\xi_2(G) \geq \min\{\xi_2(W_i) | i = 2, 3, 4, 5\} > 0$, a contradiction.

Case 2. $\varepsilon_G(v_1) = d - 1 = \varepsilon_G(v_{d-1})$. Then, the principal submatrix of $A(G)$ indexed by $\{v_0, v_d, v_1, v_{d-1}\}$ is

$$W_6 = \begin{pmatrix} 0 & d & 0 & d - 1 \\ d & 0 & d - 1 & 0 \\ 0 & d - 1 & 0 & 0 \\ d - 1 & 0 & 0 & 0 \end{pmatrix}$$

with the second largest eigenvalue $\xi_2(W_6) = \frac{1}{2}(d + \sqrt{4 - 8d + 5d^2}) > 0$, and so $\xi_2(G) \geq \xi_2(W_6) > 0$ by Lemma 2.1.

As proved above, $\text{diam}(G) \leq 2$ for any $G \in \mathcal{G}$.

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**Fig. 1:** Graphs in Lemma 2.6.

**Lemma 2.6.** No graph in $\mathcal{G}$ contains one in $\{P_4, C_4, P_3 \cup K_1\}$ as an induced subgraph.

**Proof.** By Lemma 2.5 it suffices to consider $\text{diam}(G) = 2$. Assume by the contradiction that $P_4 = v_1v_2v_3v_4 \subseteq G$. Due to $\varepsilon_G(v_i) \leq 2$ ($1 \leq i \leq 4$), $d_G(v_i, v_j) \leq 2$ for any $i, j \in \{1, 2, 3, 4\}$. Hence, we get $d_G(v_1, v_3) = 2, d_G(v_1, v_4) = 2, d_G(v_2, v_4) = 2$ and $\varepsilon_G(v_i) = 2$ ($i = 1, 2, 3, 4$). Thus, the principal submatrix of $A(G)$ indexed by these four vertices are

$$W_7 = \begin{pmatrix} 0 & 0 & 2 & 2 \\ 0 & 0 & 0 & 2 \\ 2 & 0 & 0 & 0 \\ 2 & 2 & 0 & 0 \end{pmatrix}$$

with the second largest eigenvalue $\xi_2(W_7) = \sqrt{5} - 1$. By Lemma 2.1 we get $\xi_2(G) \geq \xi_2(W_7) > 0$, a contradiction. Hence, $P_4 \not\subseteq G$. 

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6
Set $C_4 \subseteq G$. Clearly, the principal submatrix of $A(G)$ indexed by $V(C_4)$ is

$$W_8 = \begin{pmatrix}
0 & 0 & 0 & 2 \\
0 & 0 & 2 & 0 \\
0 & 2 & 0 & 0 \\
2 & 0 & 0 & 0
\end{pmatrix}$$

whose the second largest eigenvalue is $\xi_2(W_8) = 2$. Thus, $\xi_2(G) \geq 2 > 0$, a contradiction.

For $P_3 \cup K_1 \subseteq G$, the principal submatrix of $A(G)$ indexed by those vertices is

$$W_9 = \begin{pmatrix}
0 & 2 & 2 & 2 \\
2 & 0 & 0 & 2 \\
2 & 0 & 0 & 0 \\
2 & 2 & 0 & 0
\end{pmatrix}$$

with the second largest eigenvalue $\xi_2(W_9) \approx 0.6222$. So, $\xi_2(G) > 0$, a contradiction.

This completes the proof. \(\square\)

Note that the vertex set of $S(t_0, t_1, \ldots, t_k)$ is $V_0 \cup V_1 \cup \cdots \cup V_k$, where the corresponding set of $t_i$ is $V_i = \{v_{i1}, v_{i2}, \ldots, v_{it_i}\}$ $(0 \leq i \leq k)$. Let $G[v_1, \ldots, v_j]$ denote the subgraph of $G$ induced by $\{v_1, \ldots, v_j\}$.

**Lemma 2.7.** Let $G' = S(t_0, t_1, \ldots, t_k)$ with $k \geq 2$ and $t_1 \geq 1 (1 \leq i \leq k)$. If $G' \in \mathcal{G}$ and $G \in \mathcal{G}$ is the connected graph obtained from $G'$ by adding a new vertex $w$, then $w$ must be adjacent to all vertices of $V_0$.

**Proof.** For the mixed extension of star $S_{1,k}$, we get that any vertex in $V_0$ is adjacent to those ones in other $V_i$'s $(1 \leq i \leq k)$, and that the vertices in $V_i$ and the vertices in $V_j$ are mutually not adjacent $(1 \leq i \neq j \leq k)$.

Assume by way of contradiction that there exists some vertex $v_{01} \in V_0$ is not adjacent to $w$. For $v_{i1} \in V_i$ and $v_{j1} \in V_j$ ($i \neq j$), by the above statement we get $v_{01}, v_{i1}$ and $v_{01}, v_{j1}$ are adjacent. Due to $P_1 \cup P_3 \not\subseteq G$ (see Lemma 2.3), $w$ is adjacent to at least one vertex of $v_{i1}$ and $v_{j1}$. Then $G'[v_{01}, v_{i1}, w, v_{j1}] \cong C_4$ if $w$ is adjacent to both $v_{i1}$ and $v_{j1}$, and otherwise $G'[v_{01}, v_{i1}, w, v_{j1}] \cong P_4$. This contradicts Lemma 2.6.

As shown above, $w$ must be adjacent to all vertices of $V_0$. \(\square\)

**Proposition 2.8.** Let $G \in \mathcal{G}$ with order $n$. Then $G$ is the mixed extension $S(t_0, t_1, \ldots, t_k)$, where $k \geq 1$ and $t_i \geq 1 (1 \leq i \leq k)$.

**Proof.** By Lemma 2.5 if diam$(G) = 1$ we get $G \cong K_n \cong S(t_0, n-t_0)$. We next set diam$(G) = 2$. If $G$ is a tree, by diam$(G) = 2$ we get $G \cong S_{1,n-1} \cong S(1,1,\ldots,1)$ $(n \geq 3)$.

We now consider $G$ containing at least one cycle. By $C_4, P_4 \not\subseteq G$ (Lemma 2.6), then $G$ only contains the triangle $C_3$. If $n = 3$, then $G \cong C_3 \cong S(1,2)$. For $n = 4$, clearly we get $G = S(1,1,2)$ or $S(2,1,1)$. When $n \geq 5$ we show the result by the induction. Assume that the theorem holds for the graphs with order $n-1$. As $G$ contains a cycle, there exists a vertex $w$ such that $G' = G - w$ is connected. If diam$(G') = 1$, then $G' \cong K_{n-1} \cong S(t_0, n-1 - t_0) \in \mathcal{G}$. If diam$(G') \geq 3$, then $P_4 \subseteq G' \subseteq G$ contradiction to Lemma 2.6. Hence, diam$(G') = 2$.

**Claim.** For $G \in \mathcal{G}$ and $w \in V(G)$, if $G' = G - w \subseteq G$ and diam$(G') = 2$, then $G' \in \mathcal{G}$. \(\square\)
Proof of the claim. From Lemma 2.3 and $G \in \mathcal{G}$, we get $\text{diam}(G) \leq 2$. Due to $\text{diam}(G') = 2$, $\text{diam}(G) = 2$. Otherwise, $\text{diam}(G) = 1$, and so $\text{diam}(G') = \text{diam}(G - w) = 1$, a contradiction. Therefore, for any two vertices $x, y \in V(G')$ we get $d_{G'}(x, y) = d_{G}(x, y)$.

For any $u \in V(G')$, we consider the values of $\varepsilon_{G'}(u)$ and $\varepsilon_{G}(u)$. If $\varepsilon_{G'}(u) = 1$, then we get $\varepsilon_{G}(u) = 1$; otherwise, by $\text{diam}(G) = 2$ we get $\varepsilon_{G}(u) = 2$, and hence $\varepsilon_{G'}(u) = 2$, a contradiction. If $\varepsilon_{G'}(u) = 2$, we have $\varepsilon_{G}(u) = 2$; or else, by $\text{diam}(G) = 2$ we have $\varepsilon_{G}(u) = 1$, and thus $\varepsilon_{G'}(u) = 1$, a contradiction again. Therefore, we obtain for any $u \in V(G')$ that $\varepsilon_{G'}(u) = \varepsilon_{G}(u)$.

From the above discussions, we know that $G$ and $G'$ satisfy the conditions of Corollary 2.3. Hence,

$$\xi_1(G) \geq \xi_1(G') \geq \xi_2(G) \geq \xi_2(G') \geq \cdots \geq \xi_{n-1}(G') \geq \xi_n(G)$$

which, along with $G \in \mathcal{G}$, leads to $G' \in \mathcal{G}$. □

By inductive hypothesis and $G' \in \mathcal{G}$, we can set $G' = S(t_0', t_1', \ldots, t_k')$, where $\sum_{i=0}^{k} t_i' = n - 1$, $V'_i = \{v_{i1'}, \ldots, v_{i\ell'}\}$, $k \geq 2$ and $t_i' \geq 1$ ($0 \leq i \leq k$). By Lemma 2.7, we get that $w$ is adjacent to all the vertices of $V'_0$.

If $w$ is not adjacent to any vertex of $V'_0 \cup \cdots \cup V'_k$, then $G \cong S(t_0', t_1', \ldots, t_k', 1)$. If $w$ is adjacent to a vertex (say, $v_{i\ell'}$) of one set in $\{V'_1, \ldots, V'_k\}$ (say, $V'_{i_0}$), then $w$ must be adjacent to all vertices of $V'_{i_0}$. Otherwise, there exits a vertex $v_{i\ell'} \in V'_{i_0}$ such that $w$ and $v_{i\ell'}$ are not adjacent which implies $G[w, v_{i1'}, v_{i\ell'}, v_{j1'}] \cong P_3 \cup K_1 \subseteq G$, contradiction to Lemma 2.6. Consequently, $G \cong S(t_0', t_1', \ldots, t_i'+1, \ldots, t_k')$. If $w$ is adjacent to the vertices of at least two sets in $\{V'_1, \ldots, V'_k\}$ (say, $V'_i$ and $V'_j$ ($0 \leq i \neq j \leq k$)), for $v_{i\ell'} \in V'_i$ and $v_{j1'} \in V'_j$ we conclude that $w$ must be adjacent to all vertices of $V'_i \cup \cdots \cup V'_k$. Otherwise, there is a vertex $v \in V'_i \cup \cdots \cup V'_k$ satisfying that $v$ and $w$ is not adjacent. In this case, $G[w, v, v_{i\ell'}, v_{j1'}] \cong P_4$ if $v \in V'_i \cup V'_j$, or $G[w, v, v_{i\ell'}, v_{j1'}] \cong P_3 \cup K_1$ if $v \notin V'_i \cup V'_j$, a contradiction. Therefore, $w$ is adjacent to all the vertices of $V'_0 \cup \cdots \cup V'_k$, and so $G \cong S(t_0'+1, t_1', \ldots, t_k')$.

This finishes the proof. □

**Proposition 2.9.** Let $G = S(t_0, -p, t_1, \ldots, t_q)$ be a mixed extension with $p, q \geq 0$ and $t_j \geq 2$ ($1 \leq j \leq q$). If $G \in \mathcal{G}$, then

(i) $t_0 = 1$, $p + q \geq 1$;

(ii) $t_0 = 2$, $p, q \geq 0$;

(iii) $t_0 = 3$, $0 \leq q \leq 4 - p$ ($0 \leq p \leq 4$);

(iv) $t_0 = 4$, $0 \leq q \leq 3 - p$ ($0 \leq p \leq 3$);

(v) $t_0 \geq 5$, $0 \leq q \leq 2 - p$ ($0 \leq p \leq 2$).

**Proof.** Let $t_0 \geq 5$. If $p \geq 3$, then $F_1 \subseteq G$ contradiction to Lemma 2.4. Hence, $p \leq 2$. If $p = 2$, then $q = 0$ by $F_2 \notin G$ (see Lemma 2.4). If $p = 0, 1$, then $q \leq 2 - p$ by $F_3 \notin G$. Set $t_0 = 4$. Since $F_4 \notin G$, then $p \leq 3$. Due to $F_5, F_6, F_7 \notin G$, we get $q \leq 3 - p$. Let $t_0 = 3$. By $F_8 \notin G$ we obtain $p \leq 4$. In view of $F_i \notin G$ ($i = 9, 10, 11, 12$), we have $q \leq 4 - p$ ($p \leq 3$). Since the order of $G$ is at least 2, we get $p, q \geq 0$ if $t_0 = 2$ and $p + q \geq 1$ if $t_0 = 1$. □

So far, we have shown the sufficiency of Theorem 1.1. We next show it is necessary. Write $\{t_1, t_2, \ldots, t_q\}$ as the multiset $\{k_1 \cdot t_1, \ldots, k_h \cdot t_h\}$, where $k_i$ is the number of $t_i$ ($1 \leq i \leq h$). Clearly, $S(t_0, -p, t_1, \ldots, t_q) = S(t_0, -p, k_1 \cdot t_1, \ldots, k_h \cdot t_h)$ and $\sum_{i=1}^{h} k_i = q$. 

8
Proposition 2.10. Let \( G = S(t_0, -p, k_1 \cdot t_1, \cdots, k_h \cdot t_h) \) be a mixed extension with \( p, q \geq 0 \) and \( t_j \geq 2 \) \((1 \leq j \leq h)\). Under the conditions (i) – (v) in Proposition 2.9, \( G \) has exactly one positive eigenvalue. Furthermore,

(i) \( p + q \leq 1 \). For \( t_0 \geq 1 \), then \( G \cong K_n \) and

\[
\text{Spec}_A(G) = \left\{ \frac{n-1}{1} \right\}
\]

(ii) \( p + q \geq 2 \) and \( p \geq 1 \). If \( t_0 = 1, q = 0 \) or \( t_0 = 3, q = 4 - p \) or \( t_0 = 4, q = 3 - p \), we get \( \text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \right\} \)

Thus, for the other cases in conditions (i) – (v) of Proposition 2.9,

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \right\}
\]

where \( \xi_1 \in (-2t_h, -2), \xi_{5+2i} \in (-2t_{h-i}, -2t_{h-i+1}) \) \((1 \leq i \leq h - 1)\).

Otherwise, for the other cases in conditions (i) – (v) of Proposition 2.9,

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \right\}
\]

where \( \xi_0 \in (-2t_h, -2), \xi_{6+2i} \in (-2t_{h-i}, -2t_{h-i+1}) \) \((1 \leq i \leq h - 1)\).

(iii) \( p + q \geq 2 \) and \( p = 0 \). If \( t_0 = 3, q = 4 \) or \( t_0 = 4, q = 3 \), then

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \right\}
\]

where \( \xi_3 + 2t_i \in (-2t_{h-i}, -2t_{h-i+1}) \) \((1 \leq i \leq h - 1)\).

Otherwise, for the other cases in conditions (i) – (v) of Proposition 2.9,

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \right\}
\]

where \( \xi_4 + 2t_i \in (-2t_{h-i}, -2t_{h-i+1}) \) and \( 1 \leq i \leq h - 1 \).

Proof. (i) If \( p + q \leq 1 \), then \( G = K_n \) is the mixed extension \( S(t_0, n - t_0) \) with

\[
\text{Spec}_A(G) = \left\{ \frac{n-1}{1} \right\}
\]

(ii) Let \( p + q \geq 2 \) and \( p \geq 1 \). Labelling the vertices of \( G \) properly, we get

\[
\mathcal{A}(G) = \begin{pmatrix}
J - I & J & J & J & \cdots & J \\
J & 2(J - I) & 2J & 2J & \cdots & 2J \\
J & 2J & 0 & 2J & \cdots & 2J \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\
J & 2J & 2J & 2J & \cdots & 0
\end{pmatrix},
\]

with the \( \mathcal{A} \)-polynomial

\[
\phi(G, \lambda) = \lambda^{n-t_0-p-q}(\lambda + 1)^{t_0-1}(\lambda + 2)^{p-1}g_{t_0, -p, \ldots, t_q}(\lambda),
\]

where

\[
g_{t_0, -p, \ldots, t_q}(\lambda) = \prod_{i=1}^{h}(\lambda + 2t_i)^{k_i-1}h(\lambda)
\]
and

\[ h(\lambda) = (\lambda^2 - 2p\lambda - t_0\lambda + 3\lambda + t_0p - 2t_0 - 2p + 2) \prod_{i=1}^{h}(\lambda + 2t_i) - (\lambda + 2)(2\lambda - t_0 + 2) \sum_{j=1}^{h} (k_j t_j \prod_{i=1}^{h}(\lambda + 2t_i)). \]

Obviously, the polynomial \( h \) has \( q + 2 \) real roots denoted by \( \lambda_1 \geq \cdots \geq \lambda_{q+2} \). When \( k_i \geq 2 \), \( -2t_i \) is a root of \( h \) with multiplicity \( k_i - 1 \) \((1 \leq i \leq h)\). Thus, the number of these roots is \( q - h \), and hence the remaining \( h + 2 \) roots of \( h \) are the roots of \( h(\lambda) \). For \( 2 \leq i \leq h \), we have

\[
h(-2t_{i-1})h(-2t_i) = k_{i-1}t_{i-1}k_i t_i (2t_{i-1} - 2)(2t_i - 2)(4t_{i-1} + t_0 - 2)(4t_i + t_0 - 2)
\]

\[
\times [\prod_{j=1}^{i-2}(2t_j - 2t_{i-1})(2t_j - 2t_i)](t_i - t_{i-1})(t_i - t_{i-1} - t_i)
\]

\[
\times [\prod_{j=i+1}^{h}(2t_j - 2t_{i-1})(2t_j - 2t_i)].
\]

Since \( k_{i-1}t_{i-1}k_i t_i (2t_{i-1} - 2)(2t_i - 2)(4t_{i-1} + t_0 - 2)(4t_i + t_0 - 2) > 0 \), \( \prod_{j=1}^{i-2}(2t_j - 2t_{i-1})(2t_j - 2t_i) > 0 \),

\((t_i - t_{i-1})(t_i - t_{i-1} - t_i) < 0\) and \( \prod_{j=i+1}^{h}(2t_j - 2t_{i-1})(2t_j - 2t_i) > 0 \), then \( h(-2t_{i-1})h(-2t_i) < 0 \). Therefore, there is a root of \( h(\lambda) \) that is in \((-2t_{i-1}, -2t_i)\) \((2 \leq i \leq h)\). At present, we have got \( q - 1 \) roots of \( h \). For \( G \in \mathcal{G} \) we get \( \lambda_1 > 0 \), and so we need find the other two roots of \( h(\lambda) \).

Since \( p \geq 1 \), then \( h(-2t_h) = -k_h t_h (2t_h + 2)(t_0 + 4t_h - 2) \prod_{i=1}^{h-1}(-2t_h + 2t_i) < 0 \), \( h(-2) = p(t_0 + 2) \prod_{i=1}^{h}(2t_i - 2) > 0 \). Hence, \( \lambda_3 \in (-2t_h, -2) \). A direct calculation shows that \( h(-1) = t_0(p - 1) \prod_{i=1}^{h}(2t_i - 1) + t_0 \sum_{j=1}^{h} (k_j t_j \prod_{i=1}^{h}(2t_i - 1)) \) and \( h(-1) > 0 \) for \( p + q \geq 2 \). As well,

\[
h(0) = (t_0p - 2t_0 - 2p + 2) \prod_{i=1}^{h} 2t_i - 2(-t_0 + 2) \sum_{j=1}^{h} (k_j t_j \prod_{i=1}^{h}(2t_i - 1)) = 2^h(qt_0 + pt_0 - 2t_0 - 2q - 2p + 2) \prod_{i=1}^{h} t_i.
\]

We consider the conditions (i)–(v) in Proposition 2.9 If \( t_0 = 1 \), then \( q \geq 0 \). When \( q = 0 \), \( h(0) = 2^h(-q) \prod_{i=1}^{h} t_i = 0 \). Otherwise, \( h(0) < 0 \). If \( t_0 = 2 \), \( q \geq 0 \) and so \( h(0) = 2^h(-2) \prod_{i=1}^{h} t_i < 0 \).

If \( t_0 = 3 \), then \( 0 \leq q \leq 4 - p \). \( h(0) = 2^h(p + q - 4) \prod_{i=1}^{h} t_i < 0 \) for \( q < 4 - p \) and \( h(0) = 0 \) for \( q = 4 - p \). If \( t_0 = 4 \), we get \( 0 \leq q \leq 3 - p \). For \( q < 3 - p \), \( h(0) = 2^h(2p + 2q - 6) \prod_{i=1}^{h} t_i < 0 \). Or else, \( h(0) = 0 \). If \( t_0 \geq 5 \), \( 0 \leq q \leq 2 - p \) and hence \( h(0) = 2^h(3p + 3q - 8) \prod_{i=1}^{h} t_i < 0 \).

Consequently, for the cases \( t_0 = 1, q = 0 \), or \( t_0 = 3, q = 4 - p \), or \( t_0 = 4, q = 3 - p \) we get \( \lambda_2 = 0 \), and

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \quad 0 \quad \frac{\xi_3}{1} \quad 0 \quad \frac{\xi_5}{1} \quad -1 \quad -2 \quad \xi_7 \quad \cdots \quad -2t_2 \quad \xi_{2h+3} \quad -2t_1 \quad \right\},
\]

where \( \xi_5 \in (-2t_h, -2) \) and \( \xi_{5+2i} \in (-2t_{h-i}, -2t_{h-i+1}) \) \((1 \leq i \leq h - 1)\). Otherwise, \( \lambda_2 \in (-1, 0) \) and thus

\[
\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1} \quad 0 \quad \frac{\xi_3}{1} \quad 0 \quad \frac{\xi_5}{1} \quad -1 \quad -2 \quad \xi_6 \quad \cdots \quad -2t_2 \quad \xi_{2h+4} \quad -2t_1 \quad \right\},
\]
where $\xi_6 \in (-2t_h, -2)$ and $\xi_{6+2i} \in (-2t_{h-i}, -2t_{h-i+1})$ ($1 \leq i \leq h - 1$).

(iii) Let $p + q \geq 2$ and $p = 0$, i.e., $q \geq 2$. Labeling the vertices of $G$ properly, we get

$$A(G) = \begin{pmatrix} J - I & J & J & \ldots & J \\ J & 0 & 2J & \ldots & 2J \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ J & 2J & 2J & \ldots & 0 \end{pmatrix},$$

with the $A$-polynomial

$$\phi(G, \lambda) = \lambda^{n-t_0-q}(\lambda + 1)^{t_0-1} \prod_{i=1}^{h}(\lambda + 2t_i)^{k_i-1}l(\lambda)$$

where

$$l(\lambda) = (\lambda - t_0 + 1) \prod_{i=1}^{h}(\lambda + 2t_i) - (2\lambda - t_0 + 2) \sum_{j=1}^{h}(k_j t_j \prod_{i=1}^{h}(\lambda + 2t_i)).$$

A straightforward calculation shows that

$$l(-1) = -t_0 \prod_{i=1}^{h}(2t_i - 1) + t_0 \sum_{j=1}^{h}(k_j t_j \prod_{i=1}^{h}(2t_i - 1))$$

$$= t_0 \sum_{j=1}^{h}(2t_i - 1) + (t_1 - t_2) \prod_{i=1}^{h}(2t_i - 1) + \sum_{j=1}^{h}(k_j t_j \prod_{i=1}^{h}(2t_i - 1)) + \prod_{i=1}^{h}(2t_i - 1)$$

$$> 0$$

and $l(0) = (-t_0 + 1) \prod_{i=1}^{h}2t_i - (t_0 + 2) \sum_{j=1}^{h}(2k_j t_j \prod_{i=1}^{h}t_i) = 2^{h-1}(2t_0 - 2 - 2q + 2) \prod_{i=1}^{h}t_i$.

Under the conditions (i)-(v) in Proposition 2.9, we consider the following cases. If $t_0 = 1$, then $q \geq 2$ and $l(0) = 2^{h-1}q \prod_{i=1}^{h}t_i < 0$. If $t_0 = 2$, $l(0) = 2^{h} \prod_{i=1}^{h}t_i < 0$. If $t_0 = 3$, we get $2 \leq q \leq 4$. For $2 < q < 4$, $l(0) = 2^{h-1}(q - 4) \prod_{i=1}^{h}t_i < 0$. Otherwise, $l(0) = 0$. If $t_0 = 4$, $2 \leq q \leq 3$. $l(0) = 2^{h-1}(2q - 6) \prod_{i=1}^{h}t_i < 0$ for $q < 3$ and $l(0) = 0$ for $q = 3$. If $t_0 \geq 5$, then $l(0) = -2^{h} \prod_{i=1}^{h}t_i < 0$.

Consequently, for $(t_0, q) = (3, 4)$ or $(t_0, q) = (4, 3)$ we have $\lambda_2 = 0$, and

$$\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1 - n-t_0 - q + 1} \begin{array}{cccccc} 0 & -1 & -2t_h & \xi_5 & \xi_7 & \cdots & \xi_2h + 1 \\ k_1 & k_2 - 1 & k_3 - 1 & 1 & \cdots & \xi_2h + 1 \\ & \vdots & \vdots & \vdots & \ddots & \vdots \\ & & & & & 1 & k_1 - 1 \end{array} \right\}$$

where $\xi_{3+2i} \in (-2t_{h-i}, -2t_{h-i+1})$ ($1 \leq i \leq h - 1$); Otherwise, $\lambda_2 \in (-1, 0)$ and

$$\text{Spec}_A(G) = \left\{ \frac{\xi_1}{1 - n-t_0 - q + 1} \begin{array}{cccccc} 0 & \xi_3 - 1 & -2t_h & \xi_6 & \xi_8 & \cdots & \xi_2h + 2 \\ k_1 & k_2 - 1 & k_3 - 1 & 1 & \cdots & \xi_2h + 2 \\ & \vdots & \vdots & \vdots & \ddots & \vdots \\ & & & & & 1 & k_1 - 1 \end{array} \right\}$$

with $\xi_{4+2i} \in (-2t_{h-i}, -2t_{h-i+1})$ ($1 \leq i \leq h - 1$).

Proof of Theorem 1.1 This theorem follows from Propositions 2.8, 2.9 and 2.10.
Remark 2.11. Recently, Sorgun and Küçük [27] independently studied the graphs with exactly one positive $A$-eigenvalue. In their paper, $S(4,-t_1,t_2,t_3,t_4)$ and $S(3,-t_1,t_2,t_3,t_4,t_5)$ ($t_i \geq 1$) are regarded as such graphs in [26, Theorem 2.11 (iv)]. However, in Table 1 we can see that $F_7 = S(4,-1,2,2,2)$ and $F_{12} = S(3,-1,2,2,2)$ have more than one positive $A$-eigenvalues. On the other side, the first author of this paper, Jianfeng Wang, has been discussing with Sezer Sorgun about this topic. Through communications, all the authors agreed to combine these two papers into the current version.

3 Graphs with all but at most two $A$-eigenvalues equal to $-2$ and 0

Let $K_{n_1,n_2,\ldots,n_l}$ be the complete multipartite graph with $n_1 \geq n_2 \geq \cdots \geq n_l$.

Lemma 3.1. [23] Let $G \cong K_{n_0} \vee K_{n_1,\ldots,n_l}$ with $n_0 \geq 1$, $n_r \geq 2$ and $l \geq 2$ ($1 \leq r \leq l$). Then

$$\phi(G,\lambda) = (\lambda + 1)^{n_0 - 1}(\lambda + 2)^{n_l - n_0 - l}[(\lambda - n_0 + 1) \prod_{r=1}^{l}(\lambda - 2n_r + 2) - n_0 \sum_{s=1}^{l} \prod_{r \neq s} n_r(\lambda - 2n_s + 2)].$$

Lemma 3.2. [23] Let $G$ be a graph with order $n$ and the least $A$-eigenvalue $\xi_n(G)$. Then $\xi_n(G) = -2$ if and only if

(i) $G \cong K_{n_1,n_2,\ldots,n_l}$, where $l \geq 2$ and $n_r \geq 2$ ($1 \leq r \leq l$);

(ii) $G \cong K_{n_0} \vee K_{n_1,\ldots,n_l}$, where $n_r \geq 2$ ($1 \leq r \leq l$) and $2 \leq l \leq 4$ if $n_0 = 1, 2 \leq l \leq 3$ if $n_0 = 2$ or $l = 2$ if $n_0 \geq 3$.

Note that the connected graphs with order $n \geq 2$ have at least one positive $A$-eigenvalue. Let $\mathcal{S}$ denote the set of connected graphs with all but at most two $A$-eigenvalues equal to $-2$ and 0. For $G \in \mathcal{S}$, $G$ might have exactly two positive $A$-eigenvalues, or only one positive $A$-eigenvalue, or one positive and one negative $A$-eigenvalue different from $-2$ and 0. In the next lemma, we consider the first case.

Lemma 3.3. Let $G \in \mathcal{S}$ with order $n$. Then $G$ has two positive $A$-eigenvalues if and only if $G \cong K_{n_1,n_2}$ with $n_1,n_2 \geq 2$.

Proof. If $G \in \mathcal{S}$ has exactly two positive $A$-eigenvalue different from 0 and $-2$, then the least $A$-eigenvalue of $G$ is $-2$. By Lemma 3.2 we discuss the following two cases.

Case 1. $G \cong K_{n_1,n_2,\ldots,n_l}$, where $l \geq 2$ and $n_r \geq 2$ ($1 \leq r \leq l$). Since $\text{Spec}_A(K_{n_1,n_2,\ldots,n_l}) = \{2(n_1-1),2(n_2-1),\ldots,2(n_l-1),-2^{(n-l)}\}$, then $G$ has at least two positive $A$-eigenvalues. Thereby, $G \cong K_{n_1,n_2}$ with $n_1,n_2 \geq 2$.

Case 2. $G \cong K_{n_0} \vee K_{n_1,\ldots,n_l}$, where $n_0 \geq 1$, $l \geq 2$ and $n_1 \geq \cdots \geq n_l \geq 2$ ($1 \leq r \leq l$). By Lemma 3.1 we get

$$\phi(G,\lambda) = (\lambda + 1)^{n_0 - 1}(\lambda + 2)^{n_l - n_0 - l}f_{n_0,n_1,\ldots,n_l}(\lambda),$$

where $f_{n_0,n_1,\ldots,n_l}(\lambda) = (\lambda - n_0 + 1) \prod_{r=1}^{l}(\lambda - 2n_r + 2) - n_0 \sum_{s=1}^{l} \prod_{r \neq s} n_r(\lambda - 2n_s + 2)].$ If $n_0 \geq 3$, then $G$ has at least three $A$-eigenvalues (i.e., one positive $A$-eigenvalue and at least two $A$-eigenvalues $-1$) different from $-2$ and 0, a contradiction. Hence, $n_0 \leq 2$. Due to Lemma 3.2 we have $2 \leq l \leq 4$ and thus distinguish the following cases.
Subcase 2.1. \( l = 2 \). From Lemma 3.2(ii) it follows that \( n_0 \geq 1 \). By (6) we get
\[
f_{n_0,n_1,n_2}(\lambda) = (\lambda - n_0 + 1)(\lambda - 2n_1 + 2)(\lambda - 2n_2 + 2) - n_0n_1(\lambda - 2n_1 + 2) - n_0n_2(\lambda - 2n_1 + 2).
\]
By calculations we get 
\[
f_{n_0,n_1,n_2}(-2) = -4n_1n_2 < 0, 
\]
\[
f_{n_0,n_1,n_2}(-1) = (n_1 + n_2 - 1)n_0 > 0, 
\]
\[
f_{n_0,n_1,n_2}(2n_2 - 2) = 2n_0n_2(n_1 - n_2) \geq 0, 
\]
\[
f_{n_0,n_1,n_2}(2n_1 - 2) = 2n_0n_2(n_2 - n_1) \leq 0 
\]
and
\[
f_{n_0,n_1,n_2}(2(n_0 + n_1 + n_2) - 2) = 2n_0^2(4n_0 + 3n_2) + 2n_0[3n_0^2 + 2(n_0 - 1)n_0 + n_2(5n_0 - 2)] + 2n_1[4n_0^2 + n_0(5n_0 - 2) + 2n_2(5n_0 - 1)] > 0.
\]
Hence, \( G \) has more than two \( A \)-eigenvalues different from \(-2\) and \(0\) (i.e., \( \xi_1 \in [2n_1 - 2, 2(n_0 + n_1 + n_2) - 2], \xi_2 \in [2n_2 - 2, 2n_1 - 2], \xi_{n_0 + 2} \in (-2, -1) \)), a contradiction.

Subcase 2.2. \( l = 3 \). By Lemma 3.2(ii) we get \( n_0 = 1 \) or 2. If \( n_0 = 1 \), then \( G = K_1 \cup K_{n_1,n_2,n_3} \) and
\[
f_{1,n_1,n_2,n_3}(\lambda) = \lambda(\lambda - 2n_1 + 2)(\lambda - 2n_2 + 2)(\lambda - 2n_3 + 2) - n_0n_1(\lambda - 2n_1 + 2)(\lambda - 2n_2 + 2) - n_0n_2(\lambda - 2n_2 + 2)(\lambda - 2n_3 + 2) - n_0n_3(\lambda - 2n_3 + 2)(\lambda - 2n_3 + 2).
\]
We get 
\[
f_{1,n_1,n_2,n_3}(-2) = 4n_1n_2n_3 > 0, 
\]
\[
f_{1,n_1,n_2,n_3}(2n_3 - 2) = 4n_3(n_1 - n_3)(n_3 - n_2) \leq 0,
\]
\[
f_{1,n_1,n_2,n_3}(2n_1 - 2) = -4n_1(n_1 - n_2)(n_1 - n_3) \leq 0, 
\]
\[
f_{1,n_1,n_2,n_3}(2(n_1 + n_2 + n_3) - 2) = 4n_3(1 - 4n_2 + 4n_3) + n_3(2n_1 + 2n_2 + 2n_3 - 5) + (n_2 + n_3)(4n_3(1 - n_3)(n_3 - n_2) + 2n_1(n_1 + 2n_2 + 2n_3 - 5) + 2n_2(16n_3 - 11) + 2n_1(16n_3 - 5)) > 0.
\]
Therefore, \( G \) has more than two \( A \)-eigenvalues different from \(-2\) and \(0\) (i.e., \( \xi_1 \in [2n_1 - 2, 2(n_0 + n_1 + n_2) - 2], \xi_2 \in [2n_2 - 2, 2n_1 - 2], \xi_3 \in [2n_3 - 2, 2n_2 - 2], \xi_{n_0 + 3} \in (-2, -2) \)), a contradiction.

If \( n_0 = 2 \), then \( G = K_2 \cup K_{n_1,n_2,n_3} \). It is obvious that \( G \) and \( K_1 \cup K_{n_1,n_2,n_3} \) satisfy the conditions of Lemma 2.2. So, \( \mathcal{A}(K_1 \cup K_{n_1,n_2,n_3}) \) is the principle submatrix of \( \mathcal{A}(K_2 \cup K_{n_1,n_2,n_3}) \). From Corollary 2.3 by the above discussion we get \( \xi_1 \geq 2n_1 - 2, \xi_2 \geq 2n_2 - 2 \) and \( \xi_3 \geq 2n_3 - 2 \), a contradiction.

Subcase 2.3. \( l = 4 \). In view of Lemma 3.2(ii) we get \( n_0 = 1 \) and \( G = K_1 \cup K_{n_1,n_2,n_3,n_4} \). Clearly, the graphs \( G \) and \( K_1 \cup K_{n_1,n_2,n_3} \) satisfy the conditions of Lemma 2.2. Thus, \( \mathcal{A}(K_1 \cup K_{n_1,n_2,n_3}) \) is the principle submatrix of \( \mathcal{A}(K_1 \cup K_{n_1,n_2,n_3,n_4}) \). From Corollary 2.3 by Case 2.2 we obtain \( \xi_1 \geq 2n_1 - 2, \xi_2 \geq 2n_2 - 2 \) and \( \xi_3 \geq 2n_3 - 2 \), a contradiction.

As proved above, we get that \( G \cong K_{n_1,n_2} \) \((n_1,n_2 \geq 2)\) if \( G \in \mathcal{S} \) has two positive \( A \)-eigenvalues.

We next identify the graphs \( G \in \mathcal{S} \) which have only one positive \( A \)-eigenvalue, or one positive and one negative \( A \)-eigenvalue. At this moment, \( G \) has exactly one positive \( A \)-eigenvalue, and so \( G \in \mathcal{S} \) defined in Section 2.

Lemma 3.4. \( G \in \mathcal{S} \cap \mathcal{G} \) if and only if \( G \) is the star \( S_{1,p} = S(1, -p) \) with \( p \geq 1 \).

Proof. For \( G \in \mathcal{S} \), by Theorem 1.1 we get \( G \cong S(t_0, -p, t_1, \ldots, t_q) \) with those restricted conditions. Recall, \( t_1 \geq t_2 \geq \cdots \geq t_q \geq 2 \). If \( t_0 \geq 3 \), then by (14) we deduce that \( G \) has at least two \( A \)-eigenvalues \(-1\), a contradiction. Hence, \( t_0 \leq 2 \).

Case 1. \( t_0 = 1 \). By Theorem 1.1(i) we get \( p + q \geq 1 \) with \( p, q \geq 0 \).

Subcase 1.1. \( p = 0 \). Then \( q \geq 1 \), and thus \( G \cong S(1, t_1, t_2, \ldots, t_q) \) with \( t_j \geq 2 \) \((1 \leq j \leq q)\). If \( q = 1 \), then \( G \cong K_n \). \( G \in \mathcal{S} \) for \( n = 2 \) (i.e., \( K_2 = S(1, -1) \)), but \( G \not\in \mathcal{S} \) for others. If \( q \geq 2 \), set \( g_{t_0,-p,\ldots,t_q}(\lambda) \) be defined in (14).

If \( q = 2 \), then \( G \cong S(1,t_1,t_2) \). From Proposition 2.10(iii) it follows that \( G \) has three \( A \)-eigenvalues different from \(-2\) and \(0\) (i.e., \( \xi_1 > 0, \xi_{n-1} \in (-1, 0), \xi_n \in [-2t_1, -2t_2] \)), a contradiction.
If \( q = 3 \), then \( G \cong S(1, t_1, t_2, t_3) \). By Proposition \( 2.10 \) (iii) we get that \( G \) has four \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-2} \in (-1,0), \xi_{n-1} \in [-2t_2, -2t_3), \xi_n \in [-2t_1, -2t_2) \)), a contradiction.

If \( q \geq 4 \), then \( G \cong S(1, t_1, \cdots, t_q) \). Clearly, \( G \) and \( S(1, t_1, t_2, t_3) \) share the conditions of Lemma 2.2. So, \( \mathcal{A}(S(1, t_1, t_2, t_3)) \) is the principal submatrix of \( \mathcal{A}(S(1, t_1, \cdots, t_q)) \). By Corollary 2.3 and the above conclusion, we get \( \xi_1 > 0, \xi_{n-1} \leq -2t_3 \) and \( \xi_n \leq -2t_2 \), a contradiction.

Subcase 1.2. \( p = 1 \). Then \( q \geq 0 \). If \( q = 0 \), then \( G = S(1, -1) \in \mathcal{S} \cap \mathcal{G} \).

If \( q = 1 \), then \( G \cong S(1, -1, t_1) \) and \( G \) has three \( \mathcal{A} \)-different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-1} \in (-1,0), \xi_n \in (-2t_1, -2) \)) by Proposition 2.10 (ii), a contradiction.

If \( q = 2 \), then \( G \cong S(1, -1, t_1, t_2) \). From Proposition 2.10 (ii) it follows that \( G \) has four \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-2} \in (-1,0), \xi_{n-1} \in [-2t_2, -2), \xi_n \in [-2t_1, -2t_2) \)), a contradiction.

If \( q \geq 3 \), then \( G \cong S(1, -1, t_1, \cdots, t_q) \). Obviously, \( G \) and \( S(1, -1, t_1, t_2) \) possess the conditions of Lemma 2.2. Hence, \( \mathcal{A}(S(1, -1, t_1, t_2)) \) is the principal submatrix of \( \mathcal{A}(S(1, -1, t_1, \cdots, t_q)) \). By Corollary 2.1 and the above case, we get \( \xi_1 > 0, \xi_{n-1} < -2 \) and \( \xi_n \leq -2t_2 \), a contradiction.

Subcase 1.3. \( p \geq 2 \). Then \( q \geq 0 \). If \( q = 0 \), then \( G \cong S(1, -p) \) and

\[
\text{Spec}_\mathcal{A}(S(1, -p)) = \left\{ \sqrt{p^2 - p + 1 + p - 1, 0^{(n-t_0-p-q)}}, -\sqrt{p^2 - p + 1 + p - 1, -2(p-1)} \right\}.
\]

Thus, the star \( S(1, -p) \in \mathcal{S} \cap \mathcal{G} \).

If \( q = 1 \), then \( G \cong S(1, -p, t_1) \). By Proposition 2.10 we get \( G \) has three \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e. \( \xi_1 > 0, \xi_{n-p} \in (-1,0), \xi_n \in (-2t_1, -2) \)), a contradiction.

If \( q \geq 2 \), then \( G \cong S(1, -p, t_1, \cdots, t_q) \). Similarly, \( \mathcal{A}(S(1, -1, t_1, t_2)) \) is the principal submatrix of \( \mathcal{A}(S(1, -p, t_1, \cdots, t_q)) \). Analogously to the last case of Subcase 1.2 we get a conflict.

Case 2. \( t_0 = 2 \). By Theorem 1.1 we get \( p, q \geq 0 \).

Subcase 2.1. \( p = 0 \). Then \( q \geq 1 \) and \( G \cong S(2, t_1, t_2, \cdots, t_q) \). If \( q = 1 \), then \( G \cong K_n \notin \mathcal{S} \).

If \( q = 2 \), then \( G \cong S(2, t_1, t_2) \) and \( G \) has three \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-1} \in (-1,0), \xi_n \in [-2t_1, -2) \)) by Proposition 2.10 (iii), a contradiction.

If \( q \geq 3 \), then \( G \cong S(2, t_1, \cdots, t_q) \). Similarly, \( \mathcal{A}(S(1, t_1, t_2, t_3)) \) is the principal submatrix of \( \mathcal{A}(S(2, t_1, \cdots, t_q)) \). Analogously to Subcase 1.1 (when \( q = 3 \)) we get a contradiction.

Subcase 2.2. \( p = 1 \). So \( q \geq 0 \). If \( q = 0 \), then \( G \cong S(2, -1) \cong C_3 \notin \mathcal{S} \). If \( q = 1 \), then \( G \cong S(2, -1, t_1) \). By Proposition 2.10 (ii) we get that \( G \) has three \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-1} \in (-1,0), \xi_n \in (-2t_1, -2) \)), a contradiction.

If \( q \geq 2 \), then \( G \cong S(2, -1, t_1, \cdots, t_q) \). Similarly, \( \mathcal{A}(S(1, -1, t_1, t_2)) \) is the principal submatrix of \( \mathcal{A}(S(2, -1, t_1, \cdots, t_q)) \). Analogously to Subcase 1.2 (when \( q = 2 \)) we get \( G \notin \mathcal{S} \).

Subcase 2.3. \( p \geq 2 \). If \( q = 0 \), then \( G \cong S(2, -p) \) and we can get \( \mathcal{A} \)-eigenvalues of \( G \) from Proposition 2.10 (ii). Then \( G \) has three \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-p-1} \in (-1,0), \xi_{n-p} = -1 \)), a contradiction.

If \( q = 1 \), then \( G \cong S(2, -p, t_1) \). Hence, \( G \) has three \( \mathcal{A} \)-eigenvalues different from \(-2\) and 0 (i.e., \( \xi_1 > 0, \xi_{n-p-1} \in (-1,0), \xi_n \in (-2t_1, -2) \)) by Proposition 2.10 (ii), a contradiction.

If \( q \geq 2 \), then \( G \cong S(2, -p, t_1, \cdots, t_q) \). Similarly, \( \mathcal{A}(S(1, -1, t_1, t_2)) \) is the principal submatrix of \( \mathcal{A}(S(2, -p, t_1, \cdots, t_q)) \). In a similar way, \( G \notin \mathcal{S} \).

As discussed above, \( G \in \mathcal{S} \cap \mathcal{G} \) if and only if \( G \cong S(1, -p) \) with \( p \geq 2 \).

The following corollary follows from the proof of Lemma 3.4.
Corollary 3.5. No graph in $\mathcal{S}$ has only one positive $A$-eigenvalue different from $-2$ and $0$.

Clearly, the star $S_{1,p} = S(1,-p)$ is a special kind of complete bipartite graphs $K_{n_1,n_2} \cong S(-n_1,-n_2)$.

Proof of Theorem 1.2. This theorem follows from Lemma 3.3 and Corollary 3.4.

4 Hl-index of graphs with exactly one $A$-eigenvalue

In this section, we give a proof for Theorem 1.3.

Proof of Theorem 1.3. Clearly, the graph $G$ satisfies the conditions (i)-(v) in Proposition 2.9. Therefore, $\xi_{\lceil n+1 \rceil} \leq |\xi_{\lceil n+1 \rceil}| \leq 0$ and $R_A(G) = \max\{|\xi_{\lceil n+1 \rceil}|,|\xi_{\lceil n+1 \rceil}|-1\}$.

From Proposition 2.10(i), for $p \neq q \leq 1$ we get $R_A(G) = 1$. For $p + q \geq 2$, by Proposition 2.10(ii) and (iii) we consider the following cases.

Case 1. $n = t_0 + p + q$. Due to $n \geq 2$, then $\lceil \frac{n+1}{2} \rceil \geq 2 = 1 + (n - t_0 - p - q) + 1$, and thus $p + q \geq \lceil \frac{n-2t_0+2}{2} \rceil$. If $p + q = \lceil \frac{n-2t_0+2}{2} \rceil$, then $\lceil \frac{n+1}{2} \rceil = 1 + (n - t_0 - p - q) + 1$. For $t_0 = 1, q = 0$ or $t_0 = 3, q = 4 - p$ or $t_0 = 4, q = 3 - p$, $R_A(G) = |\xi_2| = 0$; otherwise, for the other cases in conditions (i)-(v) of Proposition 2.9 we get $R_A(G) = |\xi_2| \in (0,1)$.

If $\lceil \frac{n-2t_0+2}{2} \rceil \leq p + q \leq \lceil \frac{n}{2} \rceil$, then $t_0 \geq 2$ and $1 + (n - t_0 - p - q) + 1 + 1 \leq \lceil \frac{n+1}{2} \rceil \leq 1 + (n - t_0 - p - q) + 1 + (t_0 - 1)$. So, $R_A(G) = |\xi_3| = 1$ by Proposition 2.10(ii) and (iii).

If $p + q \geq \lceil \frac{n+1}{2} \rceil$, we get that $\lceil \frac{n+1}{2} \rceil \geq 1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + 1$.

Case 1.1. If $t_0 = 1, q = 0$. Then $p \geq 2$ and $q = 0 \leq \lceil \frac{n}{2} \rceil$. Hence, $1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + 1 \leq \lceil \frac{n+1}{2} \rceil \leq 1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + (p - 1)$ and $R_A(G) = |\xi_3| = 2$ by Proposition 2.10(ii). If $t_0 = 3, q = 4 - p$, then $p + q = 4 \geq \lceil \frac{n+2}{2} \rceil$ which leads to $n \leq 6 < t_0 + p + q = 7$, a contradiction. For $t_0 = 4, q = 3 - p$, then $p + q = 3 \geq \lceil \frac{n+2}{2} \rceil$ which results in $n \leq 4 < t_0 + p + q = 7$, a contradiction.

Case 1.2. For the other cases in conditions (i)-(v) of Proposition 2.9 if we assume $t_0 \geq 5$, then $p + q = 2 \geq \lceil \frac{n+2}{2} \rceil$ implying $n \leq 2 < t_0 + p + q$; if $t_0 = 4, p + q \geq 3 \geq \lceil \frac{n+2}{2} \rceil$ showing $n < 4 < t_0 + p + q$; if $t_0 = 3, p + q < 4 \geq \lceil \frac{n+2}{2} \rceil$ indicating $n < 6 < t_0 + p + q$. For any previous case, we always obtain a contradiction. Hence, $t_0 \leq 2$.

Case 1.2.1. $t_0 = 1, p \geq 2$. From Proposition 2.10(ii), we distinguish the following cases. If $q \leq \lceil \frac{n}{2} \rceil$, then $R_A(G) = |\xi_3| = 2$. If $q = \lceil \frac{n}{2} \rceil$, we get $\lceil \frac{n+1}{2} \rceil = 1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + (p - 1) + 1$, and hence $R_A(G) = |\xi_4| \in (2,2t_h)$. If $\lceil \frac{n+2}{2} \rceil \leq q \leq \lceil \frac{n+2k_h-a}{2} \rceil$, then $R_A(G) = |\xi_5|=2t_h$. If $q = \lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}}{2} \rceil$, then $1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + (p - 1) + 1 \leq \lceil \frac{n+1}{2} \rceil \leq 1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + (p - 1) + 1 + (k_h - 1)$, and therefore $R_A(G) = |\xi_{6+2i}| \in (2t_{h-i},2t_{h-i}-1) (0 \leq i \leq h - 1)$. If $\lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}+2}{2} \rceil \leq q \leq \lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}-2}{2} \rceil$, then $\lceil \frac{n+1}{2} \rceil = 1 + (n - t_0 - p - q) + 1 + (t_0 - 1) + (p - 1) + 1 + \sum_{a=0}^{i} (k_h-a-1) + i + 1$, and thus $R_A(G) = |\xi_{7+2i}| = 2t_{h-i-1} (0 \leq i \leq h - 2)$.

Case 1.2.2. $t_0 = 1, p = 1$. Then $q \geq \lceil \frac{n}{2} \rceil \geq 1$ and we discuss the following cases from Proposition 2.10(ii). If $q = \lceil \frac{n}{2} \rceil$, then $R_A(G) = |\xi_3| \in (2,2t_h)$. If $\lceil \frac{n+2}{2} \rceil \leq q \leq \lceil \frac{n+2k_h-2}{2} \rceil$, $R_A(G) = |\xi_4|=2t_h$. If $q = \lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}}{2} \rceil$, then $R_A(G) = |\xi_{5+2i}| \in (2t_{h-i},2t_{h-i}-1) (0 \leq i \leq h - 1)$. If $\lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}+2}{2} \rceil \leq q \leq \lceil \frac{n+\sum a=0^{n+1} 2k_{h-a}-2}{2} \rceil$, then $R_A(G) = |\xi_{6+2i}| = 2t_{h-i-1} (0 \leq i \leq h - 2)$. 

15
Case 1.2.3. \( t_0 = 1, p = 0 \). Then \( q \geq \left[ \frac{n+2}{2} \right] \geq 2 \). By Proposition 2.10(iii) we have the following cases. If \( \left[ \frac{n+2}{2} \right] \leq q \leq \left[ \frac{n+2k_h-2}{2} \right] \), then \( R_A(G) = |\xi_3| = 2t_h \). If \( q = \left[ \frac{n+1}{2} + \sum_{a=0}^{i} 2k_h-a \right] \), then \( R_A(G) = |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \). If \( \left[ \frac{n+2}{2} \right] \leq q \leq \left[ \frac{n+2k_h-2}{2} \right] \), then \( R_A(G) = |\xi_3| = 2t_h \). If \( q = \left[ \frac{n+1}{2} + \sum_{a=0}^{i} 2k_h-a \right] \), then \( R_A(G) = |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \).

Case 1.2.4. \( t_0 = 2, p \geq 2 \). Similarly to Case 1.2.1, we get the following cases. If \( q \leq \left[ \frac{n-2}{2} \right] \), then \( R_A(G) = |\xi_4| = 2 \). If \( q = \left[ \frac{n}{2} \right] \), then \( R_A(G) = |\xi_5| \in (2, 2t_h) \). If \( \left[ \frac{n+2}{2} \right] \leq q \leq \left[ \frac{n+2k_h-2}{2} \right] \), then \( R_A(G) = |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \). If \( n \leq t_0 + p + q \). If \( p + q \leq \left[ \frac{n-2t_0}{2} \right] \), we get \( |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \).

Case 2. \( n > t_0 + p + q \). If \( p + q \leq \left[ \frac{n-2t_0}{2} \right] \), we get \( |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \).

Case 1.2.5. \( t_0 = 2, p = 1 \). Then \( q \geq \left[ \frac{n+2}{2} \right] \). Similarly to Case 1.2.3, if \( \left[ \frac{n+2}{2} \right] \leq q \leq \left[ \frac{n+2k_h-2}{2} \right] \), then \( R_A(G) = |\xi_4| = 2t_h \). If \( q = \left[ \frac{n+1}{2} + \sum_{a=0}^{i} 2k_h-a \right] \), then \( R_A(G) = |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \).

Case 2. \( n > t_0 + p + q \). If \( p + q \leq \left[ \frac{n-2t_0}{2} \right] \), we get \( |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \). For the other cases in conditions (i)-(v) of Proposition 2.9 we get \( R_A(G) = |\xi_3| = 1 \). For the other cases, we consider the conditions (ii)-(v) of Proposition 2.10(iii) we have \( R_A(G) = |\xi_4| = 1 \). For the other cases in conditions (ii)-(v) of Proposition 2.9 we have \( R_A(G) = |\xi_3| = 1 \). For \( p + q \geq \left[ \frac{n+1}{2} \right] \), we get \( |\xi_{i+2k_h} - 2t_h - i - 1| (0 \leq i \leq h - 1) \). For the other cases in conditions (i)-(v) of Proposition 2.9 we get \( R_A(G) = |\xi_3| = 2 \). For the other cases, we consider the conditions (ii)-(v) of Proposition 2.10(ii) we have \( R_A(G) = |\xi_4| = 2 \).
As Haemers pointed out [8], the mixed extension of graphs is a special case of the so called generalized composition (see [10] for details). However, Haemers’s definition is more convenient and powerful. It is quite helpful for the classifications of graphs and further for identifying which graphs are determined by the spectra. On reflection, we propose the following problems, the first one of which is a natural step.

**Problem 1.** Which graphs with exactly one positive A-eigenvalue are determined by their A-spectra?

**Problem 2.** Determine the graphs with all but two A-eigenvalues equal to \(-2\) and \(-1\).

For the anti-adjacency matrix, we expect more general results about the HL-index \(R_A(G)\) of a graph \(G\).
Problem 3. *Investigate the HL-index w.r.t. the anti-adjacency matrices of graphs.*

Another interesting problem is the *nullity* $\eta_A(G)$ of a graph $G$, which is defined to be the multiplicity of zero as an eigenvalue of the adjacency matrix. Similarly, we consider the nullity $\eta_A(G)$ of the anti-adjacency matrix. The nullity of a graph is important in mathematics, since it is related to the singularity of (anti-)adjacency matrix. Note that the anti-adjacency matrices of graphs seem to be usually more sparse than adjacency matrices. Hence, the nullity of anti-adjacency matrix may be larger than that of adjacency matrix. For example, $\eta_A(P_{2k+1}) = 1$ and $\eta_A(P_{2k}) = 0$ for $k \geq 1$; while $\eta_A(P_{2k+1}) = 2k - 3$ and $\eta_A(P_{2k}) = 2k - 4$ for $k \geq 3$ (see [24, Lemma 2.1])

**Problem 4.** *For the anti-adjacency matrix, give lower and upper bounds of nullity involving graph parameters, and characterize the extreme graphs.*

On the other hand, it is well-know that the HL-index and the nullity of graphs are of great interest in chemistry. As a comparison in [23], it seems that the spectral radius of adjacency matrix of a graph is closely related to the chemical properties of octane isomers, while the spectral radius of anti-adjacency matrix of graphs may be more efficient for the benzenoid hydrocarbons. In the end, we pose the last one problem to finish this paper.

**Problem 5.** *With respect to the adjacency and anti-adjacency matrices of graphs, compare the HL-index and nullity of graphs and study their applications in the chemistry.*

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**References**

[1] A.E. Brouwer, W.H. Haemers, Spectra of Graphs, Springer, 2012.

[2] S.M. Cioabă, W.H. Haemers, J.R. Vermette, W. Wong, The graphs with all but two eigenvalues equal to ±1, J. Algebr. Comb. 41 (2015) 887–897.

[3] S.M. Cioabă, W.H. Haemers, J.R. Vermette, The graphs with all but two eigenvalues equal to −2 or 0, Des. Codes Cryptogr. 84 (2017) 153–163.

[4] D.M. Cvetković, M. Doob, H. Sachs, Spectra of Graphs Theory and Applications, Academic Press, New York, San Francisco, London, 1980.

[5] D.M. Cvetković, P. Rowlinson, S. Simić, Spectral Generalizations of Line Graphs: On Graphs with Least Eigenvalue −2. Cambridge University Press, Cambridge, 2004.

[6] W.H. Haemers, Spectral characterizations of graphs, a plenary talk in 2017 Meeting of the International Linear Algebra Society (or see http://members.upc.nl/w.haemers/SC-show.pdf).

[7] W.H. Haemers, Spectral characterization of mixed extensions of small graphs, Discrete Math. 342 (2019) 2760–2764.

[8] W.H. Haemers, On the spectral characterization of mixed extensions of $P_3$, Elect. J. Combin. 26(3) (2019) #P3.16
[9] X.C. He, L. Lu, On the largest and least eigenvalues of eccentricity matrix of trees, Discrete Math. 345 (2022) 112662.
[10] X.Y. Huang, Q.X. Huang, L. Lu, Graphs with at most three distance eigenvalues different from −1 and −2, Graphs Combin. 34 (2018) 395–414.
[11] L. Lu, Q.X. Huang, X.Y. Huang, The graphs with exactly two distance eigenvalues different from −1 and −3, J Algebr Comb. 45 (2017) 629–647.
[12] I. Mahato, R. Gurusamy, M.R. Kannan, S. Arockiaraj, Spectra of eccentricity matrices of graphs, Discrete Appl. Math. 285 (2020) 252–260.
[13] I. Mahato, R. Gurusamy, M.R. Kannan, S. Arockiaraj, On the spectral radius and the energy of eccentricity matrix of a graph, arXiv:1909.05609v1.
[14] B. Mohar, Median eigenvalues and the HOMO-LUMO index of graphs, J. Combin. Theory, Ser. B 112 (2015) 78–92.
[15] B. Mohar, Median Eigenvalues of Bipartite Subcubic Graphs, Combin. Probab. Comput. 25 (2016) 768–790.
[16] B. Mohar, Tayfeh-Rezaie, Median eigenvalues of bipartite graphs, J. Algebr. Comb. 41 (2015) 899–909.
[17] M. Randić, $D_{\text{MAX}}$-Matrix of dominant distances in a graph, MATCH Commun. Math. Comput. Chem. 70 (2013) 221–238.
[18] A.J. Schwenk, Almost all trees are cospectral, in: F. Harary (Ed.), New Directions in the Theory of Graphs, Academic Press, New York, 1973, pp. 275–307.
[19] A.J. Schwenk, Computing the characteristic polynomial of a graph, in: R. Bary, F. Harary(Eds.), Graphs Combinatorics, in: Lecture Notes in Mathematics, vol. 406, Springer, Berlin, 1974, pp. 153–172.
[20] S. Sorgun, H. Küçük, On the graphs having exactly one positive eccentricity eigenvalue, arXiv:2012.10933v1.
[21] H. Topcu, S. Sorgun, W. H. Haemers, The graphs cospectral with the pineapple graph, Discrete Appl. Math. 269 (2019) 52–59.
[22] F. Tura, On the eccentricity energy of complete multipartite graph, arXiv:2002.07140v1.
[23] J.F. Wang, X.Y. Lei, S.C. Li, W. Wei, On the eccentricity matrix of graphs and its applications to the boiling point of hydrocarbons, Chem. Intel. Lab. Sys. 207 (2020) 104173.
[24] J.F. Wang, L. Lu, M. Randić, G.Z. Li, Graph energy based on the eccentricity matrix, Discrete Math. 342 (2019) 2636–2646.
[25] J.F. Wang, M. Lu, F. Belardo, M. Randić, The anti-adjacency matrix of a graph: eccentricity matrix, Discrete Appl. Math. 251 (2018) 299–309.
[26] J.F. Wang, M. Lu, M. Brunetti, L. Lu, X.Y. Huang, Spectral determinations and eccentricity matrix of graphs, manuscript and submitted.
[27] J. Wang, M. Lu, L. Lu, F. Belardo, Spectral properties of the eccentricity matrix of graphs, Discrete Appl. Math. 279 (2020) 168–177.
[28] W. Wei, X.C. He, S.C. Li, Solutions for two conjectures on the eigenvalues of the eccentricity matrix, and beyond, Discrete Math. 343 (2020) 111925.