An A_α-Spectral Version of the Bhattacharya-Friedland-Peled Conjecture

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Abstract

In 1985, Brualdi and Hoffman posed the following conjecture: Let G be an n-vertex graph of size m, where $0 \leqslant m \leqslant \binom{n}{2}$. If $m = \binom{a}{2} + b$ with $0 \leqslant b < a$, then $G \cong (K_b \vee (K_{a-b} \cup K_1)) \cup (n-a-1)K_1$ is the unique graph having the largest spectral radius. This conjecture was completely resolved by Rowlinson (1988). In 2008, Bhattacharya, Friedland and Peled posed the bipartite version of Brualdi-Hoffman conjecture. Here, we consider an A_α-spectral extremal question, which may be seen as an A_α-spectral version of the Bhattacharya-Friedland-Peled conjecture: For fixed $\alpha \in [0, 1)$, which graph attains the maximum A_α-index over all bipartite graphs with n vertices and m edges? When $\frac{1}{2} \leqslant \alpha < 1$, we prove that for every pair of positive integers n, m, if $m = k(n-k)$, where k is a positive integer with $k \neq 1, n-1$, then the complete bipartite graph $K_{k,n-k}$ is the unique graph that maximizes the A_α-index over all bipartite graphs with n vertices and m edges; if $n \leqslant m \leqslant 2n-5$, then $K^m_{2,n-2}$, the graph obtained from the complete bipartite graph $K_{2,n-2}$ by deleting $2n-4-m$ edges which are incident on a common vertex of degree $n-2$, is the unique graph that maximizes the A_α-index over all bipartite graphs with n vertices and m edges; if $2n-3 \leqslant m \leqslant 2\sqrt{2}(n-4)$, then $K^m_{3,n-3}$, the graph obtained from the complete bipartite graph $K_{3,n-3}$ by deleting $3n-9-m$ edges which are incident on a common vertex of degree $n-3$, is the unique graph that maximizes the A_α-index over all bipartite graphs with n vertices and m edges. It improves some known ones of Zhang and Li (2017) and partially answers some questions posed by Zhai, Lin and Zhao (2022).

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1 Introduction

In this paper, we consider only simple and finite graphs. Unless otherwise stated, we follow the traditional notation and terminology (see, for instance, West [28], Godsil and Royle [14]).

Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. We use $n := |V(G)|$ and $m := |E(G)|$ to denote the *order* and the *size* of G, respectively. We say that two vertices u and v are *adjacent* (or *neighbours*) if they are joined by an edge and we write it as $u \sim v$. If $u \sim v$, then let $G - uv$ denote the graph obtained from G by deleting edge uv (this notation is naturally extended if more than one edge is deleted). Similarly, if $u \nsim v$, then let $G + uv$ denote the graph obtained from G by adding an edge joining u and v.

As usual, let $K_{a,b}$ be the complete bipartite graph with partite sets of sizes a and b. The *set of neighbours* of a vertex v (in a graph G) is denoted by $N_G(v)$. The *degree* $d_G(v)$ of v in a graph G is the number of edges incident with v, and it is equal to the size of $N_G(v)$ if G is simple. The *maximum degree* of G is denoted by $\Delta(G)$. A vertex $v \in V(G)$ is said to be a leaf of G if $d_G(v) = 1$.

Let G be a graph of order n, the *adjacency matrix* of G is defined as the $n \times n$ $(0, 1)$-matrix $A(G) = (a_{ij})$ with $a_{ij} = 1$ if and only if $v_i \sim v_j$. The *degree diagonal matrix* of G is defined as the $n \times n$ diagonal matrix $D(G) = \mathrm{diag}(d_G(v_1), \ldots, d_G(v_n))$. The *signless Laplacian matrix* of G is defined as $Q(G) = D(G)+A(G)$, whereas the *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$. The largest eigenvalue of $A(G)$ (resp. $Q(G), L(G)$) is called the *index* (resp. *Q-index*, *L-index*) of G, denoted by $\rho(G)$ (resp. $q(G)$, $\mu(G)$) as usual. It is known that $\mu(G) = q(G)$ if G is a bipartite graph.

In 2017, Nikiforov [22] proposed the A_α-*matrix* of G, which is a convex linear combination of $D(G)$ and $A(G)$, i.e.,

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

Note that $A_\alpha(G)$ is real symmetric, its eigenvalues are real. The largest eigenvalue of $A_\alpha(G)$ is called the A_α-*index* of G, denoted by $\lambda_\alpha(G)$ as usual. It is obvious that $A_0(G) = A(G)$, $A_{\frac{1}{2}}(G) = \frac{1}{2}Q(G)$ and $A_1(G) = D(G)$. Therefore, $\lambda_0(G) = \rho(G)$, $\lambda_{\frac{1}{2}}(G) = \frac{1}{2}q(G)$. If G is connected and $\alpha \neq 1$, then $A_\alpha(G)$ is non-negative and irreducible; by the Perron-Frobenius theory, there exists a unique positive unit eigenvector of $A_\alpha(G)$ corresponding to $\lambda_\alpha(G)$, we call this vector the *Perron vector* of $A_\alpha(G)$.

Let G and H be two graphs, define $G \cup H$ to be their disjoint union, and $G \vee H$ to be their *join*. Denote by $C_n^m = (K_b \vee (K_{a-b} \cup K_1)) \cup (n - a - 1)K_1$, where $m = \binom{a}{2} + b$ and $0 \leqslant b < a$. Let $\mathbb{G}(n, m)$ be the set of all n-vertex graphs of size m. In 1985, Brualdi and Hoffman posed the following conjecture.

Conjecture 1 ([3])**.** Let $G \in \mathbb{G}(n, m)$, where $0 \leqslant m \leqslant \binom{n}{2}$. If $m = \binom{a}{2} + b$ with $0 \leqslant b < a$, then $\rho(G) \leqslant \rho(C_n^m)$. Equality holds if and only if $G \cong C_n^m$.

Conjecture 1, confirmed for some special cases by Brualdi and Hoffman [3], Friedland [13] and Stanley [27], was completely resolved by Rowlinson [26].

Let $\mathcal{G}(n,m)$ be the subset of $\mathbb{G}(n,m)$ consisting of all connected graphs. In mathematical literature many works focused on identifying the graphs among $\mathcal{G}(n,m)$ with the maximum index. These nice results can be found in [1, 4, 10, 21, 24].

In 2010, Chang and Tam [7] determined the graphs with maximum Q-index over $\mathbb{G}(n,m)$ for $m \leqslant n+3$; and then Chang and Tam [5] determined the graphs with maximum Q-index over $\mathcal{G}(n,m)$ for $n-1 \leqslant m \leqslant 2n-3$. Based on the results in [7, 5], Zhai, Lin and Zhao [29] determined the graphs with maximum Q-index over $\mathbb{G}(n,m)$ for $n+4 \leqslant m \leqslant 2n-3$.

Recently, Li et al. [18] determined the graphs with maximum A_α-index over $\mathcal{G}(n,m)$ for $n-1 \leqslant m \leqslant 2n-3$ and $\frac{1}{2} \leqslant \alpha < 1$, extending and also providing an alternative proof for the results of Chang and Tam [5]. And then, based on the results in [18], Chang and Tam [6] determined the graphs with maximum A_α-index over $\mathbb{G}(n,m)$ for $m \leqslant 2n-3$ and $\frac{1}{2} \leqslant \alpha < 1$, extending the results of Chang and Tam [7] and Zhai, Lin and Zhao [29].

Let $\mathbb{B}(p,q,m)$ be the set of all bipartite graphs with size m and the sizes of partite sets being p and q, respectively. As an analogue of Conjecture 1, Bhattacharya, Friedland and Peled [2] posed the following conjecture.

Conjecture 2 ([2])**.** For $2 \leqslant p \leqslant q$ and $1 < m < pq$, a graph that solves $\max_{G\in\mathbb{B}(p,q,m)} \rho(G)$ is the union of $G^\star$ with possible some isolated vertices, where $G^\star$ is obtained from a complete bipartite graph by adding one vertex and a corresponding number of edges.

Conjecture 2 was confirmed for some special cases by Bhattacharya, Friedland and Peled [2], Chen et al. [8], Das et al. [11] and Liu and Weng [20]. Recently, Cheng, Liu and Weng [9] provided some counterexamples of Conjecture 2.

For $2 \leqslant p \leqslant q$ and $pq-p < m < pq$, let ${}^mK_{p,q}$ denote the bipartite graph obtained from $K_{p,q}$ by deleting $pq-m$ edges which are incident on a common vertex in the partite set of size q. Chen et al. [8] refined Conjecture 2 under the assumption that $m > pq-p$ as follows, which was confirmed by Liu and Weng [20].

Conjecture 3 ([8])**.** Let $G \in \mathbb{B}(p,q,m)$, where $2 \leqslant p \leqslant q$, $pq-p < m < pq$. Then $\rho(G) \leqslant \rho({}^mK_{p,q})$.

Motivated by Conjecture 2, Zhai, Lin and Zhao [29] asked the following question.

Question 4 ([29])**.** For $2 \leqslant p \leqslant q$ and $0 \leqslant m \leqslant pq$, what is the maximum Q-index and the corresponding extremal graphs over all graphs in $\mathbb{B}(p,q,m)$?

Zhai, Lin and Zhao [29, Theorem 1.2] answered Question 4 for $0 \leqslant m \leqslant 2q$; they found the extremal graphs in [29, Theorem 1.2] are connected only when $m = p+q-1$ or $p = 2$. Let $\mathcal{B}(p,q,m)$ be the subset of $\mathbb{B}(p,q,m)$ consisting of all connected bipartite graphs.

Question 5 ([29])**.** For $2 \leqslant p \leqslant q$ and $p+q-1 \leqslant m \leqslant pq$, what is the maximum Q-index and the corresponding extremal graphs over all graphs in $\mathcal{B}(p,q,m)$?

Zhai, Lin and Zhao showed the extremal graphs in Question 5 are double nested graphs (see Section 2); they [29, Theorem 4.1] answered Question 5 for $p+q-1 \leqslant m \leqslant 2q+p-2$.

Let $\mathbb{B}(n,m)$ be the set of all n-vertex bipartite graphs with size m, and let $\mathcal{B}(n,m)$ be the subset of $\mathbb{B}(n,m)$ consisting of all connected bipartite graphs. For $n \leqslant m \leqslant 2n-5$, Petrović and Simić [25] determined the maximum index and the corresponding extremal graphs over all graphs in $\mathcal{B}(n,m)$. For $n \leqslant m \leqslant 2n-5$ and $m = k(n-k)$, where k is an integer with $2 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$, Zhang and Li [30] determined the maximum L-index (and so the maximum Q-index) and the corresponding extremal graphs over all graphs in $\mathcal{B}(n,m)$.

In this paper, we mainly consider a question of maximizing A_α-index over $\mathbb{B}(n,m)$.

Question 6. For $1 \leqslant m \leqslant \lfloor \frac{n}{2} \rfloor \lceil \frac{n}{2} \rceil$ and $0 \leqslant \alpha < 1$, what is the maximum A_α-index and the corresponding extremal graphs over all graphs in $\mathbb{B}(n,m)$?

For $1 \leqslant p \leqslant q$ and $pq - q < m \leqslant pq$, let $K_{p,q}^m$ denote the bipartite graph obtained from $K_{p,q}$ by deleting $pq-m$ edges which are incident on a common vertex in the partite set of size p. For $\frac{1}{2} \leqslant \alpha < 1$, Feng and Wei [12], Li and Qin [16], Chang and Tam [6] determined all the graphs with maximum A_α-index over all the graphs with size m. As a product, we can obtain the following result quickly, which gives an answer to Question 6 for $1 \leqslant m \leqslant n-1$ and $\frac{1}{2} \leqslant \alpha < 1$.

Corollary 7. *Let $\frac{1}{2} \leqslant \alpha < 1$ and $1 \leqslant m \leqslant n-1$ be given. If $G \in \mathbb{B}(n,m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{1,n-1}^m)$, with equality if and only if $G \cong K_{1,n-1}^m$.*

Our first main result gives an answer to Question 6 for $m = k(n-k)$ and $\frac{1}{2} \leqslant \alpha < 1$, where k is an integer with $2 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$.

Theorem 8. *Let $\frac{1}{2} \leqslant \alpha < 1$ and $m = k(n-k)$ be given, where k is an integer with $2 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$. If $G \in \mathbb{B}(n,m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{k,n-k})$, with equality if and only if $G \cong K_{k,n-k}$.*

Our second main result gives an answer to Question 6 for $n \leqslant m \leqslant 2n-5$ and $\frac{1}{2} \leqslant \alpha < 1$.

Theorem 9. *Let $\frac{1}{2} \leqslant \alpha < 1$ and $n \leqslant m \leqslant 2n-5$ be given. If $G \in \mathbb{B}(n,m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{2,n-2}^m)$, with equality if and only if $G \cong K_{2,n-2}^m$.*

Our last main result gives an answer to Question 6 for $2n-3 \leqslant m \leqslant 2\sqrt{2}(n-4)$ and $\frac{1}{2} \leqslant \alpha < 1$.

Theorem 10. *Let $\frac{1}{2} \leqslant \alpha < 1$ and $2n-3 \leqslant m \leqslant 2\sqrt{2}(n-4)$ be given. If $G \in \mathbb{B}(n,m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{3,n-3}^m)$, with equality if and only if $G \cong K_{3,n-3}^m$.*

The remainder of this paper is organized as follows. In Section 2, we give some necessary preliminaries. In Section 3, we give the proofs of Theorems 8 and 9. The proof of Theorem 10 is presented in Section 4. Some concluding remarks are given in the last section.

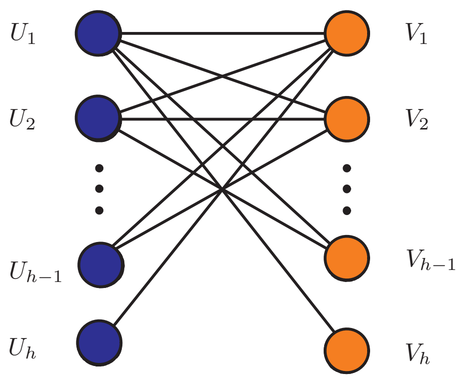

Figure 1: The structure of a double nested graph.

2 Preliminaries

Let G be a connected bipartite graph with partite sets U and V. The graph G is said to be a *double nested graph* (also known as a *chain graph* or a *difference graph*, see [2, Section 2]) if there exist partitions

$$U = U_1 \cup U_2 \cup \cdots \cup U_h \text{ and } V = V_1 \cup V_2 \cup \cdots \cup V_h,$$

such that all vertices in U_i are adjacent to all vertices in $\bigcup_{j=1}^{h+1-i} V_j$ for $1 \leqslant i \leqslant h$ (see Figure 1).

Lemma 11 ([17]). *Let G be a graph in $\mathcal{B}(n,m)$ with maximum A_α-index for some $\alpha \in [0,1)$. Then G is a double nested graph with all leaves being adjacent to a common vertex.*

By Lemma 11, the following corollary is clear.

Corollary 12. *Let G be a graph in $\mathbb{B}(p,q,m)$ with maximum A_α-index for some $\alpha \in [0,1)$. Then G is a double nested graph, possibly with some isolated vertices.*

Let M be an $n \times n$ real symmetric matrix and let $\pi : W = W_1 \cup \cdots \cup W_\ell$ be a partition of $W = \{1, \ldots, n\}$. Then corresponding to the partition π, M can be partitioned into the following block matrix:

$$M = \begin{pmatrix} M_{11} & \cdots & M_{1\ell} \\ \vdots & \ddots & \vdots \\ M_{\ell 1} & \cdots & M_{\ell\ell} \end{pmatrix}.$$

The *quotient matrix* of M with respect to π is the matrix $B = (b_{ij})_{\ell\times\ell}$, where b_{ij} is the average row sum of the block M_{ij}. The partition π is said to be *equitable* if each block M_{ij} has constant row sums for $i, j \in \{1, \ldots, \ell\}$.

Lemma 13 ([15]). *Let M be a real symmetric matrix and let B be a quotient matrix of M with respect to an equitable partition. Then the eigenvalues of B are also the eigenvalues of M. Furthermore, if M is nonnegative and irreducible, then $\lambda(M) = \lambda(B)$, where $\lambda(M)$ and $\lambda(B)$ are the largest eigenvalues of M and B, respectively.*

Lemma 14 ([19])**.** *Let G be a connected graph and let $\mathbf{x}$ be a Perron vector of $A_\alpha(G)$. Then, for each $v \in V(G)$, one has*

$$\lambda_\alpha(G)\mathbf{x}_v = \alpha d_G(v)\mathbf{x}_v + (1-\alpha)\sum_{u\sim v}\mathbf{x}_u, \tag{1}$$

$$\lambda_\alpha^2(G)\mathbf{x}_v = \alpha d_G(v)\lambda_\alpha(G)\mathbf{x}_v + \alpha(1-\alpha)\sum_{u\sim v} d_G(u)\mathbf{x}_u + (1-\alpha)^2\sum_{w\sim v}\sum_{u\sim w}\mathbf{x}_u. \tag{2}$$

Lemma 15 ([16])**.** *Let G and H be two connected graphs of order n, and let $\mathbf{x}$ and $\mathbf{y}$ be the Perron vectors of G and H, respectively. Then*

$$\mathbf{x}^T A_\alpha(G)\mathbf{y} = \alpha \sum_{uv\in E(G)}(\mathbf{x}_u\mathbf{y}_u + \mathbf{x}_v\mathbf{y}_v) + (1-\alpha)\sum_{uv\in E(G)}(\mathbf{x}_u\mathbf{y}_v + \mathbf{x}_v\mathbf{y}_u)$$

and

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

Lemma 16 ([23])**.** *Let $0 \leqslant \alpha < 1$, and let G be a connected graph with $u, v \in V(G)$. Assume that $\mathbf{x}$ is the Perron vector of $A_\alpha(G)$, and $S \subseteq N_G(v)\backslash(N_G(u)\cup\{u\})$. Let $G' = G - \{vw : w \in S\} + \{uw : w \in S\}$. If $S \neq \emptyset$ and $\mathbf{x}_u \geqslant \mathbf{x}_v$, then $\lambda_\alpha(G') > \lambda_\alpha(G)$.*

Lemma 17 ([22, 17])**.** *Let G be a double nested graph of order n. For some $\alpha \in [0, 1)$, let $\mathbf{x}$ be the Perron vector of $A_\alpha(G)$. Assume that u and v are two vertices in the same partite set of G.*

(i) *If $d_G(u) = d_G(v)$, then $\mathbf{x}_u = \mathbf{x}_v$.*

(ii) *If $d_G(u) < d_G(v)$, then $\mathbf{x}_u < \mathbf{x}_v$.*

Lemma 18 ([22])**.** *Let G be a graph with no isolated vertices, then*

$$\lambda_\alpha(G) \leqslant \max_{v\in V(G)}\left\{\alpha d_G(v) + \frac{1-\alpha}{d_G(v)}\sum_{u\sim v} d_G(u)\right\}.$$

Lemma 19. *For $\frac{1}{2} \leqslant \alpha < 1$ and $1 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$, the A_α-index of $K_{k,n-k}$ satisfies*

$$\alpha(n-k) + \frac{k(1-\alpha)^2}{\alpha} \leqslant \lambda_\alpha(K_{k,n-k}) \leqslant \alpha n.$$

Both the right and left equalities hold if and only if $\alpha = \frac{1}{2}$.

Proof. According to [22, Proposition 38], one has

$$\begin{aligned}\lambda_\alpha(K_{k,n-k}) &= \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 + 4k(n-k)(1-2\alpha)}\right) \qquad (3)\\ &= \frac{1}{2}\left(\alpha n + \sqrt{\left(\alpha(n-2k) + \frac{2k(1-\alpha)^2}{\alpha}\right)^2 + 4k^2(1-\alpha)^2\left(1 - \frac{(1-\alpha)^2}{\alpha^2}\right)}\right).\end{aligned}$$

Note that for $\frac{1}{2} \leqslant \alpha < 1$, one has $4k^2(1-\alpha)^2 \left(1 - \frac{(1-\alpha)^2}{\alpha^2}\right) \geqslant 0$, with equality if and only if $\alpha = \frac{1}{2}$. Then

$$\lambda_\alpha(K_{k,n-k}) \geqslant \alpha(n-k) + \frac{k(1-\alpha)^2}{\alpha}$$

with equality if and only if $\alpha = \frac{1}{2}$.

On the other hand, as $\alpha \geqslant \frac{1}{2}$, one has $4k(n-k)(1-2\alpha) \leqslant 0$, with equality if and only if $\alpha = \frac{1}{2}$. Then (3) gives

$$\lambda_\alpha(K_{k,n-k}) = \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 + 4k(n-k)(1-2\alpha)}\right) \leqslant \alpha n$$

with equality if and only if $\alpha = \frac{1}{2}$.

This completes the proof. □

3 Proofs of Theorems 8 and 9

In this section, we aim to give the proofs of Theorems 8 and 9.

Proof of Theorem 8. Choose G in $\mathbb{B}(n,m)$, and let U, V be two partite sets of G with $|U| \leqslant |V|$. Note that for any positive integers p, q, n with $p < q \leqslant \lfloor \frac{n}{2} \rfloor$, we have $p(n-p) < q(n-q)$. If $|U| \leqslant k-1$, then $|E(G)| \leqslant |E(K_{|U|,|V|})| = |U||V| < k(n-k) = m$, a contradiction to $G \in \mathbb{B}(n,m)$.

If $|U| \geqslant k+1$, then $|E(G)| = k(n-k) < |U||V|$, and so G is a proper subgraph of $K_{|U|,|V|}$. By the Perron-Frobenius theory and (3), one has

$$\begin{aligned}
\lambda_\alpha(G) < \lambda_\alpha(K_{|U|,|V|}) &= \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 + 4|U||V|(1-2\alpha)}\right) \\
&\leqslant \frac{1}{2}\left(\alpha n + \sqrt{\alpha^2 n^2 + 4k(n-k)(1-2\alpha)}\right) \\
&= \lambda_\alpha(K_{k,n-k}).
\end{aligned}$$

If $|U| = k$, then G is a subgraph of $K_{k,n-k}$, and so $|E(G)| \leqslant |E(K_{k,n-k})|$ $(= k(n-k) = m)$, with equality if and only if $G = K_{k,n-k}$. □

In the remainder of this section, we are going to give the proof of Theorem 9.

Let $\frac{1}{2} \leqslant \alpha < 1$, and let n, m be positive integers with $n \leqslant m \leqslant 2n-5$. Then $n \geqslant 5$. In the remainder of this section, we assume that G^* is a graph with maximum A_α-index among all graphs in $\mathbb{B}(n,m)$. Then by the Perron-Frobenius theory (see the first paragraph of the proof of [29, Lemma 2.5]), G^* has at most one non-trivial component. For convenience, we denote by $\lambda_\alpha = \lambda_\alpha(G^*)$, $\Delta = \Delta(G^*)$ and $d(v) = d_{G^*}(v)$ for $v \in V(G^*)$. As $K_{2,n-2}^m \in \mathbb{B}(n,m)$, and $K_{2,n-2}^m$ contains $K_{1,n-2}$ as a proper subgraph. By the choice of G^*, the Perron-Frobenius theory and Lemma 19, one has

$$\lambda_\alpha \geqslant \lambda_\alpha(K_{2,n-2}^m) > \lambda_\alpha(K_{1,n-2}) \geqslant \alpha(n-2) + \frac{(1-\alpha)^2}{\alpha}. \tag{4}$$

Fact 20. *$G^* = K_{2,n-2}^m$ for $n \leqslant m \leqslant 2n-6$.*

Proof. Note that G^* is a bipartite graph. Hence, in order to show $G^* = K_{2,n-2}^m$, it suffices to prove $\Delta = n-2$. Note that $\Delta = n-1$ gives $G^* = K_{1,n-1}$, and so $|E(G^*)| = n-1 < m$, a contradiction to $G^* \in \mathbb{B}(n,m)$.

Now suppose $\Delta \leqslant n-3$. Note that given real numbers $a, b > 0$, the function $f(x) = ax + \frac{b}{x}$ with $x > 0$ is convex. Let G_1 be the non-trivial component of G^*. Let v be in $V(G_1)$.

If $d(v) = 1$, then one has

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u) &= \alpha + (1-\alpha)\sum_{u\sim v} d(u)\\ &\leqslant \alpha + (1-\alpha)\Delta \leqslant \alpha + (n-3)(1-\alpha). \end{aligned} \tag{5}$$

If $d(v) \geqslant 2$, then $2 \leqslant d(v) \leqslant \Delta \leqslant n-3$. And so

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u) &\leqslant \alpha d(v) + \frac{(1-\alpha)m}{d(v)}\\ &\leqslant \max\left\{2\alpha + \frac{(1-\alpha)m}{2},\ \alpha(n-3) + \frac{(1-\alpha)m}{n-3}\right\}\\ &\leqslant \alpha(n-3) + 2(1-\alpha). \end{aligned} \tag{6}$$

Together with (5), (6) and Lemma 18, one has

$$\begin{aligned}\lambda_\alpha = \lambda_\alpha(G_1) &\leqslant \max_{v\in V(G_1)}\left\{\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u)\right\}\\ &\leqslant \max\{\alpha + (n-3)(1-\alpha),\ \alpha(n-3) + 2(1-\alpha)\}\\ &= \alpha(n-3) + 2(1-\alpha). \end{aligned} \tag{7}$$

Combining (4) with (7) gives us

$$\alpha(n-2) + \frac{(1-\alpha)^2}{\alpha} < \alpha(n-3) + 2(1-\alpha), \text{ i.e., } \frac{(2\alpha-1)^2}{\alpha} < 0,$$

a contradiction.

Therefore, $\Delta = n-2$, and so $G^* = K_{2,n-2}^m$. □

Fact 21. *For $n \leqslant m = 2n-5$, we have $n-3 \leqslant \Delta \leqslant n-2$, and $\Delta = n-2$ only if $G^* = K_{2,n-2}^m$.*

Proof. If $\Delta = n-1$, then since G^* is bipartite, G^* must be $K_{1,n-1}$. So $|E(G^*)| = n-1 < n \leqslant m$, which is a contradiction. If $\Delta = n-2$, it is clear that $G^* = K_{2,n-2}^m$. To complete the proof, it remains to rule out the possibility $\Delta \leqslant n-4$.

Suppose $\Delta \leqslant n-4$. Then for $n=5$, one has $\Delta \leqslant 1$, and so by Lemma 18, $\lambda_\alpha \leqslant \Delta = 1 < 3\alpha + \frac{(1-\alpha)^2}{\alpha}$, a contradiction to (4); for $n=6$, one has $\Delta \leqslant 2$, and so by Lemma 18, $\lambda_\alpha \leqslant \Delta \leqslant 2 < 4\alpha + \frac{(1-\alpha)^2}{\alpha}$, a contradiction to (4).

Now we consider $n \geqslant 7$. In this case, let G_1 be the non-trivial component of G^*. Let v be in $V(G_1)$. If $d(v)=1$, then one has

$$\begin{aligned} \alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u \sim v} d(u) &= \alpha + (1-\alpha) \sum_{u \sim v} d(u) \\ &\leqslant \alpha + (1-\alpha)\Delta \leqslant \alpha + (n-4)(1-\alpha). \end{aligned} \tag{8}$$

If $d(v)=2$, then one has

$$\begin{aligned} \alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u \sim v} d(u) &= 2\alpha + \frac{1-\alpha}{2} \sum_{u \sim v} d(u) \\ &\leqslant 2\alpha + (1-\alpha)\Delta \leqslant 2\alpha + (n-4)(1-\alpha). \end{aligned} \tag{9}$$

If $d(v) \geqslant 3$, then $3 \leqslant d(v) \leqslant \Delta \leqslant n-4$. And so

$$\begin{aligned} \alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u \sim v} d(u) &\leqslant \alpha d(v) + \frac{(1-\alpha)m}{d(v)} \\ &\leqslant \max\left\{3\alpha + \frac{(1-\alpha)m}{3}, \alpha(n-4) + \frac{(1-\alpha)m}{n-4}\right\} \\ &= \alpha(n-4) + (1-\alpha)(2 + \frac{3}{n-4}). \end{aligned} \tag{10}$$

Together with (8)-(10) and Lemma 18, one has

$$\begin{aligned} \lambda_\alpha &= \lambda_\alpha(G_1) \\ &\leqslant \max_{v \in V(G_1)} \left\{\alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u \sim v} d(u)\right\} \\ &\leqslant \max\{\alpha + (n-4)(1-\alpha), 2\alpha + (n-4)(1-\alpha), \alpha(n-4) + (1-\alpha)(2 + \frac{3}{n-4})\} \\ &= \alpha(n-4) + (1-\alpha)(2 + \frac{3}{n-4}). \end{aligned} \tag{11}$$

Together with (4) and (11), one has

$$\alpha(n-2) + \frac{(1-\alpha)^2}{\alpha} < \alpha(n-4) + (1-\alpha)(2 + \frac{3}{n-4}) \leqslant \alpha(n-4) + 3(1-\alpha),$$

i.e., $\frac{(2\alpha-1)(3\alpha-1)}{\alpha} < 0$, a contradiction to $\alpha \geqslant \frac{1}{2}$.

Therefore, $\Delta \geqslant n-3$, as desired. □

Fact 22. *G^* is connected for $n \leqslant m = 2n-5$.*

Proof. Suppose G^* is not connected. Let G_1 be the non-trivial component of G^*, then $|V(G_1)| \leqslant n-1$. On the other hand, by Fact 21, one has $n-3 \leqslant \Delta(G_1) \leqslant n-2$. Then G_1 is a subgraph of $K_{1,n-2}$ or $K_{2,n-3}$, and so $|E(G^*)| = |E(G_1)| \leqslant \max\{n-2,\, 2n-6\} < m$, a contradiction. □

Fact 23. *$\lambda_\alpha \leqslant \alpha(n-3) + (1-\alpha)(2+\frac{1}{n-3})$ for $6 \leqslant n \leqslant m = 2n-5$ and $\Delta = n-3$.*

Proof. Let v be in $V(G^*)$. If $d(v) = 1$, then one has

$$\alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u\sim v} d(u) = \alpha + (1-\alpha) \sum_{u\sim v} d(u) \leqslant \alpha + (n-3)(1-\alpha). \tag{12}$$

If $d(v) = 2$, then one has

$$\alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u\sim v} d(u) = 2\alpha + \frac{1-\alpha}{2} \sum_{u\sim v} d(u) \leqslant 2\alpha + (n-3)(1-\alpha). \tag{13}$$

If $d(v) \geqslant 3$, then $3 \leqslant d(v) \leqslant \Delta = n-3$. And so

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u\sim v} d(u) &\leqslant \alpha d(v) + \frac{(1-\alpha)m}{d(v)} \\ &= \max\left\{3\alpha + \frac{(1-\alpha)(2n-5)}{3},\, \alpha(n-3) + \frac{(1-\alpha)(2n-5)}{n-3}\right\} \\ &= \alpha(n-3) + (1-\alpha)(2+\frac{1}{n-3}). \end{aligned} \tag{14}$$

Together with (12)-(14) and Lemma 18, one has

$$\begin{aligned}\lambda_\alpha &\leqslant \max_{v\in V(G^*)} \left\{\alpha d(v) + \frac{1-\alpha}{d(v)} \sum_{u\sim v} d(u)\right\} \\ &\leqslant \max\{\alpha + (n-3)(1-\alpha),\, 2\alpha + (n-3)(1-\alpha),\, \alpha(n-3) + (1-\alpha)(2+\frac{1}{n-3})\} \\ &= \alpha(n-3) + (1-\alpha)(2+\frac{1}{n-3}),\end{aligned}$$

as desired.

This completes the proof. □

Fact 24. *$G^* = K^m_{2,n-2}$ for $n \leqslant 9$ and $n \leqslant m = 2n-5$.*

Proof. By Fact 21, it suffices to show $\Delta \neq n-3$. Suppose $\Delta = n-3$, recall that $n \geqslant 5$. If $n = 5$, then $m = 5$ and there exists a partite set of G^* with at most 2 vertices. And so $|E(G^*)| \leqslant 2\Delta = 2(n-3) = 4 < m$, a contradiction to $G^* \in \mathbb{B}(n,m)$. In the following, we only need to consider $6 \leqslant n \leqslant 9$.

Case 1. $n = 6$. In this case, $m = 7$. By Fact 23, one has

$$\lambda_\alpha \leqslant \alpha(n-3) + (1-\alpha)(2 + \frac{1}{n-3}) = \frac{2\alpha+7}{3}. \tag{15}$$

On the other hand, consider the partition $\pi_1 : V(K_{2,4}^7) = \{u_1\} \cup \{u_2\} \cup \{v_1, v_2, v_3\} \cup \{v_4\}$, where u_1 (resp. u_2, v_4) is the vertex of degree 4 (resp. 3, 1), v_i $(1 \leqslant i \leqslant 3)$ are the vertices of degree 2. With respect to the partition π_1, the quotient matrix of $A_\alpha(K_{2,4}^7)$ is given as

$$B_1 = \begin{pmatrix} 4\alpha & 0 & 3(1-\alpha) & 1-\alpha \\ 0 & 3\alpha & 3(1-\alpha) & 0 \\ 1-\alpha & 1-\alpha & 2\alpha & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix}.$$

By a direct calculation, the characteristic polynomial of B_1 is

$$f_1(x) = x^4 - 10\alpha x^3 + (28\alpha^2 + 14\alpha - 7)x^2 + (-18\alpha^3 - 64\alpha^2 + 32\alpha)x + 42\alpha^3 - 9\alpha^2 - 12\alpha + 3.$$

Note that the partition π_1 is equatable. By Lemma 13, $\lambda_\alpha(K_{2,4}^7)$ is equal to the largest eigenvalue of B_1, i.e., the largest zero of $f_1(x)$.

Furthermore, by a direct calculation, one has

$$f_1\left(\frac{2\alpha+7}{3}\right) = \frac{(1-\alpha)(188\alpha^3 - 1620\alpha^2 + 1497\alpha - 443}{81}. \tag{16}$$

Consider the function $g_1(\alpha) = 188\alpha^3 - 1620\alpha^2 + 1497\alpha - 443$. By a direct calculation, the first derivative of $g_1(\alpha)$ is $g_1'(\alpha) = 564\alpha^2 - 3240\alpha + 1497$, which is positive in $\left[\frac{1}{2}, \frac{270-\sqrt{49447}}{94}\right)$, and negative in $\left(\frac{270-\sqrt{49447}}{94}, 1\right)$. Therefore, $g_1(\alpha) \leqslant g_1\left(\frac{270-\sqrt{49447}}{94}\right) = -75.94 < 0$. Combining with (16) gives $f_1\left(\frac{2\alpha+7}{3}\right) < 0$, and so $\frac{2\alpha+7}{3} < \lambda_\alpha(K_{2,4}^7)$. Together with (15), one has $\lambda_\alpha < \lambda_\alpha(K_{2,4}^7)$, a contradiction to the choice of G^*.

Case 2. $n = 7$. In this case, $m = 9$. By Fact 23, one has

$$\lambda_\alpha \leqslant \alpha(n-3) + (1-\alpha)(2 + \frac{1}{n-3}) = \frac{7\alpha+9}{4}. \tag{17}$$

On the other hand, consider the partition $\pi_2 : V(K_{2,5}^9) = \{u_1\} \cup \{u_2\} \cup \{v_1, v_2, v_3, v_4\} \cup \{v_5\}$, where u_1 (resp. u_2, v_5) is the vertex of degree 5 (resp. 4, 1), v_i $(1 \leqslant i \leqslant 4)$ are the vertices of degree 2. With respect to the partition π_2, the quotient matrix of $A_\alpha(K_{2,5}^9)$ is given as

$$B_2 = \begin{pmatrix} 5\alpha & 0 & 4(1-\alpha) & 1-\alpha \\ 0 & 4\alpha & 4(1-\alpha) & 0 \\ 1-\alpha & 1-\alpha & 2\alpha & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix}.$$

By a direct calculation, the characteristic polynomial of B_2 is

$$f_2(x) = x^4 - 12\alpha x^3 + (40\alpha^2 + 18\alpha - 9)x^2 + (-28\alpha^3 - 100\alpha^2 + 50\alpha)x + 72\alpha^3 - 20\alpha^2 - 16\alpha + 4.$$

Note that the partition π_2 is equatable. By Lemma 13, $\lambda_\alpha(K^9_{2,5})$ is equal to the largest eigenvalue of B_2, i.e., the largest zero of $f_2(x)$.

Furthermore, by a direct calculation, one has

$$f_2\left(\frac{7\alpha+9}{4}\right) = -\frac{(1-\alpha)(4753\alpha^3+5853\alpha^2-11229\alpha+4079)}{256}. \tag{18}$$

Consider the function $g_2(\alpha) = 4753\alpha^3 + 5853\alpha^2 - 11229\alpha + 4079$. By a direct calculation, the first derivative of $g_2(\alpha)$ is $g_2'(\alpha) = 14259\alpha^2 + 11706\alpha - 11229$, which is negative in $\left[\frac{1}{2}, \frac{-1951+116\sqrt{1605}}{4753}\right)$, and positive in $\left(\frac{-1951+116\sqrt{1605}}{4753}, 1\right)$. Therefore, $g_2(\alpha) \geqslant g_2\left(\frac{-1951+116\sqrt{1605}}{4753}\right) = 460.23 > 0$. Combining with (18) gives $f_2\left(\frac{7\alpha+9}{4}\right) < 0$, and so $\frac{7\alpha+9}{4} < \lambda_\alpha(K^9_{2,5})$. Together with (17), one has $\lambda_\alpha < \lambda_\alpha(K^9_{2,5})$, a contradiction to the choice of G^*.

Case 3. $n = 8$. In this case, $m = 11$. By Fact 23, one has

$$\lambda_\alpha \leqslant \alpha(n-3) + (1-\alpha)(2+\frac{1}{n-3}) = \frac{14\alpha+11}{5}. \tag{19}$$

On the other hand, consider the partition $\pi_3 : V(K^{11}_{2,6}) = \{u_1\} \cup \{u_2\} \cup \{v_1, v_2, v_3, v_4, v_5\} \cup \{v_6\}$, where u_1 (resp. u_2, v_6) is the vertex of degree 6 (resp. 5, 1), v_i $(1 \leqslant i \leqslant 5)$ are the vertices of degree 2. With respect to the partition π_3, the quotient matrix of $A_\alpha(K^{11}_{2,6})$ is given as

$$B_3 = \begin{pmatrix} 6\alpha & 0 & 5(1-\alpha) & 1-\alpha \\ 0 & 5\alpha & 5(1-\alpha) & 0 \\ 1-\alpha & 1-\alpha & 2\alpha & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix}.$$

By a direct calculation, the characteristic polynomial of B_3 is

$$f_3(x) = x^4 - 14\alpha x^3 + (54\alpha^2+22\alpha-11)x^2 + (-40\alpha^3-144\alpha^2+72\alpha)x + 110\alpha^3 - 35\alpha^2 - 20\alpha + 5.$$

Note that the partition π_3 is equatable. By Lemma 13, $\lambda_\alpha(K^{11}_{2,6})$ is equal to the largest eigenvalue of B_3, i.e., the largest zero of $f_3(x)$.

Furthermore, by a direct calculation, one has

$$f_3\left(\frac{14\alpha+11}{5}\right) = -\frac{(1-\alpha)(40936\alpha^3-5738\alpha^2-34207\alpha+15509)}{625}. \tag{20}$$

Consider the function $g_3(\alpha) = 40936\alpha^3 - 5738\alpha^2 - 34207\alpha + 15509$. By a direct calculation, the first derivative of $g_3(\alpha)$ is $g_3'(\alpha) = 122808\alpha^2 - 11476\alpha - 34207$, which is negative in $\left[\frac{1}{2}, \frac{2869+5\sqrt{42338179}}{61404}\right)$, and positive in $\left(\frac{2869+5\sqrt{42338179}}{61404}, 1\right)$. Therefore, $g_3(\alpha) \geqslant g_3\left(\frac{2869+5\sqrt{42338179}}{61404}\right) = 1725.01 > 0$. Combining with (20) gives $f_3\left(\frac{14\alpha+11}{5}\right) < 0$, and so $\frac{14\alpha+11}{5} < \lambda_\alpha(K^{11}_{2,6})$. Together with (19), one has $\lambda_\alpha < \lambda_\alpha(K^{11}_{2,6})$, a contradiction to the choice of G^*.

Case 4. $n = 9$. In this case, $m = 13$. By Fact 23, one has

$$\lambda_\alpha \leqslant \alpha(n-3) + (1-\alpha)(2 + \frac{1}{n-3}) = \frac{23\alpha + 13}{6}. \tag{21}$$

On the other hand, consider the partition $\pi_4 : V(K_{2,7}^{13}) = \{u_1\} \cup \{u_2\} \cup \{v_1, v_2, v_3, v_4, v_5, v_6\} \cup \{v_7\}$, where u_1 (resp. u_2, v_7) is the vertex of degree 7 (resp. 6, 1), v_i $(1 \leqslant i \leqslant 6)$ are the vertices of degree 2. With respect to the partition π_4, the quotient matrix of $A_\alpha(K_{2,7}^{13})$ is given by

$$B_4 = \begin{pmatrix} 7\alpha & 0 & 6(1-\alpha) & 1-\alpha \\ 0 & 6\alpha & 6(1-\alpha) & 0 \\ 1-\alpha & 1-\alpha & 2\alpha & 0 \\ 1-\alpha & 0 & 0 & \alpha \end{pmatrix}.$$

By a direct calculation, the characteristic polynomial of B_4 is

$$f_4(x) = x^4 - 16\alpha x^3 + (70\alpha^2 + 26\alpha - 13)x^2 + (-54\alpha^3 - 196\alpha^2 + 98\alpha)x + 156\alpha^3 - 54\alpha^2 - 24\alpha + 6.$$

Note that the partition π_4 is equatable. By Lemma 13, $\lambda_\alpha(K_{2,7}^{13})$ is equal to the largest eigenvalue of B_4, i.e., the largest zero of $f_4(x)$.

Furthermore, by a direct calculation, one has

$$f_4\left(\frac{23\alpha + 13}{6}\right) = -\frac{(1-\alpha)(176617\alpha^3 - 92355\alpha^2 - 70857\alpha + 42755)}{1296}. \tag{22}$$

Consider the function $g_4(\alpha) = 176617\alpha^3 - 92355\alpha^2 - 70857\alpha + 42755$. By a direct calculation, the first derivative of $g_4(\alpha)$ is $g_4'(\alpha) = 529851\alpha^2 - 184710\alpha - 70857$, which is negative in $\left[\frac{1}{2}, \frac{30785+2\sqrt{1279808287}}{176617}\right)$, and positive in $\left(\frac{30785+2\sqrt{1279808287}}{176617}, 1\right)$. Therefore, $g_4(\alpha) \geqslant g_4\left(\frac{30785+2\sqrt{1279808287}}{176617}\right) = 5049.74 > 0$. Combining with (22) gives $f_4\left(\frac{23\alpha+13}{6}\right) < 0$, and so $\frac{23\alpha+13}{6} < \lambda_\alpha(K_{2,7}^{13})$. Together with (21), one has $\lambda_\alpha < \lambda_\alpha(K_{2,7}^{13})$, a contradiction to the choice of G^*.

This completes the proof. □

Now, we are ready to give the proof of Theorem 9.

Proof of Theorem 9. For $n \leqslant m \leqslant 2n - 6$ and $n \leqslant 9$, $n \leqslant m = 2n - 5$, our result follows by Facts 20 and 24, respectively. In the following, we only need consider $n \geqslant 10$ and $m = 2n - 5$. By Fact 21, it suffices to show $\Delta \neq n - 3$.

Suppose $\Delta = n - 3$. By Fact 22, G^* is connected, and so Lemma 11 implies G^* is a double nested graph with all leaves being adjacent to a common vertex.

Let u_1 be the vertex of G^* with $d(u_1) = n - 3$, and let u_2, u_3 be two vertices of G^* not adjacent to u_1. If the sizes of the partite sets of G^* are 2 and $n - 2$, say, one of the partite sets is $\{u_1, u_2\}$, then we have $d(u_2) = m - d(u_1) = (2n - 5) - (n - 3) = n - 2 > \Delta$, which is a contradiction. Hence, $\{u_1, u_2, u_3\}$ and $N_{G^*}(u_1)$ are two partite sets of G^*, and so $d(u_1) + d(u_2) + d(u_3) = m$. Without loss of generality, we assume

$d(u_3) \leqslant d(u_2) \leqslant d(u_1)$. Then according to the structure of a double nested graph, one has $N_{G^*}(u_3) \subseteq N_{G^*}(u_2) \subseteq N_{G^*}(u_1)$. For convenience, we denote by $s := d(u_3)$, $t := d(u_2)$ and $V_1 := N_{G^*}(u_3)$, $V_2 := N_{G^*}(u_2) \backslash N_{G^*}(u_3)$, $V_3 := N_{G^*}(u_1) \backslash N_{G^*}(u_2)$ (it may hold one of V_2 and V_3 is empty). Then

$$s \leqslant t \text{ and } s + t = m - d(u_1) = n - 2. \tag{23}$$

Let $\mathbf{x}$ be the Perron vector of $A_\alpha(G^*)$. For $1 \leqslant i \leqslant 3$, let $\mathbf{x}_{u_i} = a_i$. As all vertices in V_1 (resp. V_2, V_3) have the same degree 3 (resp. 2, 1). According to Lemma 17, for $1 \leqslant i \leqslant 3$, we can assume $\mathbf{x}_v = b_i$ if $v \in V_i$. Then Lemma 17 implies

$$a_3 \leqslant a_2 \leqslant a_1 \text{ and } b_3 < b_2 < b_1. \tag{24}$$

In order to complete the proof of Theorem 9, we need the following three claims.

Claim 25. *$V_3 \neq \emptyset$, and $b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha - \alpha}$.*

Proof of Claim 25. Suppose $V_3 = \emptyset$. Then $N_{G^*}(u_2) = N_{G^*}(u_1)$, and so $t = d(u_1) = n - 3$. By (23), $s = 1$, i.e., $|V_1| = 1$. Let $V_1 = \{v_1\}$, applying (1) to v_1 gives

$$\lambda_\alpha b_1 = 3\alpha b_1 + (1-\alpha)(a_1 + a_2 + a_3) \leqslant 3\alpha b_1 + 3(1-\alpha)a_1. \tag{25}$$

As $n \geqslant 10$, by (4), we have $\lambda_\alpha > 8\alpha$. Together with (25),

$$b_1 \leqslant \frac{3(1-\alpha)a_1}{\lambda_\alpha - 3\alpha} < \frac{3(1-\alpha)a_1}{5\alpha} < a_1.$$

Construct $G = G^* - u_3v_1 + u_3u_1$. Clearly, $G \in \mathbb{B}(n, m)$, and by Lemma 16, $\lambda_\alpha(G) > \lambda_\alpha(G^*)$, a contradiction to the choice of G^*. Therefore, $V_3 \neq \emptyset$.

Now, applying (1) to a vertex $v \in V_3$ gives $\lambda_\alpha b_3 = \alpha b_3 + (1-\alpha)a_1$. And so $b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha - \alpha}$, as desired. ☐

Claim 26. *It holds that $b_1 < \max\left\{\frac{2(1-\alpha)a_1}{(n-5)\alpha}, \frac{7}{2}b_3\right\}$.*

Proof of Claim 26. Applying (2) to a vertex $v \in V_1$ gives

$$\begin{aligned}\lambda_\alpha^2 b_1 &= 3\alpha\lambda_\alpha b_1 + \alpha(1-\alpha)[(n-3)a_1 + ta_2 + sa_3] \\ &\quad + (1-\alpha)^2[3sb_1 + 2(t-s)b_2 + (n-3-t)b_3] \\ &< 3\alpha\lambda_\alpha b_1 + \alpha(1-\alpha)(2n-5)a_1 + (1-\alpha)^2(2n-5)b_1,\end{aligned}$$

where the inequality follows by (23) and (24). Then

$$b_1 < \frac{\alpha(1-\alpha)(2n-5)a_1}{(\lambda_\alpha - 3\alpha)\lambda_\alpha - (1-\alpha)^2(2n-5)} = \frac{2\alpha(1-\alpha)a_1}{(\lambda_\alpha - 3\alpha)\frac{\lambda_\alpha}{n-\frac{5}{2}} - 2(1-\alpha)^2}.$$

Together with (4), one has

$$b_1 < \frac{2\alpha(1-\alpha)a_1}{(\lambda_\alpha - 3\alpha)\alpha + \frac{(\lambda_\alpha-3\alpha)\left(\frac{\alpha}{2}+\frac{(1-\alpha)^2}{\alpha}\right)}{n-\frac{5}{2}} - 2(1-\alpha)^2}. \tag{26}$$

Note that $n \geqslant 10$ and $\alpha \geqslant 1-\alpha$. By (4),

$$\begin{aligned}(\lambda_\alpha - 3\alpha)\left(\frac{\alpha}{2}+\frac{(1-\alpha)^2}{\alpha}\right) &> \left((n-5)\alpha + \frac{(1-\alpha)^2}{\alpha}\right)\left(\frac{\alpha}{2}+\frac{(1-\alpha)^2}{\alpha}\right) \\ &> \left(n-\frac{5}{2}\right)(1-\alpha)^2.\end{aligned}$$

Together with (4) and (26), one has

$$b_1 < \frac{2\alpha(1-\alpha)a_1}{(\lambda_\alpha-3\alpha)\alpha-(1-\alpha)^2} < \frac{2\alpha(1-\alpha)a_1}{\left((n-5)\alpha+\frac{(1-\alpha)^2}{\alpha}\right)\alpha-(1-\alpha)^2} = \frac{2(1-\alpha)a_1}{(n-5)\alpha}. \tag{27}$$

On the other hand, according to the first inequality of (27), one has

$$b_1 < \frac{2\alpha(1-\alpha)a_1}{(\lambda_\alpha-3\alpha)\alpha-\alpha^2} = \frac{2(1-\alpha)a_1}{\lambda_\alpha-4\alpha}. \tag{28}$$

As $n \geqslant 10$, by (4), $\lambda_\alpha > (n-2)\alpha \geqslant 8\alpha$. Together with (28) and Claim 25, one has

$$\frac{b_1}{b_3} < \frac{2(1-\alpha)a_1}{\lambda_\alpha-4\alpha}\cdot\frac{\lambda_\alpha-\alpha}{(1-\alpha)a_1} = \frac{2(\lambda_\alpha-\alpha)}{\lambda_\alpha-4\alpha} = 2+\frac{6\alpha}{\lambda_\alpha-4\alpha} < \frac{7}{2}.$$

And so $b_1 < \frac{7}{2}b_3$. This completes the proof of Claim 26. □

Claim 27. *If* $s \geqslant \frac{2n-7}{5}$, *then* $ta_2 + sa_3 < \frac{21}{5}a_1$.

Proof of Claim 27. Applying (1) to u_1 gives

$$\lambda_\alpha a_1 = \alpha(n-3)a_1 + (1-\alpha)(sb_1 + (t-s)b_2 + (n-3-t)b_3). \tag{29}$$

Applying (1) to u_2 gives us

$$\lambda_\alpha a_2 = \alpha t a_2 + (1-\alpha)(sb_1 + (t-s)b_2). \tag{30}$$

And applying (1) to u_3 yields

$$\lambda_\alpha a_3 = \alpha s a_3 + (1-\alpha)sb_1 < \alpha s a_3 + \frac{2(1-\alpha)^2 s a_1}{(n-5)\alpha}, \tag{31}$$

where the inequality follows by Claim 26. Together with (29)-(31), one has

$$a_2 < \frac{(\lambda_\alpha-\alpha(n-3))a_1}{\lambda_\alpha-\alpha t} \text{ and } a_3 < \frac{2(1-\alpha)^2 s a_1}{(\lambda_\alpha-\alpha s)(n-5)\alpha}. \tag{32}$$

Note that $s \geqslant \frac{2n-7}{5}$. Hence, by (23), one has $\frac{2n-7}{5} \leqslant s \leqslant \frac{n-2}{2} \leqslant t \leqslant \frac{3n-3}{5}$. Together with (24) and (32), one has

$$\begin{aligned}
ta_2 + sa_3 &\leqslant \frac{3n-3}{5}a_2 + \frac{2n-7}{5}a_3 \\
&< \frac{3n-3}{5} \cdot \frac{(\lambda_\alpha - \alpha(n-3))a_1}{\lambda_\alpha - \alpha t} + \frac{2n-7}{5} \cdot \frac{2(1-\alpha)^2 s a_1}{(\lambda_\alpha - \alpha s)(n-5)\alpha} \\
&\leqslant \left[\frac{3n-3}{5} \cdot \frac{5\lambda_\alpha - 5(n-3)\alpha}{5\lambda_\alpha - (3n-3)\alpha} + \frac{2(2n-7)(1-\alpha)^2}{5(n-5)\alpha} \cdot \frac{n-2}{2\lambda_\alpha - \alpha(n-2)}\right] a_1 \\
&< \left[\frac{3n-3}{5} \cdot \left(1 - \frac{2(n-6)\alpha}{5\lambda_\alpha - (3n-3)\alpha}\right) + \frac{2(2n-7)}{5(n-5)}\right] a_1 && \text{(by (4))} \\
&< \left[\frac{3n-3}{5} \cdot \left(1 - \frac{2(n-6)}{2n-1}\right) + \frac{2(2n-7)}{5(n-5)}\right] a_1 && \text{(by Fact 23)} \\
&= \frac{41n^2 - 230n + 179}{10n^2 - 55n + 25} a_1 \\
&< \frac{21}{5} a_1, && \text{(by } n \geqslant 10\text{)}
\end{aligned}$$

as desired. □

Recall that $s \leqslant t$ and $s + t = n - 2$ (see (23)). Consequently, $s \leqslant \frac{n-2}{2}$. According to the values of s and t, we consider the following two cases.

Case 1. $s \leqslant \frac{2(n-4)}{5}$, and so $t \geqslant \frac{3n-2}{5}$. In this case, $K_{2,n-2}^m = G^* - \{u_3 v | v \in V_1\} + \{u_2 v | v \in V_3\} + u_1 u_3$. By the Courant-Fischer theorem (see [15, Section 2.6]), one has

$$\begin{aligned}
\lambda_\alpha(K_{2,n-2}^m) - \lambda_\alpha &\geqslant \mathbf{x}^T (A_\alpha(K_{2,n-2}^m) - A_\alpha(G^*))\mathbf{x} \\
&= \alpha a_1^2 + 2(1-\alpha)a_1 a_3 + \alpha a_3^2 + (s-1)(\alpha a_2^2 + 2(1-\alpha)a_2 b_3 + \alpha b_3^2) \\
&\quad - s(\alpha a_3^2 + 2(1-\alpha)a_3 b_1 + \alpha b_1^2). \qquad (33)
\end{aligned}$$

Note that $a_3 \leqslant a_2$ and $b_1 < \frac{7}{2} b_3$ (see Claim 26), one has

$$\begin{aligned}
\lambda_\alpha(K_{2,n-2}^m) - \lambda_\alpha &> \alpha a_1^2 + 2(1-\alpha)a_1 a_3 + (s-1)(2(1-\alpha)a_2 b_3 + \alpha b_3^2) \\
&\quad - \frac{s}{4}(28(1-\alpha)a_3 b_3 + 49\alpha b_3^2) \\
&= \frac{\alpha}{4}(4a_1^2 - (45s+4)b_3^2) + (1-\alpha)((2(s-1)a_2 - 7sa_3)b_3 + 2a_1 a_3). \qquad (34)
\end{aligned}$$

As $b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha - \alpha}$ (see Claim 25), $\lambda_\alpha > \alpha(n-2)$ (see (4)) and $s \leqslant \frac{2}{5}(n-4)$, we obtain

$$4a_1^2 - (45s+4)b_3^2 = 4a_1^2 - \frac{(45s+4)(1-\alpha)^2 a_1^2}{(\lambda_\alpha - \alpha)^2} > 4a_1^2 - \frac{(45s+4)(1-\alpha)^2 a_1^2}{(\frac{5}{2}s+1)^2 \alpha^2} \geqslant 0 \qquad (35)$$

and

$$(2(s-1)a_2 - 7sa_3)b_3 + 2a_1 a_3 \geqslant \left(\frac{2(\lambda_\alpha - \alpha)}{1-\alpha} - 5s - 2\right) a_3 b_3 > 0. \qquad (36)$$

Combining with (34)-(36) gives $\lambda_\alpha(K_{2,n-2}^m) > \lambda_\alpha$, a contradiction to the choice of G^*.

Case 2. $s > \frac{2(n-4)}{5}$. Then $s \geqslant \frac{2n-7}{5}$, and so $t \leqslant \frac{3n-3}{5}$. Applying (2) to u_1 gives

$$\lambda_\alpha^2 a_1 = (n-3)\alpha\lambda_\alpha a_1 + \alpha(1-\alpha)[3sb_1 + 2(t-s)b_2 + (n-3-t)b_3] + (1-\alpha)^2[(n-3)a_1 + ta_2 + sa_3].$$

Together with (23), (24) and Claim 27, one has

$$\lambda_\alpha[\lambda_\alpha - (n-3)\alpha]a_1 < \alpha(1-\alpha)(2n-5)b_1 + (1-\alpha)^2(n+6/5)a_1.$$

Combining with (4) and Claim 26 gives us

$$\left[\alpha(n-2) + \frac{(1-\alpha)^2}{\alpha}\right]\left[\alpha + \frac{(1-\alpha)^2}{\alpha}\right] < \frac{2(1-\alpha)^2(2n-5)}{n-5} + (1-\alpha)^2(n+6/5).$$

By a direct calculation,

$$\alpha^2(n-2) + \frac{(1-\alpha)^4}{\alpha^2} < (1-\alpha)^2\left(\frac{31}{5} + \frac{10}{n-5}\right) \leqslant \frac{41}{5}(1-\alpha)^2. \tag{37}$$

Note that $1-\alpha \leqslant \alpha$. If $1-\alpha \leqslant \frac{\alpha}{2}$, then (37) gives

$$\alpha^2(n-2) + \frac{(1-\alpha)^4}{\alpha^2} < \frac{41}{20}\alpha^2,$$

a contradiction to $n \geqslant 10$. If $1-\alpha > \frac{\alpha}{2}$, then (37) gives

$$\alpha^2(n-2) + \frac{(1-\alpha)^2}{4} < \alpha^2(n-2) + \frac{(1-\alpha)^4}{\alpha^2} < \frac{41}{5}(1-\alpha)^2,$$

and so $n-2 < \frac{159}{20}$, a contradiction to $n \geqslant 10$.

This completes the proof. □

4 Proof of Theorem 10

In this section, we aim to give the proof of our last main result, i.e., Theorem 10.

Let $\frac{1}{2} \leqslant \alpha < 1$, and let n, m be positive integers with $2n-3 \leqslant m \leqslant 2\sqrt{2}(n-4)$. Then $n \geqslant 11$. In the remainder of this section, we assume that G^* is a graph with maximum A_α-index among all graphs in $\mathbb{B}(n,m)$. Then by the Perron-Frobenius theory (see the first paragraph of the proof of [29, Lemma 2.5]), G^* has at most one non-trivial component. Denote by $\lambda_\alpha = \lambda_\alpha(G^*)$, $\Delta = \Delta(G^*)$ and $d(v) = d_{G^*}(v)$ for $v \in V(G^*)$. As $K_{3,n-3}^m \in \mathbb{B}(n,m)$, and $K_{3,n-3}^m$ contains $K_{2,n-3}$ as a proper subgraph. By the choice of G^*, the Perron-Frobenius theory and Lemma 19, one has

$$\lambda_\alpha \geqslant \lambda_\alpha(K_{3,n-3}^m) > \lambda_\alpha(K_{2,n-3}) \geqslant \alpha(n-3) + \frac{2(1-\alpha)^2}{\alpha}. \tag{38}$$

Further on we have the following facts.

Fact 28. $\Delta = n-3$.

Proof. Since G^* is bipartite, if $\Delta = n-1$, then G^* must be $K_{1,n-1}$, and so $|E(G^*)| = n-1 < m$, a contradiction; if $\Delta = n-2$, then G^* must be a subgraph of $K_{2,n-2}$, and so $|E(G^*)| \leqslant 2(n-2) < m$, a contradiction. To complete the proof, it remains to rule out the possibility $\Delta \leqslant n-4$.

Suppose $\Delta \leqslant n-4$. Let G_1 be the non-trivial component of G^*. Let v be in $V(G_1)$. If $d(v) = 1$, then one has

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u) &= \alpha + (1-\alpha)\sum_{u\sim v} d(u)\\ &\leqslant \alpha + (1-\alpha)\Delta \leqslant \alpha + (n-4)(1-\alpha). \qquad (39)\end{aligned}$$

If $d(v) = 2$, then one has

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u) &= 2\alpha + \frac{1-\alpha}{2}\sum_{u\sim v} d(u)\\ &\leqslant 2\alpha + (1-\alpha)\Delta \leqslant 2\alpha + (n-4)(1-\alpha). \qquad (40)\end{aligned}$$

If $d(v) \geqslant 3$, then $3 \leqslant d(v) \leqslant \Delta \leqslant n-4$. And so

$$\begin{aligned}\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u) &\leqslant \alpha d(v) + \frac{(1-\alpha)m}{d(v)}\\ &\leqslant \max\left\{3\alpha + \frac{2\sqrt{2}(n-4)(1-\alpha)}{3},\ \alpha(n-4) + 2\sqrt{2}(1-\alpha)\right\}\\ &= \alpha(n-4) + 2\sqrt{2}(1-\alpha). \qquad (41)\end{aligned}$$

Together with (39)-(41) and Lemma 18, one has

$$\begin{aligned}\lambda_\alpha = \lambda_\alpha(G_1) &\leqslant \max_{v\in V(G_1)}\left\{\alpha d(v) + \frac{1-\alpha}{d(v)}\sum_{u\sim v} d(u)\right\}\\ &\leqslant \max\{\alpha + (n-4)(1-\alpha),\ 2\alpha + (n-4)(1-\alpha),\ \alpha(n-4) + 2\sqrt{2}(1-\alpha)\}\\ &= \alpha(n-4) + 2\sqrt{2}(1-\alpha). \qquad (42)\end{aligned}$$

Together with (38) and (42), one has

$$\alpha(n-3) + \frac{2(1-\alpha)^2}{\alpha} < \alpha(n-4) + 2\sqrt{2}(1-\alpha),$$

i.e., $\frac{3+2\sqrt{2}}{\alpha}\left(\alpha - \frac{2+\sqrt{2}}{3+2\sqrt{2}}\right)^2 < 0$, a contradiction.

Therefore, $\Delta = n-3$, as desired. □

Fact 29. *G^* is connected.*

Proof. Suppose G^* is not connected. Let G_1 be the non-trivial component of G^*, then $|V(G_1)| \leqslant n-1$. On the other hand, by Fact 28, one has $\Delta(G_1) = n-3$. Then G_1 is a subgraph of $K_{2,n-3}$, and so $|E(G^*)| = |E(G_1)| \leqslant 2n-6 < m$, a contradiction to $G^* \in \mathbb{B}(n,m)$. □

Now, we are ready to give the proof of Theorem 10.

Proof of Theorem 10. By Fact 29, G^* is connected, and so Lemma 11 implies G^* is a double nested graph with all leaves being adjacent to a common vertex.

Fact 28 shows $\Delta = n-3$. Let u_1 be the vertex of G^* with $d(u_1) = n-3$, and let u_2, u_3 be two vertices of G^* not adjacent to u_1. Then $\{u_1, u_2, u_3\}$ and $N_{G^*}(u_1)$ are two partite sets of G^*, and so $d(u_1)+d(u_2)+d(u_3) = m$. Without loss of generality, we assume $d(u_3) \leqslant d(u_2) \leqslant d(u_1)$. Then according to the structure of a double nested graph, one has $N_{G^*}(u_3) \subseteq N_{G^*}(u_2) \subseteq N_{G^*}(u_1)$. For convenience, we denote by $s := d(u_3)$, $t := d(u_2)$ and $V_1 := N_{G^*}(u_3)$, $V_2 := N_{G^*}(u_2)\backslash N_{G^*}(u_3)$, $V_3 := N_{G^*}(u_1)\backslash N_{G^*}(u_2)$ (it may hold one of V_2 and V_3 is empty). Then

$$s \leqslant t \text{ and } s+t = m - d(u_1) = m-n+3. \tag{43}$$

In order to show $G^* = K^m_{3,n-3}$, it suffices to prove $t = n-3$. Suppose $t \leqslant n-4$. Then $V_3 \neq \emptyset$. Let $\mathbf{x}$ be the Perron vector of $A_\alpha(G^*)$. For $1 \leqslant i \leqslant 3$, let $\mathbf{x}_{u_i} = a_i$. As all vertices in V_1 (resp. V_2, V_3) have the same degree 3 (resp. 2, 1). According to Lemma 17, for $1 \leqslant i \leqslant 3$, we can assume $\mathbf{x}_v = b_i$ if $v \in V_i$. Then Lemma 17 implies

$$a_3 \leqslant a_2 < a_1 \text{ and } b_3 < b_2 < b_1. \tag{44}$$

Let $V_1 = \{v_1, \ldots, v_s\}$, $V_2 = \{v_{s+1}, \ldots, v_t\}$ and $V_3 = \{v_{t+1}, \ldots, v_{n-3}\}$. Then

$$K^m_{3,n-3} = G^* - \{u_3v_i | m-2n+7 \leqslant i \leqslant s\} + \{u_2v_i | t+1 \leqslant i \leqslant n-3\}.$$

Let $\mathbf{y}$ be the Perron vector of $A_\alpha(K^m_{3,n-3})$. According to Lemma 17, we can assume $\mathbf{y}_{u_1} = \mathbf{y}_{u_2} = a'_1$, $\mathbf{y}_{u_3} = a'_2$, $\mathbf{y}_{v_i} = b'_1$ for $1 \leqslant i \leqslant m-2n+6$, and $\mathbf{y}_{v_i} = b'_2$ for $m-2n+7 \leqslant i \leqslant n-3$. Then Lemma 17 implies

$$a'_2 < a'_1 \text{ and } b'_2 < b'_1. \tag{45}$$

In order to complete the proof of Theorem 10, we need the following three claims.

Claim 30. *It holds that $b_1 < 4b_3$. Furthermore, if $a_2 \leqslant \frac{a_1}{2}$, then $b_1 < 3b_3$.*

Proof of Claim 30. Consider the graph G^* and the Perron vector $\mathbf{x}$. Applying (1) to a vertex $v \in V_3$ gives $\lambda_\alpha b_3 = \alpha b_3 + (1-\alpha)a_1$. And so

$$b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha - \alpha}. \tag{46}$$

Applying (2) to a vertex $v \in V_1$ gives

$$\begin{aligned}
\lambda_\alpha^2 b_1 &= 3\alpha\lambda_\alpha b_1 + \alpha(1-\alpha)[(n-3)a_1 + ta_2 + sa_3] \\
&\quad + (1-\alpha)^2[3sb_1 + 2(t-s)b_2 + (n-3-t)b_3] \qquad (47)\\
&< 3\alpha\lambda_\alpha b_1 + \alpha(1-\alpha)ma_1 + (1-\alpha)^2 mb_1, \qquad (48)
\end{aligned}$$

where the inequality in (48) follows by (43) and (44). As $m \leqslant 2\sqrt{2}(n-4)$, together with (38) and (48), one has

$$\begin{aligned}
b_1 < \frac{\alpha(1-\alpha)ma_1}{(\lambda_\alpha - 3\alpha)\lambda_\alpha - (1-\alpha)^2 m} &< \frac{2\sqrt{2}(n-4)\alpha(1-\alpha)a_1}{(\lambda_\alpha - 3\alpha)\left(\alpha(n-3) + \frac{2(1-\alpha)^2}{\alpha}\right) - 2\sqrt{2}(n-4)(1-\alpha)^2} \\
&= \frac{2\sqrt{2}\alpha(1-\alpha)a_1}{(\lambda_\alpha - 3\alpha)\alpha + \frac{(\lambda_\alpha - 3\alpha)\left(\alpha + \frac{2(1-\alpha)^2}{\alpha}\right)}{n-4} - 2\sqrt{2}(1-\alpha)^2}. \qquad (49)
\end{aligned}$$

Note that $n \geqslant 11$ and $\alpha \geqslant 1-\alpha$. By (38),

$$\begin{aligned}
(\lambda_\alpha - 3\alpha)\left(\alpha + \frac{2(1-\alpha)^2}{\alpha}\right) &> \left((n-6)\alpha + \frac{2(1-\alpha)^2}{\alpha}\right)\left(\alpha + \frac{2(1-\alpha)^2}{\alpha}\right) \\
&= (n-10)\alpha^2 + 2(n-5)(1-\alpha)^2 + 4\left(\alpha^2 + \frac{(1-\alpha)^4}{\alpha^2}\right) \\
&\geqslant (n-10)\alpha^2 + 2(n-5)(1-\alpha)^2 + 8(1-\alpha)^2 \\
&\geqslant 3(n-4)(1-\alpha)^2. \qquad (50)
\end{aligned}$$

Together with (49), one has

$$b_1 < \frac{2\sqrt{2}(1-\alpha)a_1}{\lambda_\alpha - 3\alpha}. \qquad (51)$$

As $n \geqslant 11$, by (38), we obtain $\lambda_\alpha > (n-3)\alpha \geqslant 8\alpha$. Together with (46) and (51), one has

$$\frac{b_1}{b_3} < \frac{2\sqrt{2}(1-\alpha)a_1}{\lambda_\alpha - 3\alpha} \cdot \frac{\lambda_\alpha - \alpha}{(1-\alpha)a_1} = \frac{2\sqrt{2}(\lambda_\alpha - \alpha)}{\lambda_\alpha - 3\alpha} = 2\sqrt{2} + \frac{4\sqrt{2}\alpha}{\lambda_\alpha - 3\alpha} < \frac{14\sqrt{2}}{5} < 4.$$

Consequently, $b_1 < 4b_3$.

Furthermore, if $a_2 \leqslant \frac{a_1}{2}$, then $a_3 \leqslant a_2 \leqslant \frac{a_1}{2}$. And so by (43), (44) and (47), one has

$$\lambda_\alpha^2 b_1 < 3\alpha\lambda_\alpha b_1 + \frac{\alpha(1-\alpha)(m+n-3)a_1}{2} + (1-\alpha)^2 mb_1. \qquad (52)$$

Note that $n \geqslant 11$, $m \leqslant 2\sqrt{2}(n-4)$, we have

$$m + n - 3 \leqslant (2\sqrt{2}+1)n - 8\sqrt{2} - 3 < 4(n-4).$$

Together with (38), (50) and (52), one has

$$b_1 < \frac{2\alpha(1-\alpha)a_1}{(\lambda_\alpha - 3\alpha)\alpha + \frac{(\lambda_\alpha-3\alpha)\left(\alpha+\frac{2(1-\alpha)^2}{\alpha}\right)}{n-4} - 2\sqrt{2}(1-\alpha)^2} < \frac{2(1-\alpha)a_1}{\lambda_\alpha - 3\alpha}. \tag{53}$$

As $n \geqslant 11$, by (38), one obtains $\lambda_\alpha > (n-3)\alpha \geqslant 8\alpha$. Together with (46) and (53), one has

$$\frac{b_1}{b_3} < \frac{2(1-\alpha)a_1}{\lambda_\alpha - 3\alpha} \cdot \frac{\lambda_\alpha - \alpha}{(1-\alpha)a_1} = \frac{2(\lambda_\alpha - \alpha)}{\lambda_\alpha - 3\alpha} = 2 + \frac{4\alpha}{\lambda_\alpha - 3\alpha} < \frac{14}{5} < 3.$$

Therefore, $b_1 < 3b_3$. □

Claim 31. *If* $m \geqslant 3(n-6)$, *then* $b_3 < \frac{13\alpha a_2}{24(1-\alpha)}$.

Proof of Claim 31. Consider the graph G^* and the Perron vector $\mathbf{x}$. Applying (1) to u_1 and u_2, respectively, gives us

$$\begin{aligned}\lambda_\alpha a_1 &= \alpha(n-3)a_1 + (1-\alpha)(sb_1 + (t-s)b_2 + (n-3-t)b_3)\\ &= \alpha(n-3)a_1 + (1-\alpha)(sb_1 + (t-s)b_2) + \frac{(1-\alpha)^2(n-3-t)a_1}{\lambda_\alpha - \alpha}, \qquad \text{(by (46))}\\ \lambda_\alpha a_2 &= \alpha t a_2 + (1-\alpha)(sb_1 + (t-s)b_2).\end{aligned}$$

Then

$$a_1 = \frac{(\lambda_\alpha - \alpha t)a_2}{\lambda_\alpha - \alpha(n-3) - \frac{(1-\alpha)^2(n-3-t)}{\lambda_\alpha-\alpha}}. \tag{54}$$

Recall that $m \geqslant 3(n-6)$. Together with (43), one has $t \geqslant \frac{m-n+3}{2} \geqslant n - \frac{15}{2}$. On the other hand, $m \geqslant 2n-3$, and so $t \geqslant \frac{m-n+3}{2} \geqslant \frac{n}{2}$. Together with (38) and (54), we have

$$a_1 < \frac{(\lambda_\alpha - \alpha(n-\frac{15}{2}))a_2}{\lambda_\alpha - \alpha(n-3) - \frac{(1-\alpha)^2(\frac{n}{2}-3)}{\alpha(n-4)}} < \frac{(\lambda_\alpha - \alpha(n-\frac{15}{2}))a_2}{\lambda_\alpha - \alpha(n-3) - \frac{(1-\alpha)^2}{2\alpha}}. \tag{55}$$

Now together with (46) and (55), one has

$$\begin{aligned}b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha - \alpha} &< \frac{1-\alpha}{\lambda_\alpha-\alpha} \cdot \frac{(\lambda_\alpha - \alpha(n-\frac{15}{2}))a_2}{\lambda_\alpha - \alpha(n-3) - \frac{(1-\alpha)^2}{2\alpha}}\\ &= \frac{1-\alpha}{\lambda_\alpha-\alpha} \cdot \left(1 + \frac{\frac{9\alpha}{2} + \frac{(1-\alpha)^2}{2\alpha}}{\lambda_\alpha - \alpha(n-3) - \frac{(1-\alpha)^2}{2\alpha}}\right) a_2\\ &< \frac{1-\alpha}{(n-4)\alpha + \frac{2(1-\alpha)^2}{\alpha}} \cdot \left(1 + \frac{9\alpha^2 + (1-\alpha)^2}{3(1-\alpha)^2}\right) a_2 \qquad \text{(by (38))}\\ &= \frac{1}{(n-4)\alpha + \frac{2(1-\alpha)^2}{\alpha}} \cdot \frac{9\alpha^2 + 4(1-\alpha)^2}{3(1-\alpha)} a_2. \end{aligned} \tag{56}$$

Note that $n \geqslant 11$ and $1-\alpha \leqslant \alpha$. If $1-\alpha \leqslant \frac{\sqrt{2}\alpha}{2}$, then (56) gives

$$b_3 < \frac{1}{(n-4)\alpha} \cdot \frac{9\alpha^2 + 2\alpha^2}{3(1-\alpha)} a_2 = \frac{11\alpha a_2}{3(n-4)(1-\alpha)} \leqslant \frac{11\alpha a_2}{21(1-\alpha)}. \tag{57}$$

If $\frac{\sqrt{2}\alpha}{2} < 1-\alpha \leqslant \alpha$, then (56) gives

$$b_3 < \frac{1}{(n-3)\alpha} \cdot \frac{13\alpha^2}{3(1-\alpha)} a_2 = \frac{13\alpha a_2}{3(n-3)(1-\alpha)} \leqslant \frac{13\alpha a_2}{24(1-\alpha)}. \tag{58}$$

Together with (57) and (58), one has $b_3 < \frac{13\alpha a_2}{24(1-\alpha)}$, as desired. □

Claim 32. *It holds that*

$$a'_2 < \frac{(\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3))a'_1}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}, \quad b'_2 = \frac{2(1-\alpha)a'_1}{\lambda_\alpha(K^m_{3,n-3}) - 2\alpha}.$$

Proof of Claim 32. Consider the graph $K^m_{3,n-3}$ and the Perron vector $\mathbf{y}$. Applying (1) to u_1, u_3 and v_{n-3}, respectively, gives us

$$\lambda_\alpha(K^m_{3,n-3})a'_1 = \alpha(n-3)a'_1 + (1-\alpha)((m-2n+6)b'_1 + (3n-9-m)b'_2), \tag{59}$$

$$\lambda_\alpha(K^m_{3,n-3})a'_2 = \alpha(m-2n+6)a'_2 + (1-\alpha)(m-2n+6)b'_1, \tag{60}$$

$$\lambda_\alpha(K^m_{3,n-3})b'_2 = 2\alpha b'_2 + 2(1-\alpha)a'_1. \tag{61}$$

Then (59) and (60) give

$$a'_2 = \frac{(1-\alpha)(m-2n+6)b'_1}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)} < \frac{(\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3))a'_1}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}.$$

And (61) gives

$$b'_2 = \frac{2(1-\alpha)a'_1}{\lambda_\alpha(K^m_{3,n-3}) - 2\alpha},$$

as desired. □

Recall that

$$K^m_{3,n-3} = G^* - \{u_3 v_i | m-2n+7 \leqslant i \leqslant s\} + \{u_2 v_i | t+1 \leqslant i \leqslant n-3\}.$$

According to Lemma 15, one has

$$\begin{aligned}
\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K^m_{3,n-3}) - \lambda_\alpha) &= \mathbf{x}^T(A_\alpha(K^m_{3,n-3}) - A_\alpha(G^*))\mathbf{y} \\
&= \alpha\left[\sum_{i=t+1}^{n-3}(\mathbf{x}_{u_2}\mathbf{y}_{u_2} + \mathbf{x}_{v_i}\mathbf{y}_{v_i}) - \sum_{i=m-2n+7}^{s}(\mathbf{x}_{u_3}\mathbf{y}_{u_3} + \mathbf{x}_{v_i}\mathbf{y}_{v_i})\right] \\
&\quad + (1-\alpha)\left[\sum_{i=t+1}^{n-3}(\mathbf{x}_{u_2}\mathbf{y}_{v_i} + \mathbf{x}_{v_i}\mathbf{y}_{u_2}) - \sum_{i=m-2n+7}^{s}(\mathbf{x}_{u_3}\mathbf{y}_{v_i} + \mathbf{x}_{v_i}\mathbf{y}_{u_3})\right] \\
&= (n-3-t)[\alpha(a_2a'_1 + b_3b'_2 - a_3a'_2 - b_1b'_2) \\
&\quad + (1-\alpha)(a_2b'_2 + b_3a'_1 - a_3b'_2 - b_1a'_2)].
\end{aligned}$$

Note that $t \leqslant n-4$, $a_3 \leqslant a_2$. Then

$$\frac{\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K_{3,n-3}^m)-\lambda_\alpha)}{n-3-t} \geqslant \alpha[a_2(a_1'-a_2')+b_2'(b_3-b_1)]+(1-\alpha)(a_1'b_3-a_2'b_1). \tag{62}$$

Note that $a_2 \leqslant a_1$, according to the relationship between a_1 and a_2, we consider the following two cases.

Case 1. $\frac{a_1}{2} < a_2 \leqslant a_1$. In this case, together with Claims 30, 32 and (62), one has

$$\begin{aligned}
&\frac{\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K_{3,n-3}^m)-\lambda_\alpha)}{n-3-t}\\
&> \alpha\left[a_2\left(a_1' - \frac{(\lambda_\alpha(K_{3,n-3}^m)-\alpha(n-3))a_1'}{\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6)}\right) - \frac{6(1-\alpha)a_1'b_3}{\lambda_\alpha(K_{3,n-3}^m)-2\alpha}\right]\\
&\quad + (1-\alpha)\left[a_1'b_3 - \frac{4(\lambda_\alpha(K_{3,n-3}^m)-\alpha(n-3))a_1'b_3}{\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6)}\right].
\end{aligned}$$

Then

$$\begin{aligned}
&\frac{\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K_{3,n-3}^m)-\lambda_\alpha)}{(n-3-t)a_1'}\\
&> \alpha\left[1 - \frac{\lambda_\alpha(K_{3,n-3}^m)-\alpha(n-3)}{\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6)}\right]a_2\\
&\quad + (1-\alpha)\left[1 - \frac{6\alpha}{\lambda_\alpha(K_{3,n-3}^m)-2\alpha} - \frac{4(\lambda_\alpha(K_{3,n-3}^m)-\alpha(n-3))}{\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6)}\right]b_3\\
&> \frac{(3n-9-m)\alpha^2a_2 + (1-\alpha)[-3\lambda_\alpha(K_{3,n-3}^m)+\alpha(6n-24-m)]b_3}{\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6)},
\end{aligned} \tag{63}$$

where the inequality in (63) follows by $m \geqslant 2n-3$.

Note that $m \leqslant 2\sqrt{2}(n-4) < 3n-9$, $\lambda_\alpha(K_{3,n-3}^m) > \lambda_\alpha(K_{2,n-3}) > \alpha(n-3)$. We have $\lambda_\alpha(K_{3,n-3}^m)-\alpha(m-2n+6) > 0$ and $3n-9-m > 0$.

If $-3\lambda_\alpha(K_{3,n-3}^m)+\alpha(6n-24-m) \geqslant 0$, then by (63), one has $\lambda_\alpha(K_{3,n-3}^m) > \lambda_\alpha$, a contradiction to the choice of G^*.

If $-3\lambda_\alpha(K_{3,n-3}^m)+\alpha(6n-24-m) < 0$. Note that $a_2 > \frac{a_1}{2}$, $b_3 = \frac{(1-\alpha)a_1}{\lambda_\alpha-\alpha} < \frac{(1-\alpha)a_1}{\alpha(n-4)} < \frac{a_1}{6}$. Then

$$\begin{aligned}
&(3n-9-m)\alpha^2a_2 + (1-\alpha)[-3\lambda_\alpha(K_{3,n-3}^m)+\alpha(6n-24-m)]b_3\\
&> \frac{(3n-9-m)\alpha^2a_1}{2} + \frac{\alpha[-3\lambda_\alpha(K_{3,n-3}^m)+\alpha(6n-24-m)]a_1}{6}.
\end{aligned} \tag{64}$$

As $K_{3,n-3}^m$ is a proper subgraph of $K_{3,n-3}$, by the Perron-Frobenius theory, $\lambda_\alpha(K_{3,n-3}^m) <$

$\lambda_\alpha(K_{3,n-3})$. And so by Lemma 19, $\lambda_\alpha(K^m_{3,n-3}) < \alpha n$. Together with (64),

$$
\begin{aligned}
&(3n-9-m)\alpha^2 a_2 + (1-\alpha)[-3\lambda_\alpha(K^m_{3,n-3}) + \alpha(6n-24-m)]b_3 \\
>& \frac{\alpha a_1}{6}[(9n-27-3m)\alpha - 3\alpha n + \alpha(6n-24-m)] \\
\geqslant& \frac{\alpha^2 a_1}{6}((12-8\sqrt{2})n + 32\sqrt{2} - 51) && \text{(by } m \leqslant 2\sqrt{2}(n-4))\\
\geqslant& \frac{\alpha^2 a_1}{6}(81-56\sqrt{2}) && \text{(by } n \geqslant 11)\\
>& 0.
\end{aligned}
$$

Together with (63) and $\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6) > 0$, we have $\lambda_\alpha(K^m_{3,n-3}) > \lambda_\alpha$, a contradiction to the choice of G^*.

Case 2. $a_2 \leqslant \frac{a_1}{2}$. In this case, by Claim 30, $b_1 < 3b_3$. Together with (62) and Claim 32, one has

$$
\begin{aligned}
&\frac{\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K^m_{3,n-3}) - \lambda_\alpha)}{n-3-t} \\
>& \alpha\left[a_2\left(a_1' - \frac{(\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3))a_1'}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}\right) - \frac{4(1-\alpha)a_1' b_3}{\lambda_\alpha(K^m_{3,n-3}) - 2\alpha}\right] \\
&+ (1-\alpha)\left[a_1' b_3 - \frac{3(\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3))a_1' b_3}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}\right].
\end{aligned}
$$

Then

$$
\begin{aligned}
&\frac{\mathbf{x}^T\mathbf{y}(\lambda_\alpha(K^m_{3,n-3}) - \lambda_\alpha)}{(n-3-t)a_1'} \\
>& \alpha\left[1 - \frac{\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3)}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}\right] a_2 \\
&+ (1-\alpha)\left[1 - \frac{4\alpha}{\lambda_\alpha(K^m_{3,n-3}) - 2\alpha} - \frac{3(\lambda_\alpha(K^m_{3,n-3}) - \alpha(n-3))}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}\right] b_3 \\
>& \frac{(3n-9-m)\alpha^2 a_2 + (1-\alpha)[-2\lambda_\alpha(K^m_{3,n-3}) + \alpha(5n-19-m)]b_3}{\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6)}, \qquad (65)
\end{aligned}
$$

where the inequality in (65) follows by $m \geqslant 2n-3$. Note that $3n-9-m > 0$ and $\lambda_\alpha(K^m_{3,n-3}) - \alpha(m-2n+6) > 0$.

If $-2\lambda_\alpha(K^m_{3,n-3}) + \alpha(5n-19-m) \geqslant 0$, then by (65), one has $\lambda_\alpha(K^m_{3,n-3}) > \lambda_\alpha$, a contradiction to the choice of G^*.

If $-2\lambda_\alpha(K^m_{3,n-3}) + \alpha(5n-19-m) < 0$, then we proceed by the following discussion. As $\lambda_\alpha(K^m_{3,n-3}) < \alpha n$, one has $\alpha(-2n+5n-19-m) < 0$. And so $m > 3n-19$, that is

$m \geqslant 3n-18$. By Claim 31, $b_3 < \frac{13\alpha a_2}{24(1-\alpha)}$. Note that $m \leqslant 2\sqrt{2}(n-4)$, then

$$\begin{aligned}
&(3n-9-m)\alpha^2 a_2 + (1-\alpha)[-2\lambda_\alpha(K_{3,n-3}^m) + \alpha(5n-19-m)]b_3 \\
&> (3n-9-m)\alpha^2 a_2 + \frac{13\alpha a_2}{24}[-2\lambda_\alpha(K_{3,n-3}^m) + \alpha(5n-19-m)] \\
&> (3n-9-2\sqrt{2}n+8\sqrt{2})\alpha^2 a_2 + \frac{13\alpha a_2}{24}[-2\alpha n + \alpha(5n-19-2\sqrt{2}n+8\sqrt{2})] \\
&= \frac{(111-74\sqrt{2})n - 463 + 296\sqrt{2}}{24}\alpha^2 a_2 \\
&\geqslant \frac{758-518\sqrt{2}}{24}\alpha^2 a_2 \qquad \text{(by } n \geqslant 11) \\
&> 0.
\end{aligned}$$

Together with (65) and $\lambda_\alpha(K_{3,n-3}^m) - \alpha(m-2n+6) > 0$, one has $\lambda_\alpha(K_{3,n-3}^m) > \lambda_\alpha$, a contradiction to the choice of G^*.

Therefore, $t = n-3$, and so $G^* = K_{3,n-3}^m$. □

5 Further discussions

In this paper, we give answers to Question 6 for $1 \leqslant m \leqslant 2\sqrt{2}(n-4)$, $\frac{1}{2} \leqslant \alpha < 1$ and $m = k(n-k)$, $\frac{1}{2} \leqslant \alpha < 1$, where k is an integer with $2 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$. Take $\alpha = \frac{1}{2}$ in Theorems 8-10, we may obtain the corresponding results for Q-index.

Corollary 33. *Let $m = k(n-k)$ be given, where k is an integer with $2 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$. If $G \in \mathbb{B}(n,m)$, then $q(G) \leqslant q(K_{k,n-k})$, with equality if and only if $G \cong K_{k,n-k}$.*

Corollary 34. *Let $n \leqslant m \leqslant 2n-5$ be given. If $G \in \mathbb{B}(n,m)$, then $q(G) \leqslant q(K_{2,n-2}^m)$, with equality if and only if $G \cong K_{2,n-2}^m$.*

Corollary 35. *Let $2n-3 \leqslant m \leqslant 2\sqrt{2}(n-4)$ be given. If $G \in \mathbb{B}(n,m)$, then $q(G) \leqslant q(K_{3,n-3}^m)$, with equality if and only if $G \cong K_{3,n-3}^m$.*

Note that if G is a bipartite graph, then $\mu(G) = q(G)$, i.e., the L- and Q-indices of G are coincide. As $K_{k,n-k}$ and $K_{2,n-2}^m$ are connected for all positive integers k, n, m with $n \leqslant m \leqslant 2n-5$, the main results in [30] can be deduced (see [30, Theorems 2.3, 2.4]).

On the other hand, it is clear that Corollary 33 gives an answer to Questions 4 and 5 for $2 \leqslant p \leqslant q$ and $m = pq$; Corollary 34 gives an answer to Questions 4 and 5 for $p = 2 \leqslant q$ and $q+2 \leqslant m \leqslant 2q-1$; Corollary 35 gives an answer to Questions 4 and 5 for $p = 3 \leqslant q$ and $2q+3 \leqslant m \leqslant 2\sqrt{2}(q-1)$.

Furthermore, by observing the extremal graphs in Theorems 8-10, we believe the following conjecture is true.

Conjecture 36. For $1 \leqslant k \leqslant \lfloor \frac{n}{2} \rfloor$ and $\frac{1}{2} \leqslant \alpha < 1$. If $(k-1)(n-k+1)+1 \leqslant m \leqslant k(n-k)$ and $G \in \mathbb{B}(n,m)$, then $\lambda_\alpha(G) \leqslant \lambda_\alpha(K_{k,n-k}^m)$. Equality holds if and only if $G \cong K_{k,n-k}^m$.

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