

## $A_\alpha$ -SPECTRAL EXTREMA OF GRAPHS WITH GIVEN SIZE AND MATCHING NUMBER

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ABSTRACT. In 2017, Nikiforov proposed the  $A_\alpha$ -matrix of a graph  $G$ . This novel matrix is defined as

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G), \quad \alpha \in [0, 1],$$

where  $D(G)$  and  $A(G)$  are the degree diagonal matrix and adjacency matrix of  $G$ , respectively. Recently, Zhai, Xue and Liu [39] considered the Brualdi-Hoffman-type problem for  $Q$ -spectra of graphs with given matching number. As a continuance of it, in this contribution we consider the Brualdi-Hoffman-type problem for  $A_\alpha$ -spectra of graphs with given matching number. We identify the graphs with given size and matching number having the largest  $A_\alpha$ -spectral radius for  $\alpha \in [\frac{1}{2}, 1)$ .

### 1. Introduction

Let  $G = (V(G), E(G))$  be a graph with *vertex set*  $V(G)$  and *edge set*  $E(G)$ . The number  $|E(G)|$  is called the *size* of  $G$  and is denoted by  $m(G)$ . In this paper, all the graphs considered are simple and undirected. Unless otherwise stated, we follow the traditional notation and terminology; see [1, 3].

For a vertex  $v \in V(G)$ , let  $N_G(v)$  be the neighborhood of  $v$  in  $G$ . Denote by  $d_G(v) := |N_G(v)|$  the *degree* of  $v$  in  $G$ . Here, as elsewhere, we drop the index referring to the underlying graph if the reference is clear. The number  $\Delta(G) := \max\{d(v) \mid v \in V(G)\}$  is the *maximum degree* of  $G$ . For a graph  $G$  with a vertex subset  $S \subseteq V(G)$ , denote by  $G[S]$  the subgraph of  $G$  induced by  $S$ .

For  $V_1 \subseteq V(G)$ ,  $E_1 \subseteq E(G)$ , let  $G - V_1$ ,  $G - E_1$  be the graphs formed from  $G$  by deleting the vertices in  $V_1$  and their incident edges, the edges in  $E_1$ , respectively. For convenience, denote  $G - \{v\}$  and  $G - \{uv\}$  by  $G - v$  and  $G - uv$ , respectively. Similarly,  $G + uv$  is obtained from  $G$  by adding the edge

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$uv \notin E(G)$ . For two graphs  $G$  and  $H$ , we define  $G \cup H$  to be their disjoint union. In addition, we use  $kG$  to denote the disjoint union of  $k$  copies of  $G$ .

Given a graph  $G$  with  $V(G) = \{v_1, \dots, v_n\}$ , its *adjacency matrix*  $A(G)$  is an  $n \times n$  0-1 matrix whose  $(i, j)$ -entry is 1 if and only if  $v_i v_j \in E(G)$ . Let  $D(G) = \text{diag}(d_1, d_2, \dots, d_n)$  be the diagonal matrix whose diagonal entries are the vertex degrees in  $G$ . The matrix  $Q(G) = D(G) + A(G)$  is the well-known *signless Laplacian matrix* of  $G$ .

In 2017, Nikiforov [25] introduced the  $A_\alpha$ -*matrix* of a graph  $G$ , which is a linear convex combination of  $D(G)$  and  $A(G)$ , i.e.,

$$A_\alpha(G) = \alpha D(G) + (1 - \alpha)A(G), \quad \alpha \in [0, 1].$$

Obviously,

$$(1) \quad A(G) = A_0(G), \quad Q(G) = 2A_{\frac{1}{2}}(G) \quad \text{and} \quad D(G) = A_1(G).$$

The eigenvalues of  $A_\alpha(G)$  are called the  $A_\alpha$ -*eigenvalues* of  $G$ , and the maximum modulus among them, denoted by  $\lambda(G)$ , is called the  $A_\alpha$ -*spectral radius* of  $G$ .

The silent rise of research on  $A_\alpha$ -spectra attracts more and more researchers' attention. One's study on  $A_\alpha$ -spectra gradually becomes a mainstream issue in spectral graph theory. It is interesting, important and challenging. Liu, Das and Shu [23] presented several upper and lower bounds on the  $k^{\text{th}}$  largest eigenvalue of  $A_\alpha$ -matrix and characterized the extremal graphs corresponding to some of these obtained bounds. For more results on bounds of  $A_\alpha$ -eigenvalues, one may be referred to [7, 8, 15, 17, 27, 31, 32, 40]. Cardoso, Pastén, and Rojo [5] studied the multiplicity of  $\alpha$  as an eigenvalue of  $A_\alpha(G)$  of graphs with pendant vertices. This problem was extended to the signed graph by Belardo, Brunetti, and Ciampella [2]. Wang, Fang, Geng, and Tian [30] considered the multiplicity of an arbitrary  $A_\alpha$ -eigenvalue of a connected graph. For more results along this line, we refer the readers to [20, 35, 37]. There is a rich study on the relation between the  $A_\alpha$ -eigenvalues of a (di)graph with various parameters; see [14] for  $A_\alpha$ -spectral radius and the size of  $G$  with  $\frac{1}{2} \leq \alpha \leq 1$ , [26] for  $A_\alpha$ -spectral radius and diameter, [9, 13] for  $A_\alpha$ -spectral radius, size, and diameter, [36] for  $A_\alpha$ -spectral radius and clique number, [21] for  $A_\alpha$ -spectral radius and number of cut vertices, [33, 34] for  $A_\alpha$ -spectral radius and parameters of digraphs.

The *spectrum*,  $\text{Spec}(G)$  of a graph  $G$  is the set of eigenvalues together with their multiplicities of the corresponding matrix, say  $M$ , associated with  $G$ . Two graphs are called  $M$ -*cospectral* if they share the same  $M$ -spectrum. A graph  $G$  is said to be *determined by the spectrum* ( $DS$  for short), if any cospectral graph of  $G$  is isomorphic to  $G$ . A graph  $G$  is said to be *determined by the generalized  $M$ -spectrum* ( $DGMS$  for short), if any graph  $H$  satisfying  $\text{Spec}(G) = \text{Spec}(H)$  and  $\text{Spec}(\bar{G}) = \text{Spec}(\bar{H})$ , is isomorphic to  $G$ , where  $\bar{H}$  and  $\bar{G}$  denote the complement of  $H$  and  $G$ , respectively. In fact, it is tough to determine whether a graph is  $DS$  (resp.  $DGMS$ ) in general. Lin, Liu, Xue [22] showed that lollipop graph is determined by its  $A_\alpha$ -spectrum for  $0 < \alpha < 1$  and the friendship

graph is determined by its  $A_\alpha$ -spectrum for  $\frac{1}{2} < \alpha < 1$ . Li and Sun [16] gave a simple arithmetic condition for an  $\alpha$ -controllable graph  $G$  being  $DGA_\alpha S$  for  $0 \leq \alpha < 1$ . Li and Wang [19] gave a simple criterion for an almost  $\alpha$ -controllable graph  $G$  being  $DGA_\alpha S$  for  $0 \leq \alpha < 1$ .

In 1985, Brualdi and Hoffman proposed the following extremal spectral problem:

**Problem 1** (Brualdi-Hoffman Problem). How to determine the graphs of size  $m$  having the largest  $A_0$ -spectral radius?

This problem was studied by Brualdi and Hoffman [4], Friedland [11], Rowlinson [28] and Stanley [29]. Surprisingly if one adds some more constraints, for example among graphs of given size and order, the Brualdi-Hoffman problem becomes much more difficult. In fact, for any positive integers  $m$  and  $n$ , the Brualdi-Hoffman problem for graphs of order  $n$  and size  $m$  is still open. We refer the reader to the recent article [18] and in the references cited therein for the advances on this open problem. It is still interesting to consider the Brualdi-Hoffman problem under some other constraints.

Matching theory is fundamental in graph theory, and it has many important applications in theoretical chemistry and combinatorial optimization (see [24]). A subset  $S$  of  $E(G)$  is called a *matching* if any two members of  $S$  are not adjacent in  $G$ . The *matching number*  $\mu(G)$  is the size of a maximum matching in  $G$ . A vertex is *saturated* by a matching  $M$  if it is incident with an edge of  $M$ . The matching number of a graph has a close relationship with spectral parameters. Feng, Yu, and Zhang [10] identified the graph with given matching number having the largest  $A_0$ -spectral radius. Yu [38] characterized the graph with given matching number having the largest  $A_{\frac{1}{2}}$ -spectral radius of graphs. Chen and Huang [6] determined the  $n$ -vertex extremal graphs with given matching number having maximum  $A_\alpha$ -spectral radius for  $0 \leq \alpha < 1$ . Lin, Huang, and Xue [21] characterized the  $n$ -vertex trees with given matching number having the largest  $A_\alpha$ -spectral radius for  $0 \leq \alpha < 1$ . Very recently, Zhai, Xue and Liu [39] identified the graph with given size and matching number having the largest  $A_{\frac{1}{2}}$ -spectral radius.

Motivated directly from [6,21,39], we consider the following Brualdi-Hoffman problem with the additional matching constraint.

**Problem 2.** How can we determine the graphs with given size and matching number having the largest  $A_\alpha$ -spectral radius for  $0 \leq \alpha \leq 1$ ?

In order to formulate our main result, we need to introduce some notation. Let  $\mathcal{G}_m^\mu$  be the set of graphs of size  $m$  and matching number  $\mu$ , and let  $\mathcal{G}_m^{\geq \mu}$  be the set of graphs with size  $m$  and matching number at least  $\mu$ . We use  $F_{r,s,t}$  to denote the *firefly graph* of size  $m$ , which is obtained from  $r$  triangles,  $s$  pendant paths of length 1 and  $t$  pendant paths of length 2 by sharing a common vertex; see Figure 1.

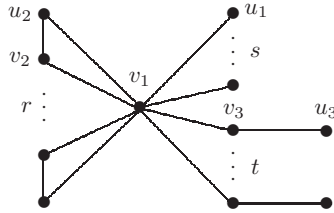


FIGURE 1. The firefly graph  $F_{r,s,t}$  with some labeled vertices, where  $3r + 2t + s = m$ .

Note that, among  $\mathcal{G}_m^1$ , it is straightforward to determine the graphs having the largest  $A_\alpha$ -spectral radius. On the other hand,  $A_1(G) = D(G)$ . When  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ , Problem 2 is solved in the following theorem.

**Theorem 1.1.** *Let  $G$  be in  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius, where  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ . Then  $G$  is isomorphic to  $F_{r,s,t}$  ( $s \geq 1$ ) with possibly some isolated edges and isolated vertices, and the matching number of  $G$  is  $\mu$ . Moreover,*

- (i) *if  $m \geq 3\mu - 1$ , then  $r = \mu - 1$ ,  $s = m - 3\mu + 3$  and  $t = 0$ ;*
- (ii) *if  $m \leq 3\mu - 2$  and  $m - \mu$  is even, then  $r = \frac{m-\mu}{2}$ ,  $s = 1$  and  $t = 0$ ;*
- (iii) *if  $m \leq 3\mu - 2$  and  $m - \mu$  is odd, then  $r = \frac{m-\mu-1}{2}$  and  $s = t = 1$ .*

The proof techniques in the paper for our main result follow the idea of Zhai, Xue and Liu [39]. Together with some new ideas we make the proofs work. The remaining part of our paper is organized as follows: In the next section we recall some important known results. In Section 3, we give some structure lemmas. In Section 4, we give the proof of Theorem 1.1. In the last section, we give some brief comments on our contribution and propose some further research questions.

### 2. Some preliminaries

In this section, we provide some known lemmas that will be used in the subsequent sections.

Let  $B$  be a real matrix whose rows and columns are indexed by  $V = \{1, \dots, n\}$ . Assume that  $B$  can be written as

$$B = \begin{pmatrix} B_{11} & \cdots & B_{1k} \\ \vdots & \ddots & \vdots \\ B_{k1} & \cdots & B_{kk} \end{pmatrix}$$

according to partition  $V = V_1 \cup \dots \cup V_k$ , wherein  $B_{ij}$  denotes the submatrix (block) of  $B$  formed by the rows in  $V_i$  and the columns in  $V_j$ . Let  $c_{ij}$  denote the average row sum of  $B_{ij}$ . Then the matrix  $C = (c_{ij})$  is called the *quotient*

matrix of  $B$ . If the row sum of each block  $B_{ij}$  is a constant, then the partition is called *equitable* and  $C$  is called the *equitable quotient matrix* of  $B$ .

**Lemma 2.1** ([3]). *Let  $B$  be a nonnegative matrix and  $C$  be the equitable quotient matrix of  $B$ . Then  $\rho(C) = \rho(B)$ , where  $\rho(C)$  and  $\rho(B)$  are the spectral radii of  $C$  and  $B$ , respectively.*

**Lemma 2.2** ([12]). *If  $B$  is a nonnegative matrix, then there is a nonnegative nonzero vector  $\mathbf{u}$  such that  $B\mathbf{u} = \rho(B)\mathbf{u}$ , where  $\rho(B)$  is the spectral radius of  $B$ .*

Since  $A_\alpha$ -matrix is a nonnegative matrix for  $\alpha \in [0, 1]$ , there exists a nonnegative nonzero unit vector  $\mathbf{x}$  such that  $A_\alpha(G)\mathbf{x} = \lambda(G)\mathbf{x}$ . We call  $\mathbf{x}$  the *principal eigenvector* of  $A_\alpha(G)$  for  $\alpha \in [0, 1]$ . For convenience, let  $x_v$  denote the coordinate of  $\mathbf{x}$  such that  $x_v$  corresponds to the vertex  $v \in V(G)$ . By a direct calculation, one has

$$(2) \quad \lambda(G)x_v = \alpha d(v)x_v + (1 - \alpha) \sum_{uv \in E(G)} x_u$$

for all  $v \in V(G)$  and  $\alpha \in [0, 1]$ .

**Lemma 2.3** ([25]). *Let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$  with  $\alpha \in [0, 1]$ .*

- (i) *If  $G$  is connected, then  $\mathbf{x}$  is positive.*
- (ii) *If  $H$  is any proper subgraph of a connected graph  $G$ , then  $\lambda(G) > \lambda(H)$ .*

Assume that  $H$  is a connected graph with  $|V(H)| \geq 3$  and let  $G \cong H \cup aK_2 \cup bK_1$  ( $a, b \geq 0$ ). Then  $\lambda(G) = \lambda(H)$  and  $\lambda(G)\mathbf{x} = A_\alpha(G)\mathbf{x}$  for  $\mathbf{x} = (\mathbf{x}|_H^T, 0, 0, \dots, 0)^T$ , where  $\mathbf{x}|_H$  is the principal eigenvector of  $A_\alpha(H)$ . Since  $H$  is connected,  $\mathbf{x}|_H$  is a positive vector by Lemma 2.3 and we get the next corollary.

**Corollary 2.4.** *Let  $H$  be a connected graph with  $|V(H)| \geq 3$  and let  $G \cong H \cup aK_2 \cup bK_1$ . If  $A_\alpha(G)\mathbf{x} = \lambda(G)\mathbf{x}$  ( $0 \leq \alpha < 1$ ), then  $x_v > 0$  for all  $v \in V(H)$ .*

**Lemma 2.5** ([14]). *For two graphs  $G$  and  $H$  with the same order, assume that the principal eigenvectors of  $A_\alpha(G)$  and  $A_\alpha(H)$  are  $\mathbf{x}$  and  $\mathbf{y}$ , respectively. Then*

$$\mathbf{x}^T(A_\alpha(G))\mathbf{y} = \sum_{uv \in E(G)} [\alpha(x_u y_u + x_v y_v) + (1 - \alpha)(x_u y_v + x_v y_u)]$$

and

$$\mathbf{x}^T\mathbf{y}(\lambda(H) - \lambda(G)) = \mathbf{x}^T(A_\alpha(H) - A_\alpha(G))\mathbf{y}.$$

**Lemma 2.6** ([25]). *Let  $G$  be a graph with the maximum degree  $\Delta \geq 1$ . If  $\alpha \in [\frac{1}{2}, 1)$ , then  $\lambda(G) \geq \alpha\Delta + (1 - \alpha)^2/\alpha$ .*

If  $\Delta \geq 3$  and  $\alpha \in [\frac{1}{2}, 1)$ , then we have  $\frac{[(\Delta+1)\alpha-2](2\alpha-1)}{2\alpha} \geq 0$ , i.e.,  $\alpha\Delta + \frac{(1-\alpha)^2}{\alpha} \geq \frac{1}{2}(\Delta + 1)$ . Then we get the next lemma.

**Lemma 2.7.** *Let  $G$  be a graph with the maximum degree  $\Delta \geq 3$ . If  $\alpha \in [\frac{1}{2}, 1)$ , then  $\lambda(G) \geq \frac{1}{2}(\Delta + 1)$ .*

### 3. Some key lemmas

In this section, we give some structure lemmas. The first one describes the effect of a graph transformation on the  $A_\alpha$ -spectral radius.

**Lemma 3.1.** *Let  $G$  be a graph and let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$  for  $\alpha \in (0, 1)$ . Assume that  $u_1u_2 \in E(G)$ ,  $v_1v_2 \notin E(G)$  and  $x_{u_1} \geq x_{u_2}$ ,  $x_{v_1} \geq x_{v_2}$ . If  $x_{v_1} > 0$  and  $x_{v_i} \geq x_{u_i}$  for  $i = 1, 2$ , then  $\lambda(G - u_1u_2 + v_1v_2) > \lambda(G)$ .*

*Proof.* It is obvious that  $\mathbf{x}$  is nonnegative. Note that  $x_{v_i} \geq x_{u_i}$  for  $i = 1, 2$ . Hence, we obtain  $x_{v_i}^2 \geq x_{u_i}^2$  and  $x_{v_1}x_{v_2} \geq x_{u_1}x_{u_2}$ . Let  $G' = G - u_1u_2 + v_1v_2$ . Then, for  $\alpha \in (0, 1)$ , by Rayleigh quotient, we have

$$\begin{aligned} \lambda(G') - \lambda(G) &\geq \mathbf{x}^T (A_\alpha(G') - A_\alpha(G)) \mathbf{x} \\ &= \sum_{uv \in E(G')} [\alpha(x_u^2 + x_v^2) + 2(1 - \alpha)x_u x_v] \\ &\quad - \sum_{uv \in E(G)} [\alpha(x_u^2 + x_v^2) + 2(1 - \alpha)x_u x_v] \\ &= \alpha(x_{v_1}^2 + x_{v_2}^2 - x_{u_1}^2 - x_{u_2}^2) + 2(1 - \alpha)(x_{v_1}x_{v_2} - x_{u_1}x_{u_2}) \\ &\geq 0. \end{aligned}$$

Hence,  $\lambda(G') \geq \lambda(G)$ .

Suppose that  $\lambda(G') = \lambda(G)$ . Then  $\lambda(G') = \mathbf{x}^T A_\alpha(G') \mathbf{x}$ , and so  $\mathbf{x}$  is also the principal eigenvector of  $A_\alpha(G')$ . Since  $\{v_1, v_2\} \neq \{u_1, u_2\}$ , we have  $v_1 \notin \{u_1, u_2\}$  or  $v_2 \notin \{u_1, u_2\}$ . Without loss of generality, assume that  $v_2 \notin \{u_1, u_2\}$ . Then  $d_{G'}(v_2) = d_G(v_2) + 1$ . By  $x_{v_1} > 0$  and  $\alpha \in (0, 1)$ , we get

$$\begin{aligned} \lambda(G')x_{v_2} &= \alpha d_{G'}(v_2)x_{v_2} + (1 - \alpha) \sum_{w \in N_{G'}(v_2)} x_w \\ &= \alpha d_G(v_2)x_{v_2} + \alpha x_{v_2} + (1 - \alpha) \sum_{w \in N_G(v_2)} x_w + (1 - \alpha)x_{v_1} \\ &> \alpha d_G(v_2)x_{v_2} + (1 - \alpha) \sum_{w \in N_G(v_2)} x_w \\ &= \lambda(G)x_{v_2}, \end{aligned}$$

which contradicts  $\lambda(G') = \lambda(G)$ . Thereby,  $\lambda(G') > \lambda(G)$ .

This completes the proof.  $\square$

Next we define a special matching for a graph  $G$ . Then we describe the relation between this matching and the principal eigenvector of  $A_\alpha(G)$ .

**Definition 3.1.** Let  $G$  be a graph and let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$ . A maximum matching  $M^* := \{u_1v_1, u_2v_2, \dots, u_{\mu(G)}v_{\mu(G)}\}$  of  $G$  is said to be extremal (with respect to  $\mathbf{x}$ ) if

$$\sum_{u_i v_i \in M^*} [\alpha(x_{u_i}^2 + x_{v_i}^2) + 2(1 - \alpha)x_{u_i}x_{v_i}] = \max_M \sum_{uv \in M} [\alpha(x_u^2 + x_v^2) + 2(1 - \alpha)x_u x_v],$$

where  $M$  takes over all the maximum matchings of  $G$ .

The next lemma establishes a relation between the principle eigenvector and an extremal matching.

**Lemma 3.2.** Let  $G$  be a graph among  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius,  $\alpha \in (0, 1)$ . Let  $M^*$  be an extremal matching of  $G$  and let  $V^*$  denote the set of vertices saturated by  $M^*$ . Then  $x_w \leq \min_{v \in V^*} x_v$  for any vertex  $w \in V(G) \setminus V^*$ .

*Proof.* Assume that  $u_1v_1 \in M^*$  satisfying  $x_{u_1} = \min_{v \in V^*} x_v$ . Then it suffices to show that  $x_w \leq x_{u_1}$  for all vertices  $w$  in  $V(G) \setminus V^*$ . In what follows, we prove it by contradiction. Suppose that  $x_w > x_{u_1}$ .

If  $wv_1 \in E(G)$ , then for  $\alpha \in (0, 1)$ , we have

$$\sum_{u_i v_i \in M^*} [\alpha(x_{u_i}^2 + x_{v_i}^2) + 2(1 - \alpha)x_{u_i}x_{v_i}] < \sum_{\substack{uv \in (M^* \setminus \{u_1v_1\}) \\ \cup \{wv_1\}}} [\alpha(x_u^2 + x_v^2) + 2(1 - \alpha)x_u x_v],$$

which contradicts the definition of  $M^*$ .

If  $wv_1 \notin E(G)$ , then let  $G' = G - u_1v_1 + wv_1$ . Obviously,  $G' \in \mathcal{G}_m^{\geq \mu}$ . Bearing in mind that the principal eigenvector  $\mathbf{x}$  is nonnegative, we have  $x_w > x_{u_1} \geq 0$ . By Lemma 3.1 we get  $\lambda(G') > \lambda(G)$ , which contradicts the maximality of  $\lambda(G)$ .

This completes the proof.  $\square$

Recall the following definition, which orders the edges in an extremal matching of  $G$ .

**Definition 3.2** ([39]). Assume that  $M^*$  is an extremal matching. Then one may arrange the edges of  $M^*$  with respect to  $\mathbf{x}$  as  $u_1v_1, u_2v_2, \dots, u_{\mu(G)}v_{\mu(G)}$  such that the followings hold:

- (i) For  $i = 1, \dots, \mu(G)$ ,  $x_{v_i} \geq x_{u_i}$ ;
- (ii) For  $i = 1, \dots, \mu(G) - 1$ ,  $x_{v_i} \geq x_{v_{i+1}}$ , and  $x_{u_i} \geq x_{u_{i+1}}$  if  $x_{v_i} = x_{v_{i+1}}$ .

The upper ordering of the edges in  $M^*$  is said to be proper with respect to  $\mathbf{x}$ .

In what follows, we always assume that the order of the edges in  $M^*$  is proper with respect to the principal eigenvector  $\mathbf{x}$  of  $A_\alpha(G)$ . By Definition 3.2 and Lemma 3.2, we have  $x_{v_1} = \max_{v \in V(G)} x_v$ . Since  $\mathbf{x} (\neq \mathbf{0})$  is nonnegative, one has  $x_{v_1} > 0$ .

The following lemma describes the local structure of the graph in  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius.

**Lemma 3.3.** *Let  $G$  be a graph among  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius, where  $\mu \geq 2$  and  $\alpha \in (0, 1)$ . Assume that  $\mathbf{x}$  is the principal eigenvector of  $A_\alpha(G)$  and  $M^*$  is an extremal matching of  $G$  whose edges are ordered properly with respect to  $\mathbf{x}$ . For  $1 \leq i < j \leq \mu(G)$ , we have  $x_{u_i} \geq x_{v_j}$  if and only if  $G[\{u_i, v_i, u_j, v_j\}] \cong 2K_2$  or  $K_4$ .*

*Proof.* ( $\Rightarrow$ ) For  $1 \leq i < j \leq \mu(G)$ , assume that  $x_{u_i} \geq x_{v_j}$  and let  $H = G[\{u_i, v_i, u_j, v_j\}]$ . Suppose  $H \not\cong 2K_2$ . Then  $E(H) \setminus \{u_i v_i, u_j v_j\} \neq \emptyset$  and there exists an edge  $uv \in E(H) \setminus \{u_i v_i, u_j v_j\}$ . If  $x_u = 0$ , then from (2), we have  $x_w = 0$  for all  $w \in N_G(u)$ . Therefore,  $v_1 \notin N_G(u)$  by  $x_{v_1} > 0$ . Let  $G' = G - uv + uv_1$ . Clearly,  $M^* \subseteq E(G')$  and so  $G' \in \mathcal{G}_m^{\geq \mu}$ . By  $x_{v_1} \geq x_v$  and Lemma 3.1, we get  $\lambda(G') > \lambda(G)$ , a contradiction. So,  $x_u > 0$ .

By (2), we have

$$\lambda(G)x_w = \alpha d_G(w)x_w + (1 - \alpha) \sum_{w' \in N_G(w)} x_{w'} \geq (1 - \alpha)x_u > 0$$

for all  $w \in N_G(u)$ , and so  $x_w > 0$ .

Suppose that  $v_i v_j \notin E(H)$ . As  $uv \in E(H) \setminus \{u_i v_i, u_j v_j\}$ , we have  $uv = u_i v_j, u_i u_j$  or  $v_i u_j$ . Let  $G'' = G - uv + v_i v_j$ . Then  $G'' \in \mathcal{G}_m^{\geq \mu}$ . From Definition 3.2, we have  $x_{v_i} \geq x_{u_i}, x_{v_j} \geq x_{u_j}$ . Then  $\lambda(G'') > \lambda(G)$  (based on Lemma 3.1). Therefore,  $v_i v_j \in E(H)$  and  $H$  is connected. By  $x_u > 0$ , we have  $x_w > 0$  for all  $w \in V(H)$ .

We first consider that  $u_i u_j \notin E(H)$ . Due to  $(M^*(G) \setminus \{u_i v_i, u_j v_j\}) \cup \{u_i u_j, v_i v_j\}$  is a matching of  $G - v_j u_j + u_i u_j$ , then  $\mu(G - v_j u_j + u_i u_j) \geq \mu(G)$ . By  $x_{u_i} \geq x_{v_j}$  and Lemma 3.1, we have  $\lambda(G - v_j u_j + u_i u_j) > \lambda(G)$ , a contradiction. Hence,  $u_i u_j \in E(H)$ .

Now we consider  $u_i v_j$  or  $v_i u_j \notin E(H)$ . In this subcase, we have  $\mu(G - u_i u_j + u_i v_j) \geq \mu(G)$  and  $\mu(G - u_i u_j + v_i u_j) \geq \mu(G)$ . By  $x_{v_j} \geq x_{u_j}, x_{v_i} \geq x_{u_i}$  and Lemma 3.1, we have  $\lambda(G - u_i u_j + u_i v_j) > \lambda(G)$  and  $\lambda(G - u_i u_j + v_i u_j) > \lambda(G)$ , a contradiction. Hence,  $u_i v_j, v_i u_j \in E(H)$ . It follows that  $H \cong K_4$ .

( $\Leftarrow$ ) Conversely, assume that  $H \cong 2K_2$  or  $K_4$  and suppose  $x_{u_i} < x_{v_j}$ . If  $H \cong 2K_2$ , let  $G''' = G - u_i v_i - u_j v_j + u_i u_j + v_i v_j$ . Then  $\mu(G''') \geq \mu(G)$ , and so  $G''' \in \mathcal{G}_m^{\geq \mu}$ . Moreover, for  $\alpha \in (0, 1)$ , one has

$$\begin{aligned} \lambda(G''') - \lambda(G) &\geq \mathbf{x}^T (A_\alpha(G''') - A_\alpha(G)) \mathbf{x} \\ &= [\alpha(x_{u_i}^2 + x_{u_j}^2) + 2(1 - \alpha)x_{u_i}x_{u_j} + \alpha(x_{v_i}^2 + x_{v_j}^2) + 2(1 - \alpha)x_{v_i}x_{v_j}] \\ &\quad - [\alpha(x_{u_i}^2 + x_{v_i}^2) + 2(1 - \alpha)x_{u_i}x_{v_i} + \alpha(x_{v_j}^2 + x_{u_j}^2) + 2(1 - \alpha)x_{v_j}x_{u_j}] \\ &= 2(1 - \alpha)(x_{v_j} - x_{u_i})(x_{v_i} - x_{u_j}). \end{aligned}$$

In view of Definition 3.2, we have  $x_{v_i} \geq x_{v_j} \geq x_{u_j}$ . If  $x_{v_i} = x_{u_j}$ , then  $x_{v_i} = x_{v_j}$ . By Definition 3.2, we have  $x_{v_i} \geq x_{u_i} \geq x_{u_j}$ . Then  $x_{v_i} = x_{u_j} = x_{u_i}$ . Together with  $x_{v_j} = x_{v_i}$ , we have  $x_{v_j} = x_{u_i}$ , a contradiction to  $x_{u_i} < x_{v_j}$ . Thus,  $x_{v_i} > x_{u_j}$ . Together with  $x_{u_i} < x_{v_j}$  and  $\alpha \in (0, 1)$ , one has

$$(3) \quad \lambda(G''') - \lambda(G) \geq 2(1 - \alpha)(x_{v_j} - x_{u_i})(x_{v_i} - x_{u_j}) > 0,$$



a contradiction. So,  $x_{u_i} \geq x_{v_j}$ .

If  $H \cong K_4$ , let  $M = (M^* \setminus \{u_i v_i, u_j v_j\}) \cup \{u_i u_j, v_i v_j\}$ . Then  $M$  is a maximum matching of  $G$ . However, from the above discussion and  $\alpha \in (0, 1)$ , we have

$$\begin{aligned} & \alpha(x_{u_i}^2 + x_{u_j}^2) + 2(1 - \alpha)x_{u_i}x_{u_j} + \alpha(x_{v_i}^2 + x_{v_j}^2) + 2(1 - \alpha)x_{v_i}x_{v_j} \\ & > \alpha(x_{u_i}^2 + x_{v_i}^2) + 2(1 - \alpha)x_{u_i}x_{v_i} + \alpha(x_{v_j}^2 + x_{u_j}^2) + 2(1 - \alpha)x_{v_j}x_{u_j}, \end{aligned}$$

which contradicts that  $M^*$  is extremal. So,  $x_{u_i} \geq x_{v_j}$ . □

Let  $M^*$  and  $V^*$  be the same as those defined in Lemma 3.2. Since  $x_{v_1} = \max_{v \in V(G)} x_v$ , we have a partition  $E(G) = E_1(G) \cup E_2(G)$ , where

$$(4) \quad E_1(G) = M^* \cup \{v_1 v \mid v \in N_G(v_1)\}, \quad E_2(G) = E(G) \setminus E_1(G).$$

The next lemma also describes the local structure of the graph in  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius.

**Lemma 3.4.** *Let  $G$  be a graph among  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius and let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$ , where  $\mu \geq 2$  and  $\alpha \in (0, 1)$ . If  $E_2(G) \neq \emptyset$ , then  $H_1 \subseteq G$  or  $H_2 \subseteq G$ , where  $H_1 = K_4 - e$ ,  $e$  is an edge of  $K_4$  and  $H_2$  is the graph obtained by attaching one pendant edge to each vertex of a cycle  $C_3$ . Furthermore, for each edge  $uv$  in  $E(G) \setminus (M^* \cup E(H_i))$  ( $i = 1, 2$ ), one has  $v_1$  is incident with  $uv$ , or  $\{u, v\} \subseteq N_G(v_1)$ .*

*Proof.* By Lemma 3.2 and Definition 3.2, we have  $x_{v_1} = \max_{v \in V(G)} x_v > 0$  and  $x_{v_2} = \max_{w \in V(G) \setminus \{u_1, v_1\}} x_w$ . Let  $uv \in E_2(G)$ . Then  $u, v \neq v_1$ . If  $u_1$  is incident with the edge  $uv$ , then without loss of generality assume that  $u = u_1$ . Hence,  $v \neq u_1$  and so  $x_v \leq \max_{w \in V(G) \setminus \{u_1, v_1\}} x_w = x_{v_2}$ . If  $u_1$  is not incident with the edge  $uv$ , then we get  $x_u, x_v \leq \max_{w \in V(G) \setminus \{u_1, v_1\}} x_w = x_{v_2} \leq x_{v_1}$ . Suppose that  $v_1 v_2 \notin E(G)$ . By  $x_{v_1} > 0$  and Lemma 3.1, we have  $\lambda(G - uv + v_1 v_2) > \lambda(G)$ . Since  $G - uv + v_1 v_2 \in \mathcal{G}_m^{\geq \mu}$ , we get a contradiction to the maximality of  $\lambda(G)$ . Hence,  $v_1 v_2 \in E(G)$  and  $G[\{u_1, v_1, u_2, v_2\}] \cong 2K_2$ .

We first consider  $x_{v_2} < x_{u_1}$ . Then by Lemma 3.3, we have  $G[\{u_1, v_1, u_2, v_2\}] \cong K_4$ . So,  $H_1 \subseteq G$ .

Next we consider  $x_{v_2} > x_{u_1} \geq 0$ . Then  $x_{v_2} = \max_{w \in V(G) \setminus \{v_1\}} x_w$  and  $\max\{x_{u_1}, x_{v_3}\} = \max_{w \in V(G) \setminus \{v_1, v_2, u_2\}} x_w$ . Note that  $uv \in E_2(G)$ . Hence,  $u, v \neq v_1$  and  $|\{u, v\} \cap \{u_2, v_2\}| \leq 1$ . If  $|\{u, v\} \cap \{u_2, v_2\}| = 1$ , set  $u \in \{u_2, v_2\}$ . We get  $x_u \leq x_{v_2}$ ,  $x_v \leq \max_{w \in V(G) \setminus \{v_1, v_2, u_2\}} x_w = \max\{x_{u_1}, x_{v_3}\}$ . If  $|\{u, v\} \cap \{u_2, v_2\}| = 0$ , then  $x_u, x_v \leq \max_{w \in V(G) \setminus \{v_1, v_2, u_2\}} x_w = \max\{x_{u_1}, x_{v_3}\} \leq x_{v_2}$ .

If  $\max\{x_{u_1}, x_{v_3}\} = x_{u_1}$ , we may obtain  $v_2 u_1 \in E(G)$  and  $u_2 v_1 \in E(G)$ . In fact, if  $v_2 u_1 \notin E(G)$ , then  $G - uv + v_2 u_1 \in \mathcal{G}_m^{\geq \mu}$ . By Lemma 3.1, we have  $\lambda(G - uv + v_2 u_1) > \lambda(G)$ , a contradiction. If  $u_2 v_1 \notin E(G)$ , then  $\mu(G - u_2 v_2 + u_2 v_1) \geq \mu(G)$  and  $\lambda(G - u_2 v_2 + u_2 v_1) > \lambda(G)$ , a contradiction. Therefore, one obtains  $H_1 \subseteq G$ .

If  $\max\{x_{u_1}, x_{v_3}\} = x_{v_3}$ , by a similar discussion as above, we have  $v_2 v_3 \in E(G)$  and  $v_1 v_3 \in E(G)$ , and so  $H_2 \subseteq G$ .

Now we prove the second part of our result. Suppose that  $v_1$  is not incident with  $uv$  and  $\{u, v\} \not\subseteq N_G(v_1)$ . Then, without loss of generality, assume that  $v$  is not in  $N_G(v_1)$ . Thus,  $\mu(G - uv + v_1v) \geq \mu(G)$ . By Lemma 3.1, we have  $\lambda(G - uv + v_1v) > \lambda(G)$ , a contradiction. Hence, either  $uv$  is an edge incident to  $v_1$  or  $\{u, v\} \subseteq N_G(v_1)$ .  $\square$

Our last lemma in what follows describes the global structure of the graphs among  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radii,  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ .

**Lemma 3.5.** *Let  $G$  be a graph in  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius, where  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ . Then  $G \cong F_{r,s,t}$  ( $s \geq 1$ ) with possibly some isolated edges and isolated vertices, where  $F_{r,s,t}$  is depicted in Figure 1.*

*Proof.* Let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$ . Let  $M^*$  be an extremal matching of  $G$  with respect to  $\mathbf{x}$ . Assume that  $v_1u_1, \dots, v_{\mu(G)}u_{\mu(G)}$  are all the edges in  $M^*$  with the proper order. By Lemma 3.2, we have  $x_{v_1} = \max_{v \in V^*} x_v = \max_{v \in V(G)} x_v$ . Then in view of (4), we may let  $E_i = E_i(G)$  for  $i \in \{1, 2\}$ . If  $E_2 = \emptyset$ , then our result follows immediately. So we suppose  $E_2 \neq \emptyset$  in what follows. We proceed by considering the following two possible cases.

**Case 1.**  $m(G) \geq \mu(G) + 5$ .

In this case, we consider two graphs  $G_1$  and  $G_2$ , which are defined as

$$G_1 = G \cup |E_2|K_1, \quad G_2 = G - E_2 + \{v_1w_i \mid i = 1, \dots, |E_2|\}.$$

Let  $\mathbf{x}_1 = (\mathbf{x}^T, 0, 0, \dots, 0)^T$ , where the number of extended zero-components is  $|E_2|$ . Evidently,  $\lambda(G_1) = \lambda(G)$  and  $\mathbf{x}_1$  is the principal eigenvector of  $A_\alpha(G_1)$ . Recall that  $m(G) \geq \mu(G) + 5$ . Hence,  $|E(G) \setminus M^*| \geq 5$ . Since  $u_1v_1 \in E(G_2)$  and all the edges of  $E(G) \setminus M^*$  are incident to  $v_1$  in  $G_2$ , we have  $d_{G_2}(v_1) \geq 6$ . By Lemma 2.7, we have  $\lambda(G_2) \geq \frac{7}{2}$  for  $\alpha \in [\frac{1}{2}, 1)$ .

Let  $\mathbf{y}$  be the principal eigenvector of  $A_\alpha(G_2)$  with coordinate  $y_v$  corresponding to  $v \in V(G_2)$ . By Lemma 2.5, we have

$$\begin{aligned} & \mathbf{x}_1^T \mathbf{y} (\lambda(G_2) - \lambda(G_1)) \\ &= \mathbf{x}_1^T (A_\alpha(G_2) - A_\alpha(G_1)) \mathbf{y} \\ &= \sum_{uv \in E(G_2)} [\alpha(x_u y_u + x_v y_v) + (1 - \alpha)(x_u y_v + x_v y_u)] \\ & \quad - \sum_{uv \in E(G_1)} [\alpha(x_u y_u + x_v y_v) + (1 - \alpha)(x_u y_v + x_v y_u)] \\ &= \sum_{i=1, \dots, |E_2|} [\alpha(x_{v_1} y_{v_1} + x_{w_i} y_{w_i}) + (1 - \alpha)(x_{v_1} y_{w_i} + x_{w_i} y_{v_1})] \\ (5) \quad & - \sum_{uv \in E_2} [\alpha(x_u y_u + x_v y_v) + (1 - \alpha)(x_u y_v + x_v y_u)], \end{aligned}$$

where

$$(6) \quad x_{w_i} = 0, \quad x_u \leq x_{v_1}, \quad x_v \leq x_{v_1}$$

for each  $uv \in E_2$ . Note that each  $w_i$  is a pendant vertex of  $G_2$ . Hence,  $\lambda(G_2)y_{w_i} = \alpha y_{w_i} + (1 - \alpha)y_{v_1}$ , and so

$$(7) \quad y_{w_i} = \frac{(1 - \alpha)y_{v_1}}{\lambda(G_2) - \alpha}$$

for  $i = 1, 2, \dots, |E_2|$ . Notice that  $v_1$  belongs to the unique connected component  $H$  of  $G_2$  other than an isolated vertex or an isolated edge and  $|V(H)| \geq 7$  (since  $d_{G_2}(v_1) \geq 6$ ). Hence, we have  $y_{v_1} > 0$  by Corollary 2.4.

On the other hand, we have  $d_{G_2}(v) \leq 2$  for all  $v \in V(G_2) \setminus \{v_1\}$ . Let  $y_{v^*} = \max_{v \in V(G_2) \setminus \{v_1\}} y_v$ . Then

$$\lambda(G_2)y_{v^*} = \alpha d_{G_2}(v^*)y_{v^*} + (1 - \alpha) \sum_{v \in N_{G_2}(v^*)} y_v \leq 2\alpha y_{v^*} + (1 - \alpha)(y_{v^*} + y_{v_1}),$$

and so  $y_{v^*} \leq \frac{(1-\alpha)y_{v_1}}{\lambda(G_2)-1-\alpha}$ . For all  $uv \in E_2$ ,

$$(8) \quad y_u \leq y_{v^*} \leq \frac{(1 - \alpha)y_{v_1}}{\lambda(G_2) - 1 - \alpha}, \quad y_v \leq y_{v^*} \leq \frac{(1 - \alpha)y_{v_1}}{\lambda(G_2) - 1 - \alpha}.$$

Combining (5), (6), (7) and (8) gives us

$$\begin{aligned} \mathbf{x}_1^T \mathbf{y} [\lambda(G_2) - \lambda(G_1)] &\geq [\alpha(x_{v_1}y_{v_1} + 0) + (1 - \alpha)(x_{v_1} \frac{(1 - \alpha)y_{v_1}}{\lambda(G_2) - \alpha} + 0)]|E_2| \\ &\quad - [\alpha(x_{v_1}y_{v^*} + x_{v_1}y_{v^*}) + (1 - \alpha)(x_{v_1}y_{v^*} + x_{v_1}y_{v^*})]|E_2| \\ &\geq \left( \alpha + \frac{(1 - \alpha)^2}{\lambda(G_2) - \alpha} \right) |E_2|x_{v_1}y_{v_1} - \frac{2(1 - \alpha)}{\lambda(G_2) - 1 - \alpha} |E_2|x_{v_1}y_{v_1} \\ (9) \quad &= \frac{\alpha\lambda^2(G_2) - (\alpha^2 + \alpha + 1)\lambda(G_2) + 3\alpha - 1}{(\lambda(G_2) - \alpha)(\lambda(G_2) - \alpha - 1)} |E_2|x_{v_1}y_{v_1}. \end{aligned}$$

By  $E_2 \neq \emptyset$ ,  $x_{v_1} = \max_{v \in V(G)} x_v > 0$  and  $y_{v_1} > 0$ , we get  $|E_2|x_{v_1}y_{v_1} > 0$ . Since  $\lambda(G_2) \geq \frac{7}{2}$ , we have  $\lambda(G_2) - \alpha > 0$  and  $\lambda(G_2) - \alpha - 1 > 0$  for  $\alpha \in [\frac{1}{2}, 1)$ . By the definition of  $G_2$ , we know that the size of  $G_2$  is equal to that of  $G$  and  $\mu(G_2) = \mu(G)$ . Therefore,  $G_2 \in \mathcal{G}_m^{\geq \mu}$ . Based on the maximality of  $\lambda(G)$ , we have  $\lambda(G_2) \leq \lambda(G) = \lambda(G_1)$ . Together with (9), we obtain  $\alpha\lambda^2(G_2) - (\alpha^2 + \alpha + 1)\lambda(G_2) + 3\alpha - 1 \leq 0$ . By some calculations, for  $\alpha \in [\frac{1}{2}, 1)$ , one has  $\frac{\alpha^2 + \alpha + 1}{2\alpha} = \frac{1}{2}(\alpha + \frac{1}{\alpha} + 1) \leq \frac{7}{4}$ ,  $\frac{1}{2\alpha}\sqrt{\alpha^4 + 2\alpha^3 - 9\alpha^2 + 6\alpha + 1} \leq \frac{\sqrt{33}}{4}$  and  $2\alpha \geq 1$ . So we obtain

$$\lambda(G_2) \leq \frac{(\alpha^2 + \alpha + 1) + \sqrt{\alpha^4 + 2\alpha^3 - 9\alpha^2 + 6\alpha + 1}}{2\alpha} \leq \frac{7 + \sqrt{33}}{4} < \frac{7}{2},$$

which contradicts  $\lambda(G_2) \geq \frac{7}{2}$ .

**Case 2.**  $m(G) \leq \mu(G) + 4$ . In this case, let  $\Psi_G(\lambda)$  denote the characteristic polynomial of  $A_\alpha(G)$ . Note that  $E_2 \neq \emptyset$ . By Lemma 3.4, we have  $H_1 \subseteq G$  or

$H_2 \subseteq G$ . Hence,  $m(G) \geq \mu(G) + 3$ . We proceed by considering the following two possible subcases.

**Subcase 2.1.**  $m(G) = \mu(G) + 3$ . In this subcase,  $G$  is isomorphic to either  $H_1$  or  $H_2$  with possibly some isolated edges and isolated vertices. Hence,  $\lambda(G) = \lambda(H_1)$  or  $\lambda(G) = \lambda(H_2)$  holds. Consider the equitable quotient matrix of  $A_\alpha(H_i)$  ( $i = 1, 2$ ), we get  $\lambda(H_1) = \frac{1}{2}(4\alpha + 1 + \sqrt{16\alpha^2 - 32\alpha + 17})$  and  $\lambda(H_2) = \alpha + 1 + \sqrt{\alpha^2 - 2\alpha + 2}$ . Let  $f(\alpha) = \lambda(H_2) - \lambda(H_1)$ . Then

$$f(\alpha) = \frac{1}{2} \left( -2\alpha + 1 + 2\sqrt{\alpha^2 - 2\alpha + 2} - \sqrt{16\alpha^2 - 32\alpha + 17} \right).$$

Clearly,  $f(\alpha)$  is a real function in  $\alpha$ . By some calculations, we get

$$f'(\alpha) = -\frac{(\alpha - 1)(8l_1(\alpha) - 2l_2(\alpha)) + l_1(\alpha)l_2(\alpha)}{l_1(\alpha)l_2(\alpha)}, \quad f''(\alpha) = -\frac{8l_1^3(\alpha) - 8l_2^3(\alpha)}{l_1^3(\alpha)l_2^3(\alpha)},$$

where  $l_1(\alpha) = 2\sqrt{\alpha^2 - 2\alpha + 2}$  and  $l_2(\alpha) = \sqrt{16\alpha^2 - 32\alpha + 17}$ . As  $\alpha \in [\frac{1}{2}, 1)$ , we have

$$l_1(\alpha) > 0, \quad l_2(\alpha) > 0, \quad l_1^2(\alpha) - l_2^2(\alpha) = -3(2\alpha - 3)(2\alpha - 1) \geq 0.$$

Then,  $l_1(\alpha) - l_2(\alpha) \geq 0$ , and so  $f''(\alpha) \leq 0$ . This shows that  $f'(\alpha)$  is a monotonically decreasing function in  $\alpha$  for  $\alpha \in [\frac{1}{2}, 1)$ . On the other hand,  $f'(\frac{1}{2}) = \frac{1}{5}(3\sqrt{5} - 5) > 0$  and  $f'(1) = -1 < 0$ . Hence, for  $\alpha \in [\frac{1}{2}, 1)$ ,

$$f(\alpha) \geq \min \left\{ f\left(\frac{1}{2}\right), f(1) \right\} = 0.$$

Thereby,  $\lambda(H_2) \geq \lambda(H_1)$ .

Now we consider a graph  $G'$  which is a disjoint union of  $F_{1,2,0}$  and  $\mu - 2$  isolated edges, i.e.,  $G' \cong F_{1,2,0} \cup (\mu - 2)K_2$ . We proceed by showing that  $G' \in \mathcal{G}_m^{\geq \mu}$  and  $\lambda(G') > \lambda(G)$ .

In fact,  $\mu(G') = \mu(G)$  and  $m(G') = \mu(G') + 3 = m(G)$ . Hence,  $G'$  is in  $\mathcal{G}_m^{\geq \mu}$ . Additionally, it is easy to see that  $\lambda(G') = \lambda(F_{1,2,0})$ . By a direct calculation, we have

$$\Psi_{F_{1,2,0}}(x) = (x - \alpha)(x - 3\alpha + 1)[x^3 - (6\alpha + 1)x^2 + (5\alpha^2 + 13\alpha - 4)x - 10\alpha^2 + 2].$$

Hence, for  $\alpha \in [\frac{1}{2}, 1)$ , one has

$$\begin{aligned} \Psi_{F_{1,2,0}}\left(\alpha + 1 + \sqrt{\frac{5}{4}}\right) &= -\frac{1}{8}\left(1 + \sqrt{\frac{5}{4}}\right)\left(2 - 2\alpha + \sqrt{\frac{5}{4}}\right)\left((16 + 16\sqrt{5})\alpha^2\right. \\ &\quad \left. - (2 + 20\sqrt{5})\alpha + 7\sqrt{5} - 4\right) < 0, \end{aligned}$$

and so

$$\lambda(G') = \lambda(F_{1,2,0}) > \alpha + 1 + \sqrt{\frac{5}{4}} \geq \alpha + 1 + \sqrt{\alpha^2 - 2\alpha + 2} = \lambda(H_2) \geq \lambda(G),$$

a contradiction.

**Subcase 2.2.**  $m(G) = \mu(G) + 4$ . Consider the graph  $G'' = F_{1,3,0} \cup (\mu - 2)K_2$ . Evidently,  $\mu(G'') = \mu(G)$  and  $m(G'') = \mu(G'') + 4 = m(G)$ . Hence,  $G'' \in \mathcal{G}_m^{\geq \mu}$ . Since  $K_{1,5}$  is a proper subgraph of  $F_{1,3,0}$ , we have, for  $\alpha \in [\frac{1}{2}, 1)$ ,

$$(10) \quad \lambda(G) \geq \lambda(G'') = \lambda(F_{1,3,0}) > \lambda(K_{1,5}) = 3\alpha + \sqrt{9\alpha^2 - 10\alpha + 5} \geq 3.$$

If  $K_4 \subseteq G$ , then  $G$  is isomorphic to  $K_4$  with possibly some isolated edges and isolated vertices. However,  $\lambda(G) = \lambda(K_4) = 3$ , which contradicts that  $\lambda(G) > 3$ . Thus,  $K_4 \not\subseteq G$ . Note that  $E_2 \neq \emptyset$ . Hence, by Lemma 3.4, one has  $H_1 \subseteq G$  or  $H_2 \subseteq G$ .

We proceed by considering the following two subcases to prove that  $G \cong H_3 \cup aK_2 \cup bK_1$  or  $G \cong H_4 \cup aK_2 \cup bK_1$ , where  $H_3$  is obtained from  $H_1$  by adding one pendant edge to a 3 degree vertex of  $H_1$ , and  $H_4$  is obtained from  $H_2$  by adding an edge to connect two vertices of distance 2 in  $H_2$ .

- $H_1 \subseteq G$ . Consider an edge  $uv \in E(G) \setminus (E(H_1) \cup M^*)$ . By the proof of Lemma 3.4 and  $K_4 \not\subseteq G$ , we get  $G[v_1, u_1, v_2, u_2] \cong H_1$  and  $u_1u_2 \notin E(G)$ . So,  $uv \neq u_1u_2$ . Then we have  $\{u, v\} \not\subseteq N_G(v_1)$ . By Lemma 3.4, the edge  $uv$  is incident to  $v_1$ . Without loss of generality, assume that  $u = v_1$ . Suppose that  $v$  is saturated by an edge, say  $u_jv_j$ , in  $M^*$  for some  $j \geq 3$ . Let  $H = G[\{u_1, v_1, u_j, v_j\}]$ . Since  $v_1v \in E(H) \setminus \{u_1v_1, u_jv_j\}$ , we have  $H \not\cong 2K_2$ . Note that  $K_4 \not\subseteq G$ . Hence, we get  $H \not\cong K_4$ . By Lemma 3.3, we have  $x_{u_1} < x_{v_j}$ , and so  $x_{v_j} > 0$ . Together with Lemma 3.1, one obtains  $\lambda(G - v_2u_1 + v_2v_j) > \lambda(G)$ . Note that  $G - v_2u_1 + v_2v_j \in \mathcal{G}_m^{\geq \mu}$ . Hence we obtain a contradiction. Thus  $v \notin V^*$  and  $v_1v$  is a pendant edge. Therefore,  $G$  is isomorphic to  $H_3$  with possibly some isolated edges and isolated vertices.

- $H_2 \subseteq G$ . By the proof of Lemma 3.4, we have  $v_1v_2, v_2v_3, v_1v_3 \in E(H_2)$ . Consider an edge  $uv \in E(G) \setminus (E(H_2) \cup M^*)$ . Then  $u, v \in V^*$ . Otherwise, without loss of generality, assume that  $v \notin V^*$ . By Lemma 3.2, we have  $x_v \leq x_{u_2}$ . Together with  $x_u \leq x_{v_1}$  and Lemma 3.1, we have  $\lambda(G - uv + v_1u_2) > \lambda(G)$ . As  $G - uv + v_1u_2$  is in  $\mathcal{G}_m^{\geq \mu}$ , we obtain a contradiction. If  $u$  is saturated by an edge, say  $u_jv_j$ , in  $M^*$  for some  $j \geq 4$ , then we get  $\{u, v\} \not\subseteq N_G(v_1)$ . By Lemma 3.4, the edge  $uv$  is incident to  $v_1$  and so  $v = v_1$ . Therefore,  $G[\{u_2, v_2, u_j, v_j\}] \cong 2K_2$ . By Lemma 3.3, we get  $x_{u_2} \geq x_u$ . By Lemma 3.1, one has  $\lambda(G - uv_1 + u_2v_1) > \lambda(G)$ . Together with  $G - uv_1 + u_2v_1 \in \mathcal{G}_m^{\geq \mu}$ , we obtain a contradiction. So,  $u \in \{u_1, u_2, u_3, v_1, v_2, v_3\}$ . Similarly, we have  $v \in \{u_1, u_2, u_3, v_1, v_2, v_3\}$ . Since  $v_1v_2, v_2v_3, v_1v_3 \in E(H_2)$ , we have  $uv \notin \{v_iv_j \mid 1 \leq i < j \leq 3\}$ . Recall that either  $uv$  is incident to  $v_1$  or  $\{u, v\} \subseteq N_G(v_1)$ , we get  $uv \notin \{u_iv_j \mid 1 \leq i < j \leq 3\}$ . It follows that  $u \in \{u_1, u_2, u_3\}$  and  $v \in \{v_1, v_2, v_3\}$ . Thus,  $G$  is isomorphic to  $H_4$  with possibly some isolated edges and isolated vertices.

Clearly,  $H_3 \subseteq H_4$ , and so  $\lambda(H_3) < \lambda(H_4)$ . By calculations, the characteristic polynomial of  $H_4$  is

$$\Psi_{H_4}(x) = x^6 - 14\alpha x^5 + l_3(\alpha)x^4 + l_4(\alpha)x^3 + l_5(\alpha)x^2 + l_6(\alpha)x + l_7(\alpha),$$

where

$$\begin{aligned} l_3(\alpha) &= 71\alpha^2 + 14\alpha - 7, \\ l_4(\alpha) &= -(158\alpha^3 + 128\alpha^2 - 70\alpha + 4), \\ l_5(\alpha) &= 149\alpha^4 + 366\alpha^3 - 186\alpha^2 - 6\alpha + 6, \\ l_6(\alpha) &= -(48\alpha^5 + 366\alpha^4 - 108\alpha^3 - 92\alpha^2 + 34\alpha - 2), \\ l_7(\alpha) &= 112\alpha^5 + 12\alpha^4 - 70\alpha^3 + 15\alpha^2 + 4\alpha - 1. \end{aligned}$$

For  $x \geq \lambda(K_{1,5}) = 3\alpha + \sqrt{9\alpha^2 - 10\alpha + 5}$ , we show that the  $i^{\text{th}}$  derivative function  $\Psi_{H_4}^{(i)}(x)$  of  $\Psi_{H_4}(x)$  is positive,  $i = 1, \dots, 5$ . In fact, by an elementary calculation, one may deduce that

$$\Psi_{H_4}^{(5)}(x) = 240(3x - 7\alpha) \geq 240 \left( 9\alpha + 3\sqrt{9\alpha^2 - 10\alpha + 5} - 7\alpha \right) > 0.$$

This shows that the fourth derivative function  $\Psi_{H_4}^{(4)}(x)$  is a monotonically increasing function in  $x$  for  $x \geq \lambda(K_{1,5})$ . Therefore,

$$\Psi_{H_4}^{(4)}(x) \geq \Psi_{H_4}^{(4)}(\lambda(K_{1,5})) = 24 \left( 20\alpha\sqrt{9\alpha^2 - 10\alpha + 5} + 131\alpha^2 - 136\alpha + 68 \right) > 0.$$

This implies that the third derivative function  $\Psi_{H_4}^{(3)}(x)$  is a monotonically increasing function in  $x$  for  $x \geq \lambda(K_{1,5})$ . So,

$$\begin{aligned} \Psi_{H_4}^{(3)}(x) &\geq \Psi_{H_4}^{(3)}(\lambda(K_{1,5})) \\ &= 12((82\alpha^2 - 72\alpha + 36)\sqrt{9\alpha^2 - 10\alpha + 5} + (167\alpha^2 - 180\alpha + 93)\alpha - 2) \\ &> 12((82\alpha^2 - 72\alpha + 36)\sqrt{9\alpha^2 - 10\alpha + 5} - 2) > 0. \end{aligned}$$

Hence, we obtain the second derivative function  $\Psi_{H_4}^{(2)}(x)$  is a monotonically increasing function in  $x$  for  $x \geq \lambda(K_{1,5})$ , and so

$$\begin{aligned} \Psi_{H_4}^{(2)}(x) &\geq \Psi_{H_4}^{(2)}(\lambda(K_{1,5})) \\ &= 2(((282\alpha^2 - 280\alpha + 158)\alpha - 12)\sqrt{9\alpha^2 - 10\alpha + 5} \\ &\quad + ((995\alpha^2 - 1734\alpha + 1578)\alpha - 702)\alpha + 171) \\ &> 2(-12\sqrt{5} - 114 + 171) > 0. \end{aligned}$$

Thus, the derivative function  $\Psi_{H_4}^{(1)}(x)$  is a monotonically increasing function in  $x$  for  $x \geq \lambda(K_{1,5})$ . Recall  $\alpha \in [\frac{1}{2}, 1)$ . So,

$$\begin{aligned} \Psi_{H_4}^{(1)}(x) &\geq \Psi_{H_4}^{(1)}(\lambda(K_{1,5})) \\ &= 2((((167\alpha^2 - 238\alpha + 190)\alpha - 62)\alpha + 11)\sqrt{9\alpha^2 - 10\alpha + 5} \\ &\quad + (((477\alpha^2 - 927\alpha + 979)\alpha - 570)\alpha + 206)\alpha - 29) \\ &> 2((105\alpha^2 - 62\alpha + 11)\sqrt{9\alpha^2 - 10\alpha + 5} + (528\alpha^2 - 570\alpha + 206)\alpha - 29) \end{aligned}$$

$$> 2 \left( 6\sqrt{2} + 52\alpha - 29 \right) > 0.$$

Therefore, we obtain that  $\Psi_{H_4}(x)$  is a monotonically increasing function in  $x$  for  $x \geq \lambda(K_{1,5})$ . On the other hand,

$$(11) \quad \Psi_{H_4}(x) \geq \Psi_{H_4}(\lambda(K_{1,5})) = 2l_8(\alpha)\sqrt{9\alpha^2 - 10\alpha + 5} + l_9(\alpha),$$

where

$$l_8(\alpha) = 63\alpha^5 - 107\alpha^4 + 115\alpha^3 - 74\alpha^2 + 36\alpha - 9,$$

$$l_9(\alpha) = 378\alpha^6 - 820\alpha^5 + 927\alpha^4 - 524\alpha^3 + 116\alpha^2 + 40\alpha - 21.$$

Clearly, both  $l_8(\alpha)$  and  $l_9(\alpha)$  are real functions in  $\alpha$ . By some calculations and  $\alpha \in [\frac{1}{2}, 1)$ , we obtain

$$(12) \quad l'_8(\alpha) = ((315\alpha^2 - 428\alpha + 345)\alpha - 148)\alpha + 36 > 199\alpha^2 - 148\alpha + 36 > 0,$$

$$(13) \quad l'''_9(\alpha) = 24[(1890\alpha^2 - 2050\alpha + 927)\alpha - 131] > 371\alpha - 131 > 0.$$

Hence, for  $\alpha \in [\frac{1}{2}, 1)$ , (12) gives us  $l_8(\alpha) \geq l_8(\frac{1}{2}) > 0$ , whereas (13) gives us  $l''_9(\alpha) \geq l''_9(\frac{1}{2}) > 0$ . Consequently,  $l'_9(\alpha) \geq l'_9(\frac{1}{2}) > 0$  by  $\alpha \in [\frac{1}{2}, 1)$ . Thus,  $l_9(\alpha) \geq l_9(\frac{1}{2}) > 0$  from  $\alpha \in [\frac{1}{2}, 1)$ . Hence, in view of (11), one has  $\Psi_{H_4}(x) \geq \Psi_{H_4}(\lambda(K_{1,5})) > 0$ . So,

$$\lambda(G) \leq \lambda(H_4) < 3\alpha + \sqrt{9\alpha^2 - 10\alpha + 5},$$

which contradicts (10). This completes the proof. □

#### 4. Proof of Theorem 1.1

In this section, we give the proof of Theorem 1.1, which identifies the graphs in  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius for  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ .

*Proof of Theorem 1.1.* Assume that  $G$  is in  $\mathcal{G}_m^{\geq \mu}$  ( $\mu \geq 2$ ) having the largest  $A_\alpha$ -spectral radius. Let  $\mathbf{x}$  be the principal eigenvector of  $A_\alpha(G)$  for  $\alpha \in [\frac{1}{2}, 1)$ . From Lemma 3.5,  $G \cong F_{r,s,t}$  ( $s \geq 1$ ) (see Figure 1) with  $b$  isolated edges and some isolated vertices. Let  $\Delta(G) = d_G(v_1)$  and let  $u_1v_1$  be a pendant edge. Then  $\mu(G) = r + t + b + 1$ . We proceed by showing three claims, as follows.

**Claim 1.**  $x_{v_1} = \max_{v \in V(G)} x_v$  and  $x_{v_1} > 0$ .

*Proof of Claim 1.* Note that  $u_1v_1$  is a pendant edge. If  $d_G(v_1) \leq 2$ , then  $F_{r,s,t}$  is a path of length at most three. Clearly,  $x_{v_1} = \max_{v \in V(G)} x_v$ . If  $d_G(v_1) \geq 3$ , one has  $\lambda(G) \geq 2$  by Lemma 2.7. Moreover, for any vertex  $v \in V(G) \setminus \{v_1\}$ ,  $d_G(v) \leq 2$ . Let  $x_{v_0} = \max_{v \in V(G) \setminus \{v_1\}} x_v$ . Then

$$\lambda(G)x_{v_0} = \alpha d_G(v_0)x_{v_0} + (1 - \alpha) \sum_{v \in N_G(v_0)} x_v \leq 2\alpha x_{v_0} + (1 - \alpha)(x_{v_0} + x_{v_1}).$$

By  $\lambda(G) \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ , we have  $x_{v_0} \leq \frac{(1-\alpha)x_{v_1}}{\lambda(G)-1-\alpha} \leq x_{v_1}$ . Therefore,  $x_{v_1} = \max_{v \in V(G)} x_v$ . Since  $\mathbf{x}$  is a nonnegative nonzero vector, we get  $x_{v_1} > 0$ . □

**Claim 2.**  $t \leq 1$ . Furthermore, if  $s \geq 2$ , then  $t = 0$  and  $b = 0$ .

*Proof of Claim 2.* Suppose that  $t \geq 2$ . Then let  $v_1v_iu_i$  and  $v_1v_ju_j$  be two pendant paths of length 2. Consider a new graph  $G' = G - u_iv_i - u_jv_j + u_iu_j + v_iv_j$ . Clearly,  $\mu(G') = \mu(G)$ . So,  $G' \in \mathcal{G}_m^{\geq \mu}$ . By a similar discussion as that of (3), one has

$$\lambda(G') - \lambda(G) \geq 2(1 - \alpha)(x_{v_j} - x_{u_i})(x_{v_i} - x_{u_j}),$$

in which  $x_{v_i} = x_{v_j}$ ,  $x_{u_i} = x_{u_j}$ . By

$$(14) \quad \lambda(G)x_{u_j} = \alpha x_{u_j} + (1 - \alpha)x_{v_j},$$

we have

$$x_{u_i} = x_{u_j} = \frac{1 - \alpha}{\lambda(G) - \alpha}x_{v_j} < x_{v_j} = x_{v_i}$$

for  $\lambda(G) \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ . So,  $x_{v_j} - x_{u_i} > 0$ ,  $x_{v_i} - x_{u_j} > 0$ . We have  $\lambda(G') > \lambda(G)$ , a contradiction. Hence,  $t \leq 1$ .

Next, we consider the case of  $s \geq 2$ . Suppose  $t = 1$ . Then let  $v_1v_ju_j$  be a pendant path of length 2. Similar to (14), by Claim 1, we have

$$\frac{\lambda(G) - \alpha}{1 - \alpha}x_{u_1} = x_{v_1} \geq x_{v_j} = \frac{\lambda(G) - \alpha}{1 - \alpha}x_{u_j}.$$

So,  $x_{u_1} \geq x_{u_j}$  and  $x_{u_1} = \frac{(1-\alpha)x_{v_1}}{\lambda(G)-\alpha} > 0$ . By Lemma 3.1, one has  $\lambda(G - v_ju_j + v_ju_1) > \lambda(G)$ . Clearly,  $\mu(G - v_ju_j + v_ju_1) = \mu(G)$ . Hence,  $G - v_ju_j + v_ju_1 \in \mathcal{G}_m^{\geq \mu}$ . We get a contradiction to the maximality of  $\lambda(G)$ . Thereby,  $t = 0$ .

Suppose that  $b \geq 1$  and let  $v_iu_i$  be an isolated edge. Then

$$x_{u_1} = \frac{1 - \alpha}{\lambda(G) - \alpha}x_{v_1} \geq \frac{1 - \alpha}{\lambda(G) - \alpha}x_{v_i} = x_{u_i}.$$

By Lemma 3.1, we obtain  $\lambda(G - v_iu_i + v_iu_1) > \lambda(G)$ . From  $\mu(G - v_iu_i + v_iu_1) = \mu(G)$ , we have  $G - v_iu_i + v_iu_1 \in \mathcal{G}_m^{\geq \mu}$ . Then we get a contradiction. So,  $b = 0$ . The claim holds.  $\square$

Note that  $G$  is in  $\mathcal{G}_m^{\geq \mu}$ . Hence,  $\mu(G) \geq \mu$ . In fact, we have the following claim.

**Claim 3.**  $\mu(G) = \mu$ .

*Proof of Claim 3.* Suppose that  $\mu(G) \geq \mu + 1$ . It suffices to show that there exists some graph  $G''$  in  $\mathcal{G}_m^{\geq \mu}$  such that  $\lambda(G'') > \lambda(G)$ . If  $t \geq 1$ , let  $G'' = G - uv + v_1v$ , where  $v_1uv$  is a pendant path of length 2 and  $v$  is a pendant vertex. Then  $\mu(G'') = \mu(G) - 1 \geq \mu$ . So,  $G'' \in \mathcal{G}_m^{\geq \mu}$ . By  $x_u \leq x_{v_1}$  and Lemma 3.1, we get  $\lambda(G'') > \lambda(G)$ , a contradiction. Hence,  $t = 0$ .

If  $b \geq 1$ , let  $G'' = G - uv + v_1v$ , where  $uv$  is an isolated edge. Then  $\mu(G'') = \mu(G) - 1 \geq \mu$ . That is,  $G'' \in \mathcal{G}_m^{\geq \mu}$ . By a similar discussion as above,  $\lambda(G'') > \lambda(G)$ , a contradiction. We get  $b = 0$ .

By  $t = b = 0$ , we have  $\mu(G) = r + 1$ . Since  $\mu(G) \geq \mu + 1$  and  $\mu \geq 2$ , we obtain  $r \geq 2$ . Assume that  $\{v_1, u_2, v_2\}$  induces a triangle in  $G$ . Let  $G'' =$



$G - u_2v_2 + v_1w$ , where  $w$  is an isolated vertex. Then  $\mu(G'') = \mu(G) - 1 \geq \mu$  and so  $G'' \in \mathcal{G}_m^{\geq \mu}$ . By a simple calculation,  $x_{u_2} = x_{v_2} = \frac{(1-\alpha)x_{v_1}}{\lambda(G)-1-\alpha}$  and  $x_w = 0$ . We have

$$\begin{aligned} \lambda(G'') - \lambda(G) &\geq \mathbf{x}^T (A_\alpha(G'') - A_\alpha(G)) \mathbf{x} \\ &= \alpha(x_{v_1}^2 + x_w^2 - x_{v_2}^2 - x_{u_2}^2) + 2(1-\alpha)(x_{v_1}x_w - x_{v_2}x_{u_2}) \\ &= \alpha x_{v_1}^2 - 2x_{v_2}^2 = \left( \alpha - \frac{2(1-\alpha)^2}{(\lambda(G)-1-\alpha)^2} \right) x_{v_1}^2 \\ &= \frac{\alpha\lambda(G)^2 - 2\alpha(\alpha+1)\lambda(G) + \alpha^3 + 5\alpha - 2}{(\lambda(G)-1-\alpha)^2} x_{v_1}^2. \end{aligned}$$

Recall  $r \geq 2$ , we have  $d_G(v_1) \geq 5$ . Therefore,  $K_{1,5}$  is a proper subgraph of  $G$ . Consequently, by Lemma 2.3,

$$(15) \quad \lambda(G) > \lambda(K_{1,5}) = 3\alpha + \sqrt{9\alpha^2 - 10\alpha + 5}.$$

For  $\alpha \in [\frac{1}{2}, 1)$ ,  $\lambda(G) - 1 - \alpha > 0$ . By the maximality of  $\lambda(G)$ , we have

$$\alpha\lambda(G)^2 - 2\alpha(\alpha+1)\lambda(G) + \alpha^3 + 5\alpha - 2 \leq 0.$$

Thereby,  $\lambda(G) \leq (1+\alpha) + (1-\alpha)\sqrt{\frac{2}{\alpha}}$ . Note that  $2\alpha > 0$ ,  $(1-\alpha)\sqrt{\frac{2}{\alpha}} > 0$ .

Recall  $\alpha \in [\frac{1}{2}, 1)$ . Then,

$$(2\alpha)^2 - \left( (1-\alpha)\sqrt{\frac{2}{\alpha}} \right)^2 = \frac{2(\alpha^2+1)(2\alpha-1)}{\alpha} \geq 0.$$

Hence, we get  $2\alpha - (1-\alpha)\sqrt{\frac{2}{\alpha}} \geq 0$ . Then,

$$\begin{aligned} \lambda(K_{1,5}) - \lambda(G) &\geq 3\alpha + \sqrt{9\alpha^2 - 10\alpha + 5} - (1+\alpha) - (1-\alpha)\sqrt{\frac{2}{\alpha}} \\ &= \sqrt{9\alpha^2 - 10\alpha + 5} - 1 + \left( 2\alpha - (1-\alpha)\sqrt{\frac{2}{\alpha}} \right) \\ &\geq \sqrt{9\alpha^2 - 10\alpha + 5} - 1 \\ &> 0, \end{aligned}$$

i.e.,  $\lambda(K_{1,5}) > \lambda(G)$ . That contradicts (15). Hence,  $\mu(G) = \mu$ . □

By Claim 3, we obtain that  $G$  is also in  $\mathcal{G}_m^\mu$  having the largest  $A_\alpha$ -spectral radius, where  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ . Then  $\mu = 1 + r + t + b$ . We complete our proof by considering the following two possible cases.

**Case 1.**  $m \geq 3\mu - 1$ . By  $m = 3r + s + 2t + b$  and  $\mu = 1 + r + t + b$ , we have

$$t + 2b + 2 - s \leq 0.$$

So,  $s \geq 2$ . By Claim 2, we have  $t = b = 0$ . Then  $r = \mu - 1$ . Hence,  $s = m - 3r = m - 3\mu + 3$  and we get (i).

**Case 2.**  $m \leq 3\mu - 2$ . By  $m = 3r + s + 2t + b$  and  $\mu = 1 + r + t + b$ , we have

$$t + 2b + 1 - s \geq 0.$$

Suppose that  $s \geq 2$ . By Claim 2, we have  $t = b = 0$ . Then  $t + 2b + 1 - s = 1 - s < 0$ , a contradiction. Hence,  $s = 1$  and so  $m - \mu = t + 2r$ . By Claim 2, we obtain  $t \in \{0, 1\}$ . If  $m - \mu$  is odd, we get  $t$  is odd, i.e.,  $t = 1$ . Then  $r = \frac{m-\mu-1}{2}$  and  $b = \frac{-m+3\mu-3}{2}$ . If  $m - \mu$  is even, we get  $t = 0$  and so  $r = \frac{m-\mu}{2}$ ,  $b = \frac{-m+3\mu-2}{2}$ . Therefore, (ii) and (iii) hold.  $\square$

## 5. Concluding remarks

In this paper we characterized the graphs among  $\mathcal{G}_m^{\geq \mu}$  having the largest  $A_\alpha$ -spectral radius. In fact, the matching number of the corresponding extremal graph is  $\mu$ . Hence, the following result is a direct consequence of Theorem 1.1.

**Corollary 5.1.** *Let  $G$  be in  $\mathcal{G}_m^\mu$  having the largest  $A_\alpha$ -spectral radius, where  $\mu \geq 2$  and  $\alpha \in [\frac{1}{2}, 1)$ . Then  $G$  is isomorphic to  $F_{r,s,t}$  ( $s \geq 1$ ) with possibly some isolated edges and isolated vertices. Moreover,*

- (i) if  $m \geq 3\mu - 1$ , then  $r = \mu - 1$ ,  $s = m - 3\mu + 3$  and  $t = 0$ ;
- (ii) if  $m \leq 3\mu - 2$  and  $m - \mu$  is even, then  $r = \frac{m-\mu}{2}$ ,  $s = 1$  and  $t = 0$ ;
- (iii) if  $m \leq 3\mu - 2$  and  $m - \mu$  is odd, then  $r = \frac{m-\mu-1}{2}$  and  $s = t = 1$ .

In view of (1), the signless Laplacian matrix  $Q$  is equal to  $2A_{\frac{1}{2}}(G)$ . Hence, the following result is also a direct consequence of Theorem 1.1.

**Corollary 5.2.** *Let  $G$  be in  $\mathcal{G}_m^{\geq \mu}$  ( $\mu \geq 2$ ) having the largest  $Q$ -spectral radius. Then  $G$  is isomorphic to  $F_{r,s,t}$  ( $s \geq 1$ ) with possibly some isolated edges and isolated vertices, and the matching number of  $G$  is  $\mu$ . Moreover,*

- (i) if  $m \geq 3\mu - 1$ , then  $r = \mu - 1$ ,  $s = m - 3\mu + 3$  and  $t = 0$ ;
- (ii) if  $m \leq 3\mu - 2$  and  $m - \mu$  is even, then  $r = \frac{m-\mu}{2}$ ,  $s = 1$  and  $t = 0$ ;
- (iii) if  $m \leq 3\mu - 2$  and  $m - \mu$  is odd, then  $r = \frac{m-\mu-1}{2}$  and  $s = t = 1$ .

By Corollary 5.2, we may deduce the main result [39, Theorem 1.1], which characterizes the graphs among  $\mathcal{G}_m^\mu$  ( $\mu \geq 2$ ) having the largest  $Q$ -spectral radius.

In fact, it is also interesting to determine the graphs among  $\mathcal{G}_m^{\geq \mu}$  ( $\mu \geq 2$ ) having the second largest  $A_\alpha$ -spectral radius. We will do it in the near future.

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