ON THE SPECTRAL RADIUS OF BIPARTITE GRAPHS WITH GIVEN ORDER AND 4-INDEPENDENCE NUMBER

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Abstract. For a positive integer k, let P_k be a path of order k. For a graph G, a subset $S \subseteq V(G)$ is called a k-independent set if the induced subgraph $G[S]$ does not contain P_k as its subgraph. The k-independence number of G, denoted by $\alpha_k(G)$, is the maximum cardinality of a k-independent set in G. Let $\mathscr{B}_{n,\alpha_k}$ be the set of bipartite graphs of order n with k-independence number α_k. What are the corresponding extremal graphs in $\mathscr{B}_{n,\alpha_k}$ with the maximum spectral radius? Lou and Guo [*Discrete Math.* **345** (2022) 112778] solved the problem for $k = 2$, and then Huang *et al.* [*Discrete Appl. Math.* **342** (2024) 368–380] provided the answer for $k = 3$. We are interested in the analogous problem for $k = 4$. In the paper, we determine the unique graph attaining the maximum spectral radius among all bipartite graphs in $\mathscr{B}_{n,\alpha_4}$.

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1. Introduction

In this paper, a graph means a simple undirected graph. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ of order $n = |V(G)|$ and edge set $E(G)$. The *adjacency matrix* $A(G)$ of G is an $n \times n$ matrix whose (i, j)-entry is 1 if vertices v_i and v_j are adjacent, and 0 otherwise. The largest eigenvalue of $A(G)$ is called the *spectral radius* of G, denoted by $\rho(G)$. By the Perron–Frobenius theorem, for a connected graph G, there exists a unique positive unit vector $\boldsymbol{x}$ called the *Perron vector* such that $A(G)\boldsymbol{x} = \rho(G)\boldsymbol{x}$. Denote by $N_G(v)$ the set of neighbors of a vertex v in G. The degree of v is $d_G(v) = |N_G(v)|$. For any vertex $v \in V(G)$ and any subset $S \subseteq V(G)$, let $N_S(v) = N_G(v) \cap S$ and $d_S(v) = |N_G(v) \cap S|$. For $X \subseteq V(G)$, let $G[X]$ be the subgraph of G induced by X. As usual, let P_n, K_n and $K_{a,b}$ be the path of order n, the complete graph of order n and the complete bipartite graph with two parts of sizes a and b, respectively.

A vertex subset $S \subseteq V(G)$ of G is called an *independent set* if no two vertices in S are adjacent. The *independence number* of G, denoted by $\alpha(G)$, is the maximum cardinality of an independent set in G. A vertex subset $S \subseteq V(G)$ is a *dissociation set* if the induced subgraph $G[S]$ has maximum degree at most 1. The *dissociation number* of G, denoted by $\varphi(G)$, is the maximum cardinality of a dissociation set in G. Note that every independent set is a dissociation set. For a positive integer k, a subset $S \subseteq V(G)$ is called a *k-independent set* if the induced subgraph $G[S]$ does not contain P_k as a subgraph. The *k-independence number* of G, denoted

by $\alpha_k(G)$, is the maximum cardinality of a k-independent set in G. It is obvious that $\alpha_2(G) = \alpha(G)$ and $\alpha_3(G) = \varphi(G)$.

In the 1960s, Erdős and Moser put forward the problem of finding the maximum number of maximal independent sets among all graphs of order n. In 1965, Moon and Moser [13] solved this problem. After that, numerous researchers began to explore the counting problems of maximal independent sets and maximum independent sets for various kinds of graphs, such as trees [16], unicyclic connected graphs [9], bipartite graphs [11], triangle-free graphs [7], among others. Based on the inspiration of the above findings, scholars started to study the counting of other graph substructures. For further results, see [1, 14, 15].

In 1986, Brualdi and Solheid [3] proposed the following interesting problem: which graph achieves the maximum or minimum spectral radius in a given class of graphs? Since then, this problem has been studied extensively. In 2016, Ji and Lu [8] determined the trees attaining the maximum spectral radius among all trees with given order n and independence number α. A connected graph is called a bi-block graph if each of its blocks is a complete bipartite graph. In 2021, Das and Mohanty [4] characterized the extremal graph attaining the maximum spectral radius among all bi-block graphs of order n and independence number α. Subsequently, Lou and Guo [12] extended the above result to general bipartite graphs. In 2024, Huang *et al.* [6] characterized the connected graphs (resp. bipartite graphs, trees) that attain the maximum spectral radius among all connected graphs (resp. bipartite graphs, trees) with given order n and dissociation number φ. Furthermore, they proved that the connected graph of order n with dissociation number φ attaining the minimum spectral radius is a tree, where $\varphi \geq \lceil \frac{2}{3}n \rceil$. Additionally, they determined the extremal graphs attaining the minimum spectral radius with fixed order n and dissociation number $\varphi \in \{2, \lceil \frac{2n}{3} \rceil, n-1, n-2\}$.

For an integer $k \geq 2$, a vertex subset $S \subseteq V(G)$ is called a *generalized k-independent set* if the induced subgraph $G[S]$ does not contain a k-tree (a tree with k vertices) as a subgraph. The *generalized k-independence number* of G is the maximum cardinality of a generalized k-independent set in G. By definition, the generalized k-independence number is a natural generalization of the independence number and the dissociation number. Note that every generalized k-independent set is a k-independent set, but the reverse implication does not hold for $k \geq 4$. A canonical example is the star graph $K_{1,t}$ (where $t \geq 3$), which contains $K_{1,3}$ (a 4-tree) as a subgraph but does not contain P_4. Recently, Li and Zhou [10] determined the connected graphs (resp. bipartite graphs, trees) attaining the maximum spectral radius among all connected graphs (resp. bipartite graphs, trees) with fixed order and generalized 4-independence number.

Motivated by the aforementioned spectral extremal results, we are interested in investigating the extremal graph that attains the maximum spectral radius among all bipartite graphs with fixed order n and 4-independence number α_4. In the paper, we establish a complete solution to this problem. Let $\mathscr{B}_{n,\alpha_4}$ be the set of bipartite graphs of order n with 4-independence number α_4. Our main result is as follows.

Theorem 1. *Let* $G \in \mathscr{B}_{n,\alpha_4}$. *Then* $\rho(G) \leq \sqrt{(\alpha_4 - 1)(n - \alpha_4 + 1)}$, *with equality if and only if* $G \cong K_{\alpha_4-1, n-\alpha_4+1}$.

2. Proof of Theorem 1

In this section, we present the proof of Theorem 1. First, we list the lemmas that will be used later.

Lemma 1 ([5]). *Let G be a connected graph and G' be a proper subgraph of G. Then $\rho(G') < \rho(G)$.*

Lemma 2 ([2]). *Let G be a connected graph and $\rho(G)$ be the spectral radius of $A(G)$. Let u, v be two vertices of G. Suppose that $v_1, v_2, \ldots, v_s \in N_G(v) \setminus N_G(u)$ with $1 \leq s \leq d_G(v)$, and G^* is the graph obtained from G by deleting the edges vv_i and adding the edges uv_i for $1 \leq i \leq s$. Let $\boldsymbol{x}$ be the Perron vector of $A(G)$. If $x_u \geq x_v$, then $\rho(G) < \rho(G^*)$.*

Let M be a real $n \times n$ matrix, and let $V = \{1, 2, \ldots, n\}$. Given a partition $\Pi = \{V_1, V_2, \ldots, V_k\}$ with $V = V_1 \cup V_2 \cup \cdots \cup V_k$. The matrix M is described in the following block form:

$$M = \begin{pmatrix} M_{11} & M_{12} & \cdots & M_{1k} \\ M_{21} & M_{22} & \cdots & M_{2k} \\ \vdots & \vdots & \ddots & \vdots \\ M_{k1} & M_{k2} & \cdots & M_{kk} \end{pmatrix}.$$

The *quotient matrix* of M with respect to Π is defined as the $k \times k$ matrix $B_\Pi(M) = (b_{ij})_{i,j=1}^k$, where b_{ij} is the average row sum of M_{ij}. The partition Π is called an *equitable partition* if each block M_{ij} has constant row sum b_{ij}. Additionally, we say that the quotient matrix $B_\Pi(M)$ is *equitable* if Π is an equitable partition of M.

Lemma 3 ([2]). *Let M be a real symmetric matrix, and let $\rho(M)$ be the spectral radius of M. If $B_\Pi(M)$ is an equitable quotient matrix of M, then the eigenvalues of $B_\Pi(M)$ are also eigenvalues of M. Furthermore, if M is a nonnegative irreducible matrix, then $\rho(M) = \rho(B_\Pi(M))$.*

Now, we shall give the proof of Theorem 1, which determines the unique graph attaining the maximum spectral radius among all bipartite graphs in $\mathscr{B}_{n,\alpha_4}$.

Proof of Theorem 1. Suppose that $G' = (X, Y)$ is the connected bipartite graph that attains the maximum spectral radius in $\mathscr{B}_{n,\alpha_4}$. Without loss of generality, assume that $|X| \geq |Y|$. Let S be a maximum 4-independent set of G'. Then $\alpha_4 = |S| \geq |X| + 1 \geq \lceil \frac{n}{2} \rceil + 1$.

If $n = 2$, then $G' \cong K_2$. If $n = 3$, then $G' \cong K_{2,1}$. If $n \geq 4$ and $\alpha_4 = |X| + 1$, then $G' \cong K_{\alpha_4-1, n-\alpha_4+1}$ by Lemma 1. In the following, we may assume that $n \geq 4$ and $\alpha_4 > |X| + 1$. Then S can be partitioned as $S = X_1 \cup Y_2$ with $X_1 \subseteq X$ and $Y_2 \subseteq Y$. Let $X_2 = X \setminus X_1$ and $Y_1 = Y \setminus Y_2$, and let $|X_1| = a$, $|Y_1| = b$, $|X_2| = c$ and $|Y_2| = d$. Set $X_1 = \{v_1, \ldots, v_a\}$, $Y_1 = \{z_1, \ldots, z_b\}$, $X_2 = \{u_1, \ldots, u_c\}$, and $Y_2 = \{w_1, \ldots, w_d\}$. Since $|X_1 \cup Y_2| = |S| > |X| + 1 \geq |Y| + 1$, we can deduce that $d > c + 1$ and $a > b + 1$. Consequently, $d \geq 2$ and $a \geq 2$. By the maximality of $\rho(G')$ and Lemma 1, we obtain that the subgraphs induced by (X_1, Y_1) and (X_2, Y) are complete bipartite graphs, and (X_1, Y_2) contains edges as many as possible such that it contains no P_4. We distinguish the following three cases according to the values of a and d.

Case 1. $a = d$.

Since G' is connected and the induced subgraph $G'[X_1 \cup Y_2]$ does not contain P_4 as its subgraph, we have $\max\{b, c\} \geq 1$. Then $a = d \geq 3$. Now, we divide this case into the following three subcases.

Subcase 1.1. $b = 0$.

For $b = 0$, we have $c \geq 1$ and $d_{G'}(v) = d_{Y_2}(v) \geq 1$ for all $v \in X_1$.

Subcase 1.1.1. $d_{G'}(v_i) = 1$ for all $1 \leq i \leq a$.

We claim that $N_{G'}(v_i) = N_{G'}(v_j)$ for $i \neq j$. Otherwise, assume that $d_{G'}(w_1) = \max\{d_{G'}(w_i) \mid 1 \leq i \leq d\}$. Then $d_{X_1}(w_1) = \max\{d_{X_1}(w_i) \mid 1 \leq i \leq d\}$ due to $d_{X_2}(w_i) = c$. Let $\boldsymbol{x}$ be the Perron vector of $A(G')$. By symmetry, we may assume that $x_{u_1} = x_{u_j}$ for $2 \leq j \leq c$ and $x_v = x'_i$ for $v \in N_{X_1}(w_i)$, where $1 \leq i \leq d$. Therefore, from $A(G')\boldsymbol{x} = \rho(G')\boldsymbol{x}$, we have

$$\rho(G')x_{w_i} = d_{X_1}(w_i)x'_i + cx_{u_1}$$

and

$$\rho(G')x'_i = x_{w_i},$$

where $1 \leq i \leq d$. From which we get

$$\left(\rho^2(G') - d_{X_1}(w_1)\right)x_{w_1} = \left(\rho^2(G') - d_{X_1}(w_i)\right)x_{w_i}.$$

Note that G' contains $K_{1,d_{X_1}(w_1)}$ as a proper subgraph. Then $\rho(G') > \rho(K_{1,d_{X_1}(w_1)}) = \sqrt{d_{X_1}(w_1)}$. Thus, we can deduce that $x_{w_1} = \frac{\rho^2(G')-d_{X_1}(w_i)}{\rho^2(G')-d_{X_1}(w_1)}x_{w_i} \geq x_{w_i}$ for $2 \leq i \leq d$. Let $G_1 = G' - \{vw_i \mid v \in X_1 \setminus N_{X_1}(w_1), 2 \leq i \leq d\} + \{vw_1 \mid v \in X_1 \setminus N_{X_1}(w_1)\}$. Clearly, $G_1 \in \mathscr{B}_{n,\alpha_4}$ and $N_{G_1}(v_i) = \{w_1\}$ for $1 \leq i \leq a$. According to Lemma 2, we have $\rho(G_1) > \rho(G')$, which contradicts the maximality of $\rho(G')$. Therefore, the partition $\Pi_1 : V(G') = X_1 \cup X_2 \cup \{w_1\} \cup Y_2 \setminus \{w_1\}$ is an equitable partition of G', and the corresponding quotient matrix can be written as follows:

$$B_{\Pi_1}(G') = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & a-1 \\ a & c & 0 & 0 \\ 0 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_4 - B_{\Pi_1}(G')) = \lambda^4 - a(1+c)\lambda^2 + ac(a-1).$$

Consider the following real function

$$f(t) = t^4 - a(1+c)t^2 + ac(a-1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $f(t) = 0$. Some direct calculations show that

$$f\left(\sqrt{(2a-1)(c+1)}\right) = (2a-1)(c+1)^2(a-1) + ac(a-1) > 0$$

and

$$f'\left(\sqrt{(2a-1)(c+1)}\right) = 2(c+1)(3a-2)\sqrt{(2a-1)(c+1)} > 0.$$

Note that the derivative function of $f'(t)$ is $f''(t) = 12t^2 - 2a(1+c)$. Obviously, $f''(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. Thus, $f''(t) > f''(\sqrt{(2a-1)(c+1)}) = 2(c+1)(11a-6) > 0$. Therefore, $f'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. It follows that $f'(t) > f'(\sqrt{(2a-1)(c+1)}) > 0$, and then $f(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. Consequently, $\rho(G') < \sqrt{(2a-1)(c+1)} = \rho(K_{2a-1,c+1})$, which contradicts the choice of G' since $\alpha_4(K_{2a-1,c+1}) = 2a = \alpha_4(G')$.

Subcase 1.1.2. $d_{G'}(v_i) \geq 2$ for some $1 \leq i \leq a$.

Observe that if there exists a vertex $v \in X_1$ with $d_{G'}(v) \geq 2$, then there must exist at least one vertex $w \in Y_2$ such that $d_{X_1}(w) \geq 2$. Moreover, we have $d_{X_1}(w) \geq 1$ for all $w \in Y_2$. If not, there exist a vertex $v_i \in X_1$ with $d_{G'}(v_i) \geq 2$ and a vertex $w_j \in Y_2$ with $d_{X_1}(w_j) = 0$. Let $G'' = G' + \{v_iw_j\}$. Then $\rho(G'') > \rho(G')$, contradicting the maximality of $\rho(G')$. Without loss of generality, assume that $d_{G'}(v_1) = \max\{d_{G'}(v_i) \mid 1 \leq i \leq a\}$ and $d_{G'}(w_d) = \max\{d_{G'}(w_j) \mid 1 \leq j \leq d\}$. Since $d_{G'}(v_i) = d_{Y_2}(v_i)$ and $d_{X_2}(w_j) = c$, we have $d_{Y_2}(v_1) = \max\{d_{Y_2}(v_i) \mid 1 \leq i \leq a\}$ and $d_{X_1}(w_d) = \max\{d_{X_1}(w_j) \mid 1 \leq j \leq d\}$. Let $\boldsymbol{y}$ be the Perron vector of $A(G')$. For any vertex $v \in X_1$ with $d_{G'}(v) = 1$, let $w_i \in N_{Y_2}(v)$. Then $d_{X_1}(w_d) \geq d_{X_1}(w_i)$. From $A(G')\boldsymbol{y} = \rho(G')\boldsymbol{y}$, we can deduce that

$$\left(\rho^2(G') - d_{X_1}(w_d)\right)y_{w_d} = \left(\rho^2(G') - d_{X_1}(w_i)\right)y_{w_i}.$$

Note that G' contains $K_{1,d_{X_1}(w_d)}$ as a proper subgraph. Then $\rho(G') > \rho(K_{1,d_{X_1}(w_d)}) = \sqrt{d_{X_1}(w_d)}$. Thus, $y_{w_d} = \frac{\rho^2(G')-d_{X_1}(w_i)}{\rho^2(G')-d_{X_1}(w_d)}y_{w_i} \geq y_{w_i}$, where $w_i \in N_{Y_2}(v)$ for any vertex $v \in X_1$ with $d_{G'}(v) = 1$. For any vertex $v' \in X_1$ with $d_{G'}(v') \geq 2$, let $w_j \in N_{Y_2}(v')$. Then $d_{X_1}(w_j) = 1$ and $d_{G'}(v_1) \geq d_{G'}(v')$. Similarly, we can deduce that $y_{v_1} \geq y_{v'}$. Assume that $E_1 = \{vw_d \mid v \in X_1 \setminus N_{X_1}(w_d), d_{G'}(v) = 1\} + \{v_1w_i \mid w_i \in N_{Y_2}(v), v \in X_1 \setminus N_{X_1}(w_d), d_{G'}(v) = 1\} + \{w_jv_1 \mid w_j \in N_{Y_2}(v'), v' \in X_1 \setminus \{v_1\}, d_{G'}(v') \geq 2\} + \{v'w_d \mid v' \in X_1 \setminus \{v_1\}, d_{G'}(v') \geq 2\}$, $E_2 = \{vw_i \mid v \in X_1 \setminus N_{X_1}(w_d), d_{G'}(v) = 1, w_i \in N_{Y_2}(v)\} + \{w_jv' \mid w_j \in N_{Y_2}(v'), v' \in X_1 \setminus \{v_1\}, d_{G'}(v') \geq 2\}$ and $G_2 = G' + E_1 - E_2$. Clearly, $G_2 \in \mathscr{B}_{n,\alpha_4}$, $N_{Y_2}(v_i) = \{w_d\}$ for $2 \leq i \leq a$, and $N_{X_1}(w_j) = \{v_1\}$ for $1 \leq j \leq d-1$. According to Lemma 2, we have $\rho(G_2) > \rho(G')$, which contradicts the maximality of $\rho(G')$. Therefore, the

partition $\Pi_2 : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup X_2 \cup Y_2 \setminus \{w_d\} \cup \{w_d\}$ is an equitable partition of G', and the corresponding quotient matrix can be written as follows:

$$B_{\Pi_2}(G') = \begin{pmatrix} 0 & 0 & 0 & a-1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & a-1 & 1 \\ 1 & 0 & c & 0 & 0 \\ 0 & a-1 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_2}(G')) = \lambda^5 - (ac + 2a - 2)\lambda^3 + \left(1 - 2a + a^2 - ac + a^2 c\right)\lambda.$$

We may consider the real function

$$g(t) = t^4 - (ac + 2a - 2)t^2 + \left(1 - 2a + a^2 - ac + a^2 c\right)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $g(t) = 0$. Some direct calculations show that

$$g\left(\sqrt{(2a-1)(c+1)}\right) = (2a-1)(c+1)(ac - c + 1) + (a-1)(ac + a - 1) > 0$$

and

$$g'\left(\sqrt{(2a-1)(c+1)}\right) = 2(3ac + 2a - 2c)\sqrt{(2a-1)(c+1)} > 0.$$

Note that the derivative function of $g'(t)$ is $g''(t) = 12t^2 - 2(ac + 2a - 2)$. Obviously, $g''(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. Thus, $g''(t) > g''(\sqrt{(2a-1)(c+1)}) = 2(11ac + 10a - 6c - 4) > 0$. It follows that $g'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. Therefore, $g'(t) > g'(\sqrt{(2a-1)(c+1)}) > 0$, and then $g(t)$ is monotone increasing when $t > \sqrt{(2a-1)(c+1)}$. Consequently, $\rho(G') < \sqrt{(2a-1)(c+1)} = \rho(K_{2a-1,c+1})$, which contradicts the choice of G' since $\alpha_4(K_{2a-1,c+1}) = 2a = \alpha_4(G')$.

Subcase 1.2. $c = 0$.

Based on the previous assumptions that $|X| \geq |Y|$ and $a = d$, we have $c \geq b$. If $c = 0$, then $b = 0$, which contradicts $\max\{b, c\} \geq 1$. Thus, $c = 0$ is excluded.

Subcase 1.3. $b \geq 1$ and $c \geq 1$.

Recall that G' is the graph with the maximum spectral radius in $\mathscr{B}_{n,\alpha_4}$. By Lemma 1, each vertex in X_1 is adjacent to all vertices in Y_1, and each vertex in X_2 is adjacent to all vertices in Y. Consequently, G' is connected. Based on the assumptions that $|X| \geq |Y|$ and $a = d$, we have $c \geq b$. Furthermore, if $d_{Y_2}(v) \leq 1$ for each vertex $v \in X_1$, then in fact $d_{Y_2}(v) = 1$ for all $v \in X_1$. Otherwise, assume that there exists a vertex $v' \in X_1$ such that $d_{Y_2}(v') = 0$. Then there exists a vertex $w \in Y_2$ with $d_{X_1}(w) = 0$. Let $G^* = G' + \{v'w\}$. Then $\rho(G^*) > \rho(G')$, contradicting the maximality of $\rho(G')$. Similarly, we can obtain that if $d_{X_1}(w) \leq 1$ for every vertex $w \in Y_2$, then $d_{X_1}(w) = 1$ for all $w \in Y_2$. In the following, we consider three subcases.

Subcase 1.3.1. $d_{Y_2}(v_i) = 1$ for all $1 \leq i \leq a$.

Observe that either $d_{X_1}(w_l) = 1$ for all $1 \leq l \leq d$ or $d_{X_1}(w_l) \geq 2$ for some $1 \leq l \leq d$. Furthermore, we claim that $N_{G'}(v_i) = N_{G'}(v_j)$ for $i \neq j$. Otherwise, assume that $d_{G'}(w_1) = \max\{d_{G'}(w_i) \mid 1 \leq i \leq d\}$. Then $d_{X_1}(w_1) = \max\{d_{X_1}(w_i) \mid 1 \leq i \leq d\}$ since $d_{X_2}(w_i) = c$. Let $\boldsymbol{x}$ be the Perron vector of $A(G')$. By symmetry, we may assume that $x_{u_1} = x_{u_i}$ for $2 \leq i \leq c$, $x_{z_1} = x_{z_j}$ for $2 \leq j \leq b$ and $x_v = x_i'$ for $v \in N_{X_1}(w_i)$, where $1 \leq i \leq d$. Therefore, from $A(G')\boldsymbol{x} = \rho(G')\boldsymbol{x}$, we have

$$\rho(G')x_{w_i} = d_{X_1}(w_i)x_i' + cx_{u_1}$$

and

$$\rho(G')x_i' = x_{w_i} + bx_{z_1},$$

where $1 \leq i \leq d$. Thus we obtain

$$\left(\rho^2(G') - d_{X_1}(w_1)\right)x_{w_1} - \left(\rho^2(G') - d_{X_1}(w_i)\right)x_{w_i} = (d_{X_1}(w_1) - d_{X_1}(w_i))bx_{z_1} \geq 0.$$

Note that G' contains $K_{1,d_{X_1}(w_1)}$ as a proper subgraph. Then $\rho(G') > \rho(K_{1,d_{X_1}(w_1)}) = \sqrt{d_{X_1}(w_1)}$. Thus, $x_{w_1} \geq \frac{\rho^2(G') - d_{X_1}(w_i)}{\rho^2(G') - d_{X_1}(w_1)}x_{w_i} \geq x_{w_i}$ for $2 \leq i \leq d$. Let $G_3 = G' - \{vw_i \mid v \in X_1 \setminus N_{X_1}(w_1), 2 \leq i \leq d\} + \{vw_1 \mid v \in X_1 \setminus N_{X_1}(w_1)\}$. Clearly, $G_3 \in \mathscr{B}_{n,\alpha_4}$ and $N_{Y_2}(v_i) = \{w_1\}$ for $1 \leq i \leq a$. According to Lemma 2, we have $\rho(G_3) > \rho(G')$, which contradicts the maximality of $\rho(G')$. Therefore, the partition $\Pi_3 : V(G') = X_1 \cup X_2 \cup \{w_1\} \cup Y_2 \setminus \{w_1\} \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix can be written as follows:

$$B_{\Pi_3}(G') = \begin{pmatrix} 0 & 0 & 1 & 0 & b \\ 0 & 0 & 1 & a-1 & b \\ a & c & 0 & 0 & 0 \\ 0 & c & 0 & 0 & 0 \\ a & c & 0 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_3}(G')) = \lambda^5 - (bc + ac + ab + a)\lambda^3 + ac(ab + a - b - 1)\lambda.$$

We may consider the real function

$$h(t) = t^4 - (bc + ac + ab + a)t^2 + ac(ab + a - b - 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $h(t) = 0$. Some direct calculations show that

$$h\left(\sqrt{(2a-1)(b+c+1)}\right) = (2a-1)(b+c+1)[ab + (a-b-1)(c+1)] + ac(ab+a-b-1) > 0$$

and

$$h'\left(\sqrt{(2a-1)(b+c+1)}\right) = 2[2(a-b-1)(c+1) + a(3b+c+1) + bc]\sqrt{(2a-1)(b+c+1)} > 0.$$

Note that the derivative function of $h'(t)$ is $h''(t) = 12t^2 - 2(bc + ac + ab + a)$. Obviously, $h''(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Thus, $h''(t) > h''(\sqrt{(2a-1)(b+c+1)}) = 2[6(a-b-1)(c+1)+5(ac+a+bc)+11ab] > 0$. It follows that $h'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Therefore, $h'(t) > h'(\sqrt{(2a-1)(b+c+1)}) > 0$, and then $h(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Hence, $\rho(G') < \sqrt{(2a-1)(b+c+1)} = \rho(K_{2a-1,b+c+1})$, which contradicts the choice of G' since $\alpha_4(K_{2a-1,b+c+1}) = 2a = \alpha_4(G')$.

Subcase 1.3.2. $d_{Y_2}(v_i) \geq 2$ for some $1 \leq i \leq a$ and $d_{X_1}(w_j) = 1$ for all $1 \leq j \leq d$.

We claim that $N_{G'}(w_i) = N_{G'}(w_j)$ for $i \neq j$. Otherwise, assume that $d_{G'}(v_1) = \max\{d_{G'}(v_i) \mid 1 \leq i \leq a\}$. Then $d_{Y_2}(v_1) = \max\{d_{Y_2}(v_i) \mid 1 \leq i \leq a\}$ due to $d_{Y_1}(v_i) = b$. Let $\boldsymbol{y}$ be the Perron vector of $A(G')$. By symmetry, we may assume that $y_{u_1} = y_{u_l}$ for $2 \leq l \leq c$, $y_{z_1} = y_{z_j}$ for $2 \leq j \leq b$ and $y_w = y_i'$ for $w \in N_{Y_2}(v_i)$, where $1 \leq i \leq a$. Therefore, from $A(G')\boldsymbol{y} = \rho(G')\boldsymbol{y}$, we can deduce that

$$\left(\rho^2(G') - d_{Y_2}(v_1)\right)y_{v_1} - \left(\rho^2(G') - d_{Y_2}(v_i)\right)y_{v_i} = (d_{Y_2}(v_1) - d_{Y_2}(v_i))cy_{u_1} \geq 0.$$

Note that G' contains $K_{1,d_{Y_2}(v_1)}$ as a proper subgraph. Then $\rho(G') > \rho(K_{1,d_{Y_2}(v_1)}) = \sqrt{d_{Y_2}(v_1)}$. Thus, $y_{v_1} \geq \frac{\rho^2(G') - d_{Y_2}(v_i)}{\rho^2(G') - d_{Y_2}(v_1)}y_{v_i} \geq y_{v_i}$ for $2 \leq i \leq a$. Let $G_4 = G' - \{wv_i \mid w \in Y_2 \setminus N_{Y_2}(v_1), 2 \leq i \leq a\} + \{wv_1 \mid w \in Y_2 \setminus N_{Y_2}(v_1)\}$.

Clearly, $G_4 \in \mathscr{B}_{n,\alpha_4}$ and $N_{X_1}(w_i) = \{v_1\}$ for $1 \le i \le d$. According to Lemma 2, we have $\rho(G_4) > \rho(G')$, which contradicts the maximality of $\rho(G')$. Therefore, the partition $\Pi_4 : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup X_2 \cup Y_2 \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_4}(G') = \begin{pmatrix} 0 & 0 & 0 & a & b \\ 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & a & b \\ 1 & 0 & c & 0 & 0 \\ 1 & a-1 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_4}(G')) = \lambda^5 - (bc + ac + ab + a)\lambda^3 + ab(ac + a - c - 1)\lambda.$$

We consider the following real function

$$p(t) = t^4 - (bc + ac + ab + a)t^2 + ab(ac + a - c - 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $p(t) = 0$. Some direct calculations show that

$$p\left(\sqrt{(2a-1)(b+c+1)}\right) = (2a-1)(b+c+1)[(a-b-1)(c+1) + ab] + ab(a-1)(c+1) > 0$$

and

$$p'\left(\sqrt{(2a-1)(b+c+1)}\right) = 2[2(a-b-1)(c+1) + a(3b+c+1) + bc]\sqrt{(2a-1)(b+c+1)} > 0.$$

Note that the derivative function of $p'(t)$ is $p''(t) = 12t^2 - 2(bc + ac + ab + a)$. Obviously, $p''(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Thus, $p''(t) > p''(\sqrt{(2a-1)(b+c+1)}) = 2[6(a-b-1)(c+1) + 5(ac+a+bc) + 11ab] > 0$. It follows that $p'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Therefore, $p'(t) > p'(\sqrt{(2a-1)(b+c+1)}) > 0$, and then $p(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Hence, $\rho(G') < \sqrt{(2a-1)(b+c+1)} = \rho(K_{2a-1,b+c+1})$, which contradicts the maximality of $\rho(G')$.

Subcase 1.3.3. $d_{Y_2}(v_i) \ge 2$ for some $1 \le i \le a$ and $d_{X_1}(w_j) \ge 2$ for some $1 \le j \le d$.

We first infer that $d_{Y_2}(v) \ge 1$ for all $v \in X_1$. Otherwise, suppose that there exist a vertex $v_i \in X_1$ with $d_{Y_2}(v_i) = 0$ and a vertex $w_j \in Y_2$ with $d_{X_1}(w_j) \ge 2$. Let $G^\star = G' + \{v_i w_j\}$. Then $\rho(G^\star) > \rho(G')$ by Lemma 1, contradicting the maximality of $\rho(G')$. Similarly, we can obtain that $d_{X_1}(w) \ge 1$ for all $w \in Y_2$. Without loss of generality, assume that $d_{G'}(v_1) = \max\{d_{G'}(v_i) \mid 1 \le i \le a\}$ and $d_{G'}(w_d) = \max\{d_{G'}(w_j) \mid 1 \le j \le d\}$. Then $d_{Y_2}(v_1) = \max\{d_{Y_2}(v_i) \mid 1 \le i \le a\}$ and $d_{X_1}(w_d) = \max\{d_{X_1}(w_j) \mid 1 \le j \le d\}$ due to $d_{Y_1}(v_i) = b$ and $d_{X_2}(w_j) = c$. Let $\boldsymbol{z}$ be the Perron vector of $A(G')$. For any vertex $v \in X_1$ with $d_{Y_2}(v) = 1$, let $w_i \in N_{Y_2}(v)$. Then $d_{X_1}(w_d) \ge d_{X_1}(w_i)$. Therefore, from $A(G')\boldsymbol{z} = \rho(G')\boldsymbol{z}$, we can deduce that

$$\left(\rho^2(G') - d_{X_1}(w_d)\right)z_{w_d} - \left(\rho^2(G') - d_{X_1}(w_i)\right)z_{w_i} = (d_{X_1}(w_d) - d_{X_1}(w_i))bz_{z_1} \ge 0.$$

Note that G' contains $K_{1,d_{X_1}(w_d)}$ as a proper subgraph. Then $\rho(G') > \rho(K_{1,d_{X_1}(w_d)}) = \sqrt{d_{X_1}(w_d)}$. Thus, $z_{w_d} \ge \frac{\rho^2(G') - d_{X_1}(w_i)}{\rho^2(G') - d_{X_1}(w_d)}z_{w_i} \ge z_{w_i}$, where $w_i \in N_{Y_2}(v)$ for any vertex $v \in X_1$ with $d_{Y_2}(v) = 1$. For any vertex $v' \in X_1$ with $d_{Y_2}(v') \ge 2$, let $w_j \in N_{Y_2}(v')$. Then $d_{X_1}(w_j) = 1$ and $d_{Y_2}(v_1) \ge d_{Y_2}(v')$. Similarly, we can deduce that $z_{v_1} \ge z_{v'}$. Assume that $E_1' = \{vw_d \mid v \in X_1 \setminus N_{X_1}(w_d), d_{Y_2}(v) = 1\} + \{v_1 w_i \mid w_i \in N_{Y_2}(v), v \in X_1 \setminus N_{X_1}(w_d), d_{Y_2}(v) = 1\} + \{w_j v_1 \mid w_j \in N_{Y_2}(v'), v' \in X_1 \setminus \{v_1\}, d_{Y_2}(v') \ge 2\} + \{v'w_d \mid v' \in X_1 \setminus \{v_1\}, d_{Y_2}(v') \ge 2\}$, $E_2' = \{vw_i \mid v \in X_1 \setminus N_{X_1}(w_d), d_{Y_2}(v) = 1, w_i \in N_{Y_2}(v)\} + \{w_j v' \mid w_j \in N_{Y_2}(v'), v' \in X_1 \setminus \{v_1\}, d_{Y_2}(v') \ge 2\}$ and $G_5 = G' + E_1' - E_2'$. Clearly, $G_5 \in \mathscr{B}_{n,\alpha_4}$, $N_{Y_2}(v_i) = \{w_d\}$ for $2 \le i \le a$ and $N_{X_1}(w_j) = \{v_1\}$ for $1 \le j \le d-1$. By Lemma 2, we have $\rho(G_5) > \rho(G')$, which contradicts the maximality of $\rho(G')$. Therefore, the partition

$\Pi_5 : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup X_2 \cup Y_2 \setminus \{w_d\} \cup \{w_d\} \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_5}(G') = \begin{pmatrix} 0 & 0 & 0 & a-1 & 0 & b \\ 0 & 0 & 0 & 0 & 1 & b \\ 0 & 0 & 0 & a-1 & 1 & b \\ 1 & 0 & c & 0 & 0 & 0 \\ 0 & a-1 & c & 0 & 0 & 0 \\ 1 & a-1 & c & 0 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_6 - B_{\Pi_5}(G')) = \lambda^6 - (bc + ac - 2 + ab + 2a)\lambda^4$$
$$+ \left(2bc - 2abc - ac + a^2bc + a^2c + 1 - 2a - ab + a^2 + a^2b\right)\lambda^2 + bc\left(2a - 1 - a^2\right).$$

We consider the real function

$$q(t) = t^6 - (bc + ac - 2 + ab + 2a)t^4 + \left(2bc - 2abc - ac + a^2bc + a^2c + 1 - 2a - ab + a^2 + a^2b\right)t^2$$
$$+ bc\left(2a - 1 - a^2\right)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $q(t) = 0$. Some direct calculations show that

$$q\left(\sqrt{(2a-1)(b+c+1)}\right)$$
$$= (2a-1)^2(b+c+1)^2[c(a-b-1) + b(a-1) + 1] + 2a^2(a-2)\left(b^2 + 3bc + c^2 + 2b + 2c + 1\right)$$
$$+ abc(a-2)(2a-1)(b+c) + b(a-1)(2c^2 + 1 + 2bc) + 2a\left(b^2c + 2b + bc^2 + c + 5bc + 2\right)$$
$$+ a\left(b^2 + c^2\right) + 3c(a-b-1) + a^2\left(c^2 + b^2 - 1\right) + 2c - 1 > 0$$

and

$$q'(t) = 6t^5 - 4(bc + ac - 2 + ab + 2a)t^3 + 2\left(2bc - 2abc - ac + a^2bc + a^2c + 1 - 2a - ab + a^2 + a^2b\right)t$$
$$= 2t\left[3t^4 - 2(bc + ac - 2 + ab + 2a)t^2 + \left(2bc - 2abc - ac + a^2bc + a^2c + 1 - 2a - ab + a^2 + a^2b\right)\right].$$

Next, we consider the real function

$$q_*(t) = 3t^4 - 2(bc + ac - 2 + ab + 2a)t^2 + \left(2bc - 2abc - ac + a^2bc + a^2c + 1 - 2a - ab + a^2 + a^2b\right)$$

in t with $t > 0$. Some direct calculations show that

$$q_*\left(\sqrt{(2a-1)(b+c+1)}\right) = (2a-1)(b+c+1)[3c(a-b-1) + 3b(a-1) + a(b+c+2) + bc + 1]$$
$$+ ac(a-b-1) + 2bc + ab(a-1)(c+1) + (a-1)^2 > 0$$

and

$$q_*'\left(\sqrt{(2a-1)(b+c+1)}\right) = 4[b(2a-c) + 3(a-1)(b+c) + 2a(c+2) - 1]\sqrt{(2a-1)(b+c+1)} > 0.$$

Note that the derivative function of $q_*'(t)$ is $q_*''(t) = 36t^2 - 4(bc + ac - 2 + ab + 2a)$. Clearly, $q_*''(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Thus, $q_*''(t) > q_*''(\sqrt{(2a-1)(b+c+1)}) = 36(a-1)(b+c) + 4b(8a - c) + 32a(c+2) - 28 > 0$. It follows that $q_*'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Therefore, $q_*'(t) > q_*'(\sqrt{(2a-1)(b+c+1)}) > 0$, and then $q_*(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Thus, $q_*(t) > q_*(\sqrt{(2a-1)(b+c+1)}) > 0$. This implies that $q'(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$, and $q'(t) > q'(\sqrt{(2a-1)(b+c+1)}) > 0$. Hence, $q(t)$ is monotone increasing when $t > \sqrt{(2a-1)(b+c+1)}$. Consequently, $\rho(G') < \sqrt{(2a-1)(b+c+1)} = \rho(K_{2a-1,b+c+1})$, which contradicts the choice of G' since $\alpha_4(K_{2a-1,b+c+1}) = 2a = \alpha_4(G')$.

Case 2. $a < d$.

Given that $|X_1 \cup Y_2| > |X| + 1 \geq |Y| + 1$, it follows that $d > c + 1$ and $a > b + 1$. Furthermore, from $|X| \geq |Y|$ and $a < d$, we have $c > b$.

Subcase 2.1. $b = 0$.

If $b = 0$, then $c \geq 1$ and $a \geq 2$. Furthermore, we have $d_{G'}(v) = d_{Y_2}(v) \geq 1$ for all $v \in X_1$.

Subcase 2.1.1. $d_{G'}(v_i) = 1$ for all $1 \leq i \leq a$.

Following analogous analysis to Subcase 1.1.1, we obtain that $N_{G'}(v_i) = \{w_1\}$ for $1 \leq i \leq a$. Therefore, the partition $\Pi_6 : V(G') = X_1 \cup X_2 \cup \{w_1\} \cup Y_2 \setminus \{w_1\}$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_6}(G') = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & d-1 \\ a & c & 0 & 0 \\ 0 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_4 - B_{\Pi_6}(G')) = \lambda^4 - (a + cd)\lambda^2 + ac(d-1).$$

Consider the following real function

$$f_1(t) = t^4 - (a + cd)t^2 + ac(d-1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $f_1(t) = 0$. Some direct calculations show that

$$f_1\left(\sqrt{(a+d-1)(c+1)}\right) = (a+d-1)(c+1)(ac + d - c - 1) + ac(d-1) > 0$$

and

$$f_1'\left(\sqrt{(a+d-1)(c+1)}\right) = 2[2ac + cd + a + 2(d-c-1)]\sqrt{(a+d-1)(c+1)} > 0.$$

Note that the derivative function of $f_1'(t)$ is $f_1''(t) = 12t^2 - 2(a + cd)$. Obviously, $f_1''(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. Thus, $f_1''(t) > f_1''(\sqrt{(a+d-1)(c+1)}) = 2[6(ac + d - c - 1) + 5(a + cd)] > 0$. Therefore, $f_1'(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. This implies that $f_1'(t) > f_1'(\sqrt{(a+d-1)(c+1)}) > 0$, and then $f_1(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. Consequently, $\rho(G') < \sqrt{(a+d-1)(c+1)} = \rho(K_{a+d-1,c+1})$, which contradicts the choice of G' since $\alpha_4(K_{a+d-1,c+1}) = a + d = \alpha_4(G')$.

Subcase 2.1.2. $d_{G'}(v_i) \geq 2$ for some $1 \leq i \leq a$.

We first assert that $d_{X_1}(w) \geq 1$ for all $w \in Y_2$. If not, there exist a vertex $v_i \in X_1$ with $d_{G'}(v_i) \geq 2$ and a vertex $w_j \in Y_2$ with $d_{X_1}(w_j) = 0$. Let $G^\star = G' + \{v_i w_j\}$. Then $\rho(G^\star) > \rho(G')$ by Lemma 1, contradicting the maximality of $\rho(G')$. Note that $a \geq 2$ and G' is connected. There exists at least one vertex $w \in Y_2$ such that $w \notin N_{G'}(v_1)$. Without loss of generality, assume that $d_{G'}(v_1) = \max\{d_{G'}(v_i) \mid 1 \leq i \leq a\}$ and $w_d \notin N_{G'}(v_1)$. Let $\boldsymbol{y}$ be the Perron vector of $A(G')$. If $d_{X_1}(w_i) = 1$ for all $1 \leq i \leq d$, then we can deduce that $y_{v_1} \geq y_{v_i}$, where $2 \leq i \leq a$. Let $G_1' = G' - \{wv_i \mid w \in Y_2 \setminus (N_{G'}(v_1) \cup \{w_d\}), 2 \leq i \leq a\} + \{wv_1 \mid w \in Y_2 \setminus (N_{G'}(v_1) \cup \{w_d\})\} + \{w_d v_i \mid 2 \leq i \leq a\}$. Clearly, $G_1' \in \mathscr{B}_{n,\alpha_4}$. By Lemma 2, we have $\rho(G_1') > \rho(G')$, contradicting the maximality of $\rho(G')$. Consequently, $N_{Y_2}(v_i) = \{w_d\}$ for $2 \leq i \leq a$ and $N_{X_1}(w_j) = \{v_1\}$ for $1 \leq j \leq d-1$. If there exists at least one vertex $w \in Y_2$ such that $d_{X_1}(w) \geq 2$. Without loss of generality, assume that $d_{X_1}(w_d) = \max\{d_{X_1}(w_j) \mid 1 \leq j \leq d\}$. Similarly, we also deduce that $N_{Y_2}(v_i) = \{w_d\}$ for $2 \leq i \leq a$ and

$N_{X_1}(w_j) = \{v_1\}$ for $1 \le j \le d-1$. Therefore, the partition $\Pi_7 : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup X_2 \cup Y_2 \setminus \{w_d\} \cup \{w_d\}$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_7}(G') = \begin{pmatrix} 0 & 0 & 0 & d-1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & d-1 & 1 \\ 1 & 0 & c & 0 & 0 \\ 0 & a-1 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_7}(G')) = \lambda^5 - (cd - 2 + a + d)\lambda^3 + (acd + ad - ac - a - d + 1)\lambda.$$

We consider the real function

$$g_1(t) = t^4 - (cd - 2 + a + d)t^2 + (acd + ad - ac - a - d + 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $g_1(t) = 0$. Some direct calculations show that

$$g_1\left(\sqrt{(a+d-1)(c+1)}\right) = (a+d-1)(c+1)(ac - c + 1) + d(ac - 1) + a(d - c - 1) + 1 > 0$$

and

$$g_1'\left(\sqrt{(a+d-1)(c+1)}\right) = 2[2c(a-1) + cd + a + d]\sqrt{(a+d-1)(c+1)} > 0.$$

Note that the derivative function of $g_1'(t)$ is $g_1''(t) = 12t^2 - 2(cd - 2 + a + d)$. Obviously, $g_1''(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. Thus, $g_1''(t) > g_1''(\sqrt{(a+d-1)(c+1)}) = 12c(a-1) + 10(a + d + cd) - 8 > 0$. It follows that $g_1'(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. Therefore, $g_1'(t) > g_1'(\sqrt{(a+d-1)(c+1)}) > 0$, and then $g_1(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(c+1)}$. Consequently, $\rho(G') < \sqrt{(a+d-1)(c+1)} = \rho(K_{a+d-1,c+1})$, which contradicts the choice of G' since $\alpha_4(K_{a+d-1,c+1}) = a + d = \alpha_4(G')$.

Subcase 2.2. $c = 0$.

Based on the previous assumptions that $|X| \ge |Y|$ and $a < d$, we have $c > b$. Thus, $c = 0$ is excluded.

Subcase 2.3. $b \ge 1$ and $c \ge 1$.

Recall that G' is the graph with the maximum spectral radius in $\mathscr{B}_{n,\alpha_4}$. By Lemma 1, every vertex in X_1 is adjacent to all vertices in Y_1, and every vertex in X_2 is adjacent to all vertices in Y. Consequently, G' is connected. Moreover, if $d_{X_1}(w) \le 1$ for each $w \in Y_2$, then actually $d_{X_1}(w) = 1$ for all $w \in Y_2$. Otherwise, suppose there exists a vertex $w' \in Y_2$ with $d_{X_1}(w') = 0$. Let $G_2' = G' + \{w'v_1\}$. Then $\rho(G_2') > \rho(G')$ by Lemma 1, contradicting the maximality of $\rho(G')$. Similarly, we can deduce that if $d_{Y_2}(v) \le 1$ for each $v \in X_1$, then $d_{Y_2}(v) = 1$ for all $v \in X_1$. In the following, we consider three subcases.

Subcase 2.3.1. $d_{X_1}(w_i) = 1$ for all $1 \le i \le d$.

Since $a < d$, there exists at least one vertex $v \in X_1$ with $d_{Y_2}(v) \ge 2$. Following analogous analysis to Subcase 1.3.2, we have $N_{X_1}(w_i) = \{v_1\}$ for $1 \le i \le d$. Therefore, the partition $\Pi_8 : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup X_2 \cup Y_2 \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_8}(G') = \begin{pmatrix} 0 & 0 & 0 & d & b \\ 0 & 0 & 0 & 0 & b \\ 0 & 0 & 0 & d & b \\ 1 & 0 & c & 0 & 0 \\ 1 & a-1 & c & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_8}(G')) = \lambda^5 - (bc + cd + ab + d)\lambda^3 + bd(ac + a - c - 1)\lambda.$$

We consider the following real function

$$p_1(t) = t^4 - (bc + cd + ab + d)t^2 + bd(ac + a - c - 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $p_1(t) = 0$. Some direct calculations show that

$$p_1\left(\sqrt{(a + d - 1)(b + c + 1)}\right) = (a + d - 1)(b + c + 1)[(c + 1)(a - b - 1) + bd] + bd(a - 1)(c + 1) > 0$$

and

$$p_1'\left(\sqrt{(a + d - 1)(b + c + 1)}\right) = 2[2(a - b - 1)(c + 1) + d(2b + c + 1) + b(a + c)]\sqrt{(a + d - 1)(b + c + 1)} > 0.$$

Note that the second derivative of the function $p_1(t)$ is $p_1''(t) = 12t^2 - 2(bc + cd + ab + d)$. It is obvious that $p_1''(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. It follows that $p_1''(t) > p_1''(\sqrt{(a + d - 1)(b + c + 1)}) = 2[6(a - b - 1)(c + 1) + 5(ab + cd + d + bc) + 6bd] > 0$. This implies that $p_1'(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Therefore, $p_1'(t) > p_1'(\sqrt{(a + d - 1)(b + c + 1)}) > 0$, and then $p_1(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Consequently, $\rho(G') < \sqrt{(a + d - 1)(b + c + 1)} = \rho(K_{a+d-1,b+c+1})$. Combining this with $\alpha_4(K_{a+d-1,b+c+1}) = a + d = \alpha_4(G')$, which contradicts the maximality of $\rho(G')$.

Subcase 2.3.2. $d_{X_1}(w_i) \geq 2$ for some $1 \leq i \leq d$ and $d_{Y_2}(v_j) = 1$ for all $1 \leq j \leq a$.

Following analogous analysis to Subcase 1.3.1, we have $N_{Y_2}(v_i) = \{w_1\}$ for $1 \leq i \leq a$. Therefore, the partition $\Pi_9 : V(G') = X_1 \cup X_2 \cup \{w_1\} \cup Y_2 \setminus \{w_1\} \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_9}(G') = \begin{pmatrix} 0 & 0 & 1 & 0 & b \\ 0 & 0 & 1 & d-1 & b \\ a & c & 0 & 0 & 0 \\ 0 & c & 0 & 0 & 0 \\ a & c & 0 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_9}(G')) = \lambda^5 - (bc + cd + ab + a)\lambda^3 + ac(d - b + bd - 1)\lambda.$$

We consider the following real function

$$h_1(t) = t^4 - (bc + cd + ab + a)t^2 + ac(d - b + bd - 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $h_1(t) = 0$. Some direct calculations show that

$$h_1\left(\sqrt{(a + d - 1)(b + c + 1)}\right) = (a + d - 1)(b + c + 1)[(b + 1)(d - c - 1) + ac] + ac(d - 1)(b + 1) > 0$$

and

$$h_1'\left(\sqrt{(a + d - 1)(b + c + 1)}\right) = 2[2(d - c - 1)(b + 1) + a(b + 2c + 1) + c(b + d)]\sqrt{(a + d - 1)(b + c + 1)} > 0.$$

Note that the second derivative of the function $h_1(t)$ is $h_1''(t) = 12t^2 - 2(bc + cd + ab + a)$. It is obvious that $h_1''(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. It follows that $h_1''(t) > h_1''(\sqrt{(a + d - 1)(b + c + 1)}) = 2[6(d - c - 1)(b + 1) + 5(ab + bc + a + cd) + 6ac] > 0$. This implies that $h_1'(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. It follows that $h_1'(t) > h_1'(\sqrt{(a + d - 1)(b + c + 1)}) > 0$. Therefore, $h_1(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Consequently, $\rho(G') < \sqrt{(a + d - 1)(b + c + 1)} = \rho(K_{a+d-1,b+c+1})$. Combining this with $\alpha_4(K_{a+d-1,b+c+1}) = a + d = \alpha_4(G')$, which contradicts the maximality of $\rho(G')$.

Subcase 2.3.3. $d_{X_1}(w_i) \geq 2$ for some $1 \leq i \leq d$ and $d_{Y_2}(v_j) \geq 2$ for some $1 \leq j \leq a$.

Following analogous analysis to Subcase 1.3.3, we obtain that $N_{X_1}(w_i) = \{v_1\}$ for $1 \leq i \leq d-1$ and $N_{Y_2}(v_j) = \{w_d\}$ for $2 \leq j \leq a$. Therefore, the partition $\Pi_{10} : V(G') = \{v_1\} \cup X_1 \backslash \{v_1\} \cup X_2 \cup Y_2 \backslash \{w_d\} \cup \{w_d\} \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_{10}}(G') = \begin{pmatrix} 0 & 0 & 0 & d-1 & 0 & b \\ 0 & 0 & 0 & 0 & 1 & b \\ 0 & 0 & 0 & d-1 & 1 & b \\ 1 & 0 & c & 0 & 0 & 0 \\ 0 & a-1 & c & 0 & 0 & 0 \\ 1 & a-1 & c & 0 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_6 - B_{\Pi_{10}}(G')) = \lambda^6 - (bc + cd - 2 + ab + a + d)\lambda^4 + (2bc - bcd - abc + abcd - ac + acd$$
$$+ 1 - d - bd - a + ad + abd)\lambda^2 + bc(d + a - 1 - ad).$$

We consider the real function

$$q_1(t) = t^6 - (bc + cd - 2 + ab + a + d)t^4 + (2bc - bcd - abc + abcd - ac + acd + 1 - d - bd - a + ad + abd)t^2$$
$$+ bc(d + a - 1 - ad)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $q_1(t) = 0$. Some direct calculations show that

$$q_1\left(\sqrt{(a+d-1)(b+c+1)}\right)$$
$$= (a+d-1)^2(b+c+1)^2[c(a-b-1) + b(d-1) + 1] + ad(a-b-1)(3bc+1) + d(2c+1)$$
$$+ (d-c-1)\left(3abcd + 2a^2b + 2a^2c + 3b + 1\right) + a\left(3b^2c + 2b + 3bc^2 + 3c + 5bc + 2 + c^2\right)$$
$$+ ad(d-c-2)(2b + 2c + 1) + b^2d(a-2)(a+cd) + bc(d-1)\left(a^2b + a^2c + 2b + 2c\right)$$
$$+ bd^2(c-1)(b+2c) + (b-1)\left(a^2 + d^2\right) + cd^2(ac-1) + bc^2d^2(a-3) + bd^2(ab-3)$$
$$+ a^2c^2(d+1) + b\left(bcd + c^2d + 5cd + 2 + bd\right) > 0$$

and

$$q_1'(t) = 6t^5 - 4(bc + cd - 2 + ab + a + d)t^3 + 2(2bc - bcd - abc + abcd - ac + acd + 1 - d - bd - a + ad + abd)t$$
$$= 2t\left[3t^4 - 2(bc + cd - 2 + ab + a + d)t^2 + (2bc - bcd - abc + abcd - ac + acd + 1 - d - bd - a\right.$$
$$\left. + ad + abd)\right].$$

Next, we consider the real function

$$q_\star(t) = 3t^4 - 2(bc + cd - 2 + ab + a + d)t^2 + (2bc - bcd - abc + abcd - ac + acd + 1 - d - bd - a + ad + abd)$$

in t with $t > 0$. Some direct calculations show that

$$q_\star\left(\sqrt{(a+d-1)(b+c+1)}\right)$$
$$= (a+d-1)(b+c+1)[3c(a-b-1) + 3b(d-1) + a(b+1) + d(c+1) + bc + 1] + d(ac-1)$$
$$+ ab(d-c) + a(d-c-1) + bd(bc-1) + bcd(a-b-1) + 2bc + 1 > 0$$

and

$$q_\star'\left(\sqrt{(a+d-1)(b+c+1)}\right) = 4[3c(a-b-1) + 3b(d-1) + 2(ab + a + cd + d + bc) - 1]$$
$$\times \sqrt{(a+d-1)(b+c+1)} > 0.$$

Note that the derivative function of $q'_\star(t)$ is $q''_\star(t) = 36t^2 - 4(bc + cd - 2 + ab + a + d)$. It is obvious that $q''_\star(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Therefore, $q''_\star(t) > q''_\star(\sqrt{(a + d - 1)(b + c + 1)}) = 36b(d - c - 1) + 36c(a - 1) + 32(ab + a + cd + d + bc) - 28 > 0$. This implies that $q'_\star(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Therefore, $q'_\star(t) > q'_\star(\sqrt{(a + d - 1)(b + c + 1)}) > 0$. It follows that $q_\star(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$, and then $q_\star(t) > q_\star(\sqrt{(a + d - 1)(b + c + 1)}) > 0$. Thus, $q'_1(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$, and then $q'_1(t) > q'_1(\sqrt{(a + d - 1)(b + c + 1)}) > 0$. This implies that $q_1(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + c + 1)}$. Consequently, $\rho(G') < \sqrt{(a + d - 1)(b + c + 1)} = \rho(K_{a+d-1,b+c+1})$, which contradicts the choice of G' since $\alpha_4(K_{a+d-1,b+c+1}) = a + d = \alpha_4(G')$.

Case 3. $a > d$.

From the assumption that $|X_1 \cup Y_2| > |X| + 1 \geq |Y| + 1$, we have $d > c + 1$ and $a > b + 1$. Moreover, given $|X| \geq |Y|$ and $a > d$, there exists a subcase where $c = 0$.

Subcase 3.1. $c = 0$.

For $c = 0$, we have $d \geq 2$ and $d_{G'}(w) = d_{X_1}(w) \geq 1$ for all $w \in Y_2$. Furthermore, since $a > d$ and G is connected, we have $b \geq 1$.

Subcase 3.1.1. $d_{G'}(w_i) = 1$ for all $1 \leq i \leq d$.

Following analogous analysis to Subcase 1.1.1, we obtain that $N_{G'}(w_i) = \{v_1\}$ for $1 \leq i \leq d$. Therefore, the partition $\Pi_{11} : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup Y_2 \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_{11}}(G') = \begin{pmatrix} 0 & 0 & d & b \\ 0 & 0 & 0 & b \\ 1 & 0 & 0 & 0 \\ 1 & a-1 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_4 - B_{\Pi_{11}}(G')) = \lambda^4 - (d + ab)\lambda^2 + bd(a - 1).$$

We consider the following real function

$$f_2(t) = t^4 - (d + ab)t^2 + bd(a - 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $f_2(t) = 0$. Some direct calculations show that

$$f_2\left(\sqrt{(a + d - 1)(b + 1)}\right) = (a + d - 1)(b + 1)(bd + a - b - 1) + bd(a - 1) > 0$$

and

$$f'_2\left(\sqrt{(a + d - 1)(b + 1)}\right) = 2[2bd + ab + d + 2(a - b - 1)]\sqrt{(a + d - 1)(b + 1)} > 0.$$

Note that the derivative function of $f'_2(t)$ is $f''_2(t) = 12t^2 - 2(d + ab)$. Obviously, $f''_2(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + 1)}$. Thus, $f''_2(t) > f''_2(\sqrt{(a + d - 1)(b + 1)}) = 2[6(bd + a - b - 1) + 5(d + ab)] > 0$. Therefore, $f'_2(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + 1)}$. This implies that $f'_2(t) > f'_2(\sqrt{(a + d - 1)(b + 1)}) > 0$, and then $f_2(t)$ is monotone increasing when $t > \sqrt{(a + d - 1)(b + 1)}$. Consequently, $\rho(G') < \sqrt{(a + d - 1)(b + 1)} = \rho(K_{a+d-1,b+1})$, which contradicts the choice of G' since $\alpha_4(K_{a+d-1,b+1}) = a + d = \alpha_4(G')$.

Subcase 3.1.2. $d_{G'}(w_i) \geq 2$ for some $1 \leq i \leq d$.

Following analogous analysis to Subcase 2.1.2, we obtain that $N_{X_1}(w_i) = \{v_1\}$ for $1 \leq i \leq d-1$ and $N_{Y_2}(v_j) = \{w_d\}$ for $2 \leq j \leq a$. Therefore, it is obvious that $\Pi_{12} : V(G') = \{v_1\} \cup X_1 \setminus \{v_1\} \cup Y_2 \setminus \{w_d\} \cup \{w_d\} \cup Y_1$ is an equitable partition of G', and the corresponding quotient matrix is given by

$$B_{\Pi_{12}}(G') = \begin{pmatrix} 0 & 0 & d-1 & 0 & b \\ 0 & 0 & 0 & 1 & b \\ 1 & 0 & 0 & 0 & 0 \\ 0 & a-1 & 0 & 0 & 0 \\ 1 & a-1 & 0 & 0 & 0 \end{pmatrix}.$$

Therefore,

$$\det(\lambda I_5 - B_{\Pi_{12}}(G')) = \lambda^5 - (ab - 2 + a + d)\lambda^3 + (abd + ad - bd - a - d + 1)\lambda.$$

We may consider the real function

$$g_2(t) = t^4 - (ab - 2 + a + d)t^2 + (abd + ad - bd - a - d + 1)$$

in t with $t > 0$. In view of Lemma 3, one finds that $\rho(G')$ is the largest root of $g_2(t) = 0$. Some direct calculations show that

$$g_2\left(\sqrt{(a+d-1)(b+1)}\right) = (a+d-1)(b+1)(bd-b+1) + a(bd-1) + d(a-b-1) + 1 > 0$$

and

$$g_2'\left(\sqrt{(a+d-1)(b+1)}\right) = 2[2b(d-1) + ab + a + d]\sqrt{(a+d-1)(b+1)} > 0.$$

Note that the derivative function of $g_2'(t)$ is $g_2''(t) = 12t^2 - 2(ab - 2 + a + d)$. Obviously, $g_2''(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(b+1)}$. Thus, $g_2''(t) > g_2''(\sqrt{(a+d-1)(b+1)}) = 12b(d-1) + 10(a + d + ab) - 8 > 0$. It follows that $g_2'(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(b+1)}$. Therefore, $g_2'(t) > g_2'(\sqrt{(a+d-1)(b+1)}) > 0$, and then $g_2(t)$ is monotone increasing when $t > \sqrt{(a+d-1)(b+1)}$. Consequently, $\rho(G') < \sqrt{(a+d-1)(b+1)} = \rho(K_{a+d-1,b+1})$, which contradicts the choice of G' since $\alpha_4(K_{a+d-1,b+1}) = a + d = \alpha_4(G')$.

For the remaining subcases where either $b = 0$ or $b \geq 1$ with $c \geq 1$, the contradiction can be derived in a similar way to Case 2, and thus the procedure is omitted here.

From the above results, we conclude that $G' \cong K_{\alpha_4-1,n-\alpha_4+1}$. A simple calculation gives $\rho(K_{\alpha_4-1,n-\alpha_4+1}) = \sqrt{(\alpha_4 - 1)(n - \alpha_4 + 1)}$.

In the following, suppose that $G' \in \mathscr{B}_{n,\alpha_4}$ is a disconnected bipartite graph attaining the maximum spectral radius with $G' = \bigcup_{i=1}^k G_i$, where G_i is a connected bipartite graph of order n_i and 4-independence number α_4^i. Then $1 \leq n_i < n$, $\alpha_4^i < \alpha_4$ $(1 \leq i \leq k)$ and

$$\sum_{i=1}^k (n_i - \alpha_4^i) = \sum_{i=1}^k n_i - \sum_{i=1}^k \alpha_4^i = n - \alpha_4.$$

Thus, $n_i - \alpha_4^i < n - \alpha_4$ for each $1 \leq i \leq k$, where $k \geq 2$. Therefore,

$$\rho(G') = \max\{\rho(G_i) \mid 1 \leq i \leq k\} = \max\left\{\sqrt{(\alpha_4^i - 1)(n_i - \alpha_4^i + 1)} \mid 1 \leq i \leq k\right\}$$
$$< \sqrt{(\alpha_4 - 1)(n - \alpha_4 + 1)} = \rho(K_{\alpha_4-1,n-\alpha_4+1}),$$

a contradiction.

We complete the proof. $\qquad\square$

CONFLICTS OF INTEREST

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

DATA AVAILABILITY STATEMENT

No data was used for the research described in the article.

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