Extremal results for graphs with binding number strictly less than $1/r$

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Abstract

The binding number $b(G)$ of a graph, introduced by Woodall [J. Combin. Theory, Ser. B, 1973], is a central topic of both structural and extremal graph theory. It is closely related to fundamental combinatorial and structural properties of graphs.

The graphs with $b(G) \geqslant 1$ exhibit strong expansion properties and a highly connected global structure. In contrast, the structure for graphs with $b(G) < 1$ remains far less well understood. Kane et al. [J. Graph Theory, 1981] proved that if $b(G) < 1$, then every binding set of G is independent. Goddard and Swart [Quaest. Math., 1990] showed that if $b(G) \leqslant 1$, then the toughness $\tau(G) \leqslant b(G)$. This makes it particularly interesting to investigate extremal problems for graphs with $b(G) < 1$. For any integer $r \geqslant 1$, we completely characterize the unique extremal graph that maximizes the size (spectral radius) among all graphs of order n satisfying $b(G) < \frac{1}{r}$.

For any bipartite graph $G = (X, Y)$ on n vertices, it is readily seen that $b(G) \leqslant \min\{|X|/|Y|, |Y|/|X|\} \leqslant 1$. Notably, the complete balanced bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ achieves the maximum size (spectral radius) among all bipartite graphs with $b(G) = 1$. In this paper, we completely determine the extremal graphs maximizing the size or the spectral radius among all bipartite graphs with $b(G) < \frac{1}{r}$, where $r \geqslant 1$ is an integer.

Mathematics Subject Classifications: 05C50, 05C35

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The order and size of G are denoted by $|V(G)| = n$ and $|E(G)| = e(G)$, respectively. Let G_1 and G_2 be two vertex-disjoint graphs, and let $G_1 \cup G_2$ denote their disjoint union. The join $G_1 \vee G_2$ is the graph obtained from $G_1 \cup G_2$ by adding all possible edges between $V(G_1)$ and $V(G_2)$. For a vertex subset $S \subseteq V(G)$, let $G[S]$ and $|S|$ be the subgraph of G induced by S and the size of S, respectively. For a graph G of order n, its adjacency matrix is the 0-1

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matrix $A(G) = (a_{ij})_{n\times n}$, where $a_{ij} = 1$ if $v_i \sim v_j$ and $a_{ij} = 0$ otherwise. Note that $A(G)$ is a real nonnegative symmetric matrix. So all its eigenvalues are real and can be ordered non-increasingly as $\lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_n(G)$. The largest eigenvalue $\rho(G) = \lambda_1(G)$ is called the *spectral radius* of G. For undefined terminology and notation, one can refer to [2, 5].

The binding number of graphs was introduced by Woodall [20]. For any vertex $v \in V(G)$, let $N_G(v)$ denote its neighborhood in G, and for $S \subseteq V(G)$, define $N_G(S) = \bigcup_{v\in S} N_G(v)$. The *binding number* $b(G)$ of a graph G is given by

$$b(G) = \min\left\{\frac{|N_G(S)|}{|S|} : \emptyset \neq S \subseteq V(G), N_G(S) \neq V(G)\right\}.$$

As a fundamental graph invariant, the binding number possesses wide-ranging applications in numerous fields, such as graph theory, network science, quantum sensing, and information processing. A central problem concerning the binding number lies in characterizing its bounds via fundamental graph structural parameters, including the degree sequence [4], minimum degree [3], and connectivity [20].

The binding number of a graph is closely related to the combinatorial structural properties of the graph. The graphs with $b(G) \geqslant 1$ exhibit strong expansion properties and a highly connected global structure. Some fundamental graph properties that are guaranteed by lower bounds on $b(G)$ include Hamilton cycle [20, 21], k-factor [14, 15], k-extendibility [6, 19], k-clique [17]. In contrast, for graphs with $b(G) < 1$, the structure is still not well characterized. Kane et al.[16] established the following useful result. A non-empty subset $S \subseteq V(G)$ is a *binding set* if and only if $b(G) = |N(S)|/|S|$.

Theorem 1 (Kane et al. [16])**.** *Let G be a graph. If $b(G) < 1$, then every binding set S is independent.*

The *toughness* $\tau(G) = \min\{\frac{|S|}{c(G-S)} : S$ is a cut set of vertices in $G\}$ for $G \ncong K_n$, which is initially proposed by Chvátal [7]. Goddard and Swart [10] discovered the relationship between $\tau(G)$ and $b(G)$ when $b(G) \leqslant 1$.

Theorem 2 (Goddard and Swart [10])**.** *Let G be a graph. If $b(G) \leqslant 1$, then $b(G) \geqslant \tau(G)$.*

Naturally, one wonders about extremal results of graphs with $b(G) < 1$. So we propose the following intriguing problem.

Problem 3. What is the maximum size (spectral radius) among all graphs of order n satisfying $b(G) < \frac{1}{r}$, where $r \geqslant 1$ is an integer?

Note that $b(G) = 0$ if and only if G contains isolated vertices. It is easy to see that the graph $K_{n-1} \cup K_1$ attains the maximum size (spectral radius) among all graphs with $b(G) = 0$. Therefore, for Problem 3, it suffices to restrict our attention to graphs without isolated vertices. Let $\mathcal{G}_{n,r}$ be the family of graphs without isolated vertices of order n such that $b(G) < \frac{1}{r}$ for every $G \in \mathcal{G}_{n,r}$, where $r \geqslant 1$ is an integer.

Theorem 4. *Let $r \geqslant 1$ and $n \geqslant r+13$ be two integers, and let $G \in \mathcal{G}_{n,r}$. Then*

$$e(G) \leqslant \binom{n-r-1}{2} + r + 1$$

with equality if and only if $G \cong K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$.

Theorem 5. *Let $r \geqslant 1$ and $n \geqslant 2r+15$ be two integers, and let $G \in \mathcal{G}_{n,r}$. Then*

$$\rho(G) \leqslant \rho(K_1 \vee (K_{n-r-2} \cup (r+1)K_1))$$

with equality if and only if $G \cong K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$.

By taking $r = 1$ in Theorems 4 and 5, one can get the following result for $n \geqslant 17$.

Corollary 6 (Fan and Lin [8])**.** *Let G be a connected graph of order $n \geqslant 17$ with $b(G) < 1$. Each of the following holds.*
(i) $e(G) \leqslant \binom{n-2}{2} + 2$ with equality if and only if $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$.
(ii) $\rho(G) \leqslant \rho(K_1 \vee (K_{n-3} \cup 2K_1))$ with equality if and only if $G \cong K_1 \vee (K_{n-3} \cup 2K_1)$.

The research concerning the binding number of bipartite graphs has not yet been involved in the literature. For any bipartite graph $G = (X, Y)$ on n vertices, it is readily seen that $b(G) \leqslant \min\{|X|/|Y|, |Y|/|X|\} \leqslant 1$. Notably, the complete balanced bipartite graph $K_{\frac{n}{2},\frac{n}{2}}$ achieves the maximum size (spectral radius) over all bipartite graphs with $b(G) = 1$. This naturally leads to an interesting problem.

Problem 7. What is the maximum size (spectral radius) among all bipartite graphs of order n satisfying $b(G) < \frac{1}{r}$, where $r \geqslant 1$ is an integer?

Note that $b(G) = 0$ if and only if G contains isolated vertices. It is easy to see that the graph $K_{\lfloor \frac{n-1}{2} \rfloor, \lceil \frac{n-1}{2} \rceil} \cup K_1$ attains the maximum size (spectral radius) among all bipartite graphs with $b(G) = 0$. Consequently, when addressing Problem 7, it is sufficient to focus on graphs that do not contain isolated vertices. Let $\mathcal{B}_{n,r}$ be the family of n-vertex bipartite graphs without isolated vertices satisfying $b(G) < \frac{1}{r}$ for each $G \in \mathcal{B}_{n,r}$, where $r \geqslant 1$ is an integer.

A connected bipartite graph $G = (X, Y)$ is called a *double nested graph* if its vertex sets admit partitions $X = X_1 \cup X_2 \cup \cdots \cup X_h$ and $Y = Y_1 \cup Y_2 \cup \cdots \cup Y_h$, where X_i and Y_j are independent sets, and all vertices in X_i are adjacent to every vertex in $\bigcup_{j=1}^{h+1-i} Y_j$ for $1 \leqslant i \leqslant h$. In the following figure, large solid circles stand for independent sets, and each line between two large solid circles means that all vertices in one large solid circle are adjacent to all vertices in the other one. Let $|X_i| = p_i$ and $|Y_i| = q_i$ for $i = 1, 2, \ldots, h$. We denote the double nested graph by $D(p_1, p_2, \ldots, p_h; q_1, q_2, \ldots, q_h)$ (see Fig. 1).

Define $f(n,r) = \left\lfloor \frac{n-1}{r+1} \right\rfloor \left(n - \left\lfloor \frac{n-1}{r+1} \right\rfloor\right)$ and $g(n,r) = \left\lfloor \frac{n-r-1}{2} \right\rfloor \left\lceil \frac{n-r-1}{2} \right\rceil + r + 1$. Focusing on Problem 7, we prove the following results.

Theorem 8. *Let $r \geqslant 1$ and $n \geqslant r^2 + r + 1$ be two integers, and let $G \in \mathcal{B}_{n,r}$.*

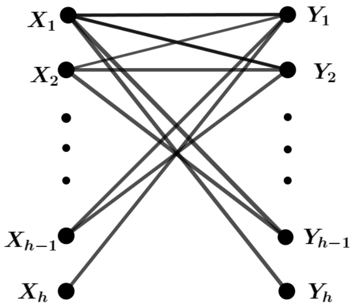

Figure 1: Graph $D(p_1, p_2, \ldots, p_h; q_1, q_2, \ldots, q_h)$.

(i) *If* $r = 1$, *then* $e(G) \leqslant f(n,1)$ *with equality if and only if* $G \cong K_{n-\lfloor \frac{n-1}{2} \rfloor, \lfloor \frac{n-1}{2} \rfloor}$.

(ii) *If* $r \geqslant 2$ *and* $f(n,r) > g(n,r)$, *then* $e(G) \leqslant f(n,r)$ *with equality if and only if* $G \cong K_{n-\lfloor \frac{n-1}{r+1} \rfloor, \lfloor \frac{n-1}{r+1} \rfloor}$.

(iii) *If* $r \geqslant 2$ *and* $f(n,r) < g(n,r)$, *then* $e(G) \leqslant g(n,r)$ *with equality if and only if* $G \in \left\{ D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right), D\left(\left\lfloor \frac{n-r-1}{2} \right\rfloor, r+1; 1, \left\lceil \frac{n-r-1}{2} \right\rceil - 1\right) \right\}$.

(iv) *If* $r \geqslant 2$ *and* $f(n,r) = g(n,r)$, *then* $e(G) \leqslant f(n,r)$ *with equality if and only if* $G \in$

$$\left\{ K_{n-\lfloor \frac{n-1}{r+1} \rfloor, \lfloor \frac{n-1}{r+1} \rfloor}, D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right), \right.$$
$$\left. D\left(\left\lfloor \frac{n-r-1}{2} \right\rfloor, r+1; 1, \left\lceil \frac{n-r-1}{2} \right\rceil - 1\right) \right\}.$$

Let $\rho' = \rho\left(K_{n-\lfloor \frac{n-1}{r+1} \rfloor, \lfloor \frac{n-1}{r+1} \rfloor}\right)$ and $\rho'' = \rho\left(D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)\right)$.

Theorem 9. *Let* $r \geqslant 1$ *and* $n \geqslant r^2 + r + 2$ *be two integers, and let* $G \in \mathcal{B}_{n,r}$.

(i) *If* $r = 1$ *then* $\rho(G) \leqslant \rho'$ *with equality if and only if* $G \cong K_{n-\lfloor \frac{n-1}{2} \rfloor, \lfloor \frac{n-1}{2} \rfloor}$.

(ii) *If* $r \geqslant 2$ *and* $\rho' > \rho''$, *then* $\rho(G) \leqslant \rho'$ *with equality if and only if* $G \cong K_{n-\lfloor \frac{n-1}{r+1} \rfloor, \lfloor \frac{n-1}{r+1} \rfloor}$.

(iii) *If* $r \geqslant 2$ *and* $\rho' < \rho''$, *then* $\rho(G) \leqslant \rho''$ *with equality if and only if*

$$G \cong D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right).$$

(iv) *If* $r \geqslant 2$ *and* $\rho' = \rho''$, *then* $\rho(G) \leqslant \rho'$ *with equality if and only if*

$$G \in \left\{ K_{n-\lfloor \frac{n-1}{r+1} \rfloor, \lfloor \frac{n-1}{r+1} \rfloor}, \quad D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right) \right\}.$$

2 Proofs of Theorems 4 and 5

Before proving our main theorems, we present several auxiliary lemmas.

Lemma 10 (Brouwer and Haemers [2], Godsil and Royle [9], Haemers [11])**.** *Let M be a real symmetric matrix and $R(M)$ its quotient matrix. The eigenvalues of every quotient matrix of M interlace those of M. If $R(M)$ is equitable, then the eigenvalues of $R(M)$ are also the eigenvalues of M. Furthermore, if M is nonnegative and irreducible, then the spectral radius of $R(M)$ equals the spectral radius of M.*

Lemma 11 (Godsil and Royle [9])**.** *If H is a spanning subgraph of a connected graph G, then $\rho(H) \leqslant \rho(G)$ with equality if and only if $H \cong G$.*

Lemma 12. $b(K_1 \vee (K_{n-r-2} \cup (r+1)K_1)) < \frac{1}{r}$.

Proof. Let $G = K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$. The vertex set of G can be partitioned as $V(G) = V(K_1) \cup V(K_{n-r-2}) \cup V((r+1)K_1)$. Take $S = V((r+1)K_1)$. Then $b(G) \leqslant \frac{|N_G(S)|}{|S|} = \frac{1}{r+1} < \frac{1}{r}$. □

Now we are ready to provide the proof of Theorem 4.

Proof of Theorem 4. Let G_e^* be the graph with the maximum size in $\mathcal{G}_{n,r}$. Note that $b(G_e^*) < \frac{1}{r}$ for integer $r \geqslant 1$. Let S be a binding set. Then $b(G_e^*) = \frac{|N_{G_e^*}(S)|}{|S|} < \frac{1}{r}$ and $N_{G_e^*}(S) \neq V(G_e^*)$. By Theorem 1, S is an independent set, which implies that $S \cap N_{G_e^*}(S) = \emptyset$. Define $T_1 = N_{G_e^*}(S)$ and $T_2 = V(G_e^*) \setminus (S \cup N_{G_e^*}(S))$. Let $|T_i| = t_i$ for $i = 1, 2$ and $|S| = s$. Then we have

$$s \geqslant rt_1 + 1. \tag{1}$$

By Lemma 12, $K_1 \vee (K_{n-r-2} \cup (r+1)K_1) \in \mathcal{G}_{n,r}$, and hence

$$e(G_e^*) \geqslant e(K_1 \vee (K_{n-r-2} \cup (r+1)K_1)) = \binom{n-r-1}{2} + r + 1. \tag{2}$$

Claim 13. $G_e^*[T_1 \cup T_2] \cong K_{t_1+t_2}$ *and* $G_e^*[T_1 \cup S] \cong K_{t_1} \vee sK_1$.

Proof. If $|T_1 \cup T_2| = 1$, then the result follows. Next we consider $|T_1 \cup T_2| \geqslant 2$. Suppose to the contrary that $G_e^*[T_1 \cup T_2] \ncong K_{t_1+t_2}$. Then there exist two vertices $u, v \in T_1 \cup T_2$ such that $uv \notin E(G_e^*)$. Let $G' = G_e^* + uv$. Then $b(G') \leqslant \frac{|N_{G'}(S)|}{|S|} = \frac{|N_{G_e^*}(S)|}{|S|} < \frac{1}{r}$, which implies that $G' \in \mathcal{G}_{n,r}$. However, $e(G') > e(G_e^*)$, which contradicts the maximality of G_e^*. So $G_e^*[T_1 \cup T_2] \cong K_{t_1+t_2}$. Similarly, $G_e^*[T_1 \cup S] \cong K_{t_1} \vee sK_1$. ◊

By Claim 13, we have $G_e^* \cong K_{t_1} \vee (K_{n-t_1-s} \cup sK_1)$.

Claim 14. $t_2 \geqslant 2$.

Proof. By contradiction, assume that $t_2 \leqslant 1$. If $t_2 = 0$, then $n = s + t_1$. By (1), we have $s \geqslant \left\lceil \frac{nr+1}{r+1} \right\rceil \geqslant \frac{nr+1}{r+1}$. Note that $G_e^* \cong K_{n-s} \vee sK_1$. Then we have

$$\begin{aligned} e(G_e^*) &= e(K_{n-s} \vee sK_1) = \frac{n(n-1)}{2} - \frac{s(s-1)}{2} \\ &\leqslant \frac{n(n-1)}{2} - \frac{nr+1}{2(r+1)} \left(\frac{nr+1}{r+1} - 1 \right) \\ &< \binom{n-r-1}{2} + r + 1, \end{aligned}$$

which contradicts (2). Next we consider $t_2 = 1$. Let $S' = S \cup T_2$. Note that G_e^* is connected. Then $N_{G_e^*}(S') = N_{G_e^*}(S) = T_1$, and hence $b(G_e^*) \leqslant \frac{|N_{G_e^*}(S')|}{|S'|} = \frac{t_1}{s+1} < \frac{t_1}{s} = b(G_e^*)$, a contradiction. Hence $t_2 \geqslant 2$. ♢

Claim 15. $s = rt_1 + 1$.

Proof. Note that $b(K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1 + 1)K_1)) \leqslant \frac{t_1}{rt_1+1} < \frac{1}{r}$. Then $K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1) \in \mathcal{G}_{n,r}$. By (1), $s \geqslant rt_1 + 1$. If $s \geqslant rt_1 + 2$, then G_e^* is a proper subgraph of $K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)$. Hence $e(K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)) > e(G_e^*)$, which contradicts the maximality of G_e^*. ♢

By Claim 15, we have $G_e^* \cong K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1 + 1)K_1)$. Note that $T_1 \neq \emptyset$. Then $t_1 \geqslant 1$. Suppose that $t_1 \geqslant 2$. By (1), $s + t_1 + t_2 = n$, and Claim 14, we have $2 \leqslant t_1 \leqslant \left\lfloor \frac{n-3}{r+1} \right\rfloor$. Define

$$f_1(x) = -\left(\frac{r^2}{2} + r \right) x^2 + \left(nr - \frac{3r}{2} - 1 \right) x + n - 1.$$

The quadratic function $f_1(x)$ has axis of symmetry $x = \frac{1}{r^2+2r}(nr - \frac{3r}{2} - 1) > \frac{1}{2}\left(1 + \left\lfloor \frac{n-3}{r+1} \right\rfloor\right)$, hence $f_1(x) > f_1(1) = \frac{(r+1)(2n-r-4)}{2}$ for $2 \leqslant x \leqslant \left\lfloor \frac{n-3}{r+1} \right\rfloor$. Combining (2), we have

$$\begin{aligned} \binom{n-r-1}{2} + r + 1 &\leqslant e(G_e^*) = e(K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1 + 1)K_1)) \\ &= \frac{n(n-1)}{2} - \left[-\left(\frac{r^2}{2} + r \right) t_1^2 + \left(nr - \frac{3r}{2} - 1 \right) t_1 + n - 1 \right] \\ &< \frac{n(n-1)}{2} - \frac{(r+1)(2n-r-4)}{2} \\ &= \binom{n-r-1}{2} + r + 1, \end{aligned}$$

a contradiction. Hence $t_1 = 1$. Then we have $G_e^* \cong K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$. □

Now we are ready to present the proof of Theorem 5.

Proof of Theorem 5. Let G^*_ρ be the graph with the maximum spectral radius in $\mathcal{G}_{n,r}$. Note that $b(G^*_\rho) < \frac{1}{r}$ for integer $r \geqslant 1$. Let S be a binding set. Then $b(G^*_\rho) = \frac{|N_{G^*_\rho}(S)|}{|S|} < \frac{1}{r}$ and $N_{G^*_\rho}(S) \neq V(G^*_\rho)$. By Theorem 1, S is an independent set, which implies that $S \cap N_{G^*_\rho}(S) = \emptyset$. Define $T_1 = N_{G^*_\rho}(S)$ and $T_2 = V(G^*_\rho) \setminus (S \cup N_{G^*_\rho}(S))$. Let $|T_i| = t_i$ for $i = 1, 2$ and $|S| = s$. Then

$$s \geqslant rt_1 + 1. \tag{3}$$

By Lemma 12, $K_1 \vee (K_{n-r-2} \cup (r+1)K_1) \in \mathcal{G}_{n,r}$, and hence

$$\rho(G^*_\rho) \geqslant \rho(K_1 \vee (K_{n-r-2} \cup (r+1)K_1)) > n - r - 2. \tag{4}$$

Claim 16. *G^*_ρ is connected.*

Proof. Suppose to the contrary that G^*_ρ is disconnected. Let $G_1, G_2, \ldots, G_c$ be the connected components of G^*_ρ, where $c \geqslant 2$. Then there exists a connected component G_i such that $S \cap V(G_i) \neq \emptyset$. Without loss of generality, assume that $S \cap V(G_1) = S_1 \neq \emptyset$. Note that G^*_ρ contains no isolated vertices. Then $N_{G_1}(S_1) \neq \emptyset$. Construct $G' = G^*_\rho + uv_2 + uv_3 + \cdots + uv_c$, where $u \in V(N_{G_1}(S_1))$ and $v_i \in V(G_i)$ for $2 \leqslant i \leqslant c$. Recall that $S \cap N_{G^*_\rho}(S) = \emptyset$. Then $S_1 \cap N_{G_1}(S_1) = \emptyset$. Therefore, $b(G') \leqslant \frac{|N_{G'}(S)|}{|S|} = \frac{|N_{G^*_\rho}(S)|}{|S|} < \frac{1}{r}$, implying that $G' \in \mathcal{G}_{n,r}$. Note that G' is connected and G^*_ρ is a spanning subgraph of G'. By Lemma 11, $\rho(G') > \rho(G^*_\rho)$, which contradicts the maximality of G^*_ρ. $\Diamond$

Claim 17. *$G^*_\rho[T_1 \cup T_2] \cong K_{t_1+t_2}$ and $G^*_\rho[T_1 \cup S] \cong K_{t_1} \vee sK_1$.*

Proof. If $|T_1 \cup T_2| = 1$, then the result follows. Next we consider $|T_1 \cup T_2| \geqslant 2$. Suppose to the contrary that $G^*_\rho[T_1 \cup T_2] \ncong K_{t_1+t_2}$. Then there exist two vertices $u, v \in T_1 \cup T_2$ such that $uv \notin E(G^*_\rho)$. Let $G'' = G^*_\rho + uv$. Then $b(G'') \leqslant \frac{|N_{G''}(S)|}{|S|} = \frac{|N_{G^*_\rho}(S)|}{|S|} < \frac{1}{r}$, which implies that $G'' \in \mathcal{G}_{n,r}$. However, by Claim 16 and Lemma 11, $\rho(G'') > \rho(G^*_\rho)$, which contradicts the maximality of G^*_ρ. So $G^*_\rho[T_1 \cup T_2] \cong K_{t_1+t_2}$. Similarly, $G^*_\rho[T_1 \cup S] \cong K_{t_1} \vee sK_1$. $\Diamond$

By Claim 17, we have $G^*_\rho \cong K_{t_1} \vee (K_{n-t_1-s} \cup sK_1)$.

Claim 18. $t_2 \geqslant 2$.

Proof. By contradiction, assume that $t_2 \leqslant 1$. If $t_2 = 0$, then $n = s + t_1$. By (3), we deduce that $s \geqslant \left\lceil \frac{nr+1}{r+1} \right\rceil = n - \left\lfloor \frac{n-1}{r+1} \right\rfloor$. Note that $G^*_\rho \cong K_{n-s} \vee sK_1$. For convenience, let $\alpha = \left\lfloor \frac{n-1}{r+1} \right\rfloor$. Note that $K_{n-s} \vee sK_1$ is a spanning subgraph of $K_\alpha \vee (n-\alpha)K_1$. By (4) and Lemma 11, we have

$$n - r - 2 < \rho(G^*_\rho) = \rho(K_{n-s} \vee sK_1) \leqslant \rho(K_\alpha \vee (n-\alpha)K_1). \tag{5}$$

Notice that $A(K_\alpha \vee (n-\alpha)K_1)$ has an equitable quotient matrix

$$R(A(K_\alpha \vee (n-\alpha)K_1)) = \begin{bmatrix} \alpha - 1 & n - \alpha \\ \alpha & 0 \end{bmatrix}.$$

Then the characteristic polynomial of $R(A(K_\alpha \vee (n-\alpha)K_1))$ is $f_2(x) = x^2 - (\alpha-1)x + \alpha(\alpha-n)$. The axis of symmetry of $f_2(x)$ is $x = \frac{\alpha-1}{2} < n-r-2$, which implies that $f_2(x)$ is increasing for $x \geqslant n-r-2$. By $n \geqslant 2r+15$, we have

$$f_2(x) \geqslant f_2(n-r-2) = n(n-2r-2\alpha-3) + r^2 + (\alpha+3)r + \alpha^2 + 2\alpha + 2 > 0.$$

Hence $\rho(K_\alpha \vee (n-\alpha)K_1) < n-r-2$. Combining (5), we have

$$n-r-2 < \rho(G^*_\rho) \leqslant \rho(K_\alpha \vee (n-\alpha)K_1) < n-r-2,$$

a contradiction. Next we consider $t_2 = 1$. Let $S^* = S \cup T_2$. By Claim 16, G^*_ρ is connected. Then $N_{G^*_\rho}(S^*) = N_{G^*_\rho}(S) = T_1$, and hence $b(G^*_\rho) \leqslant \frac{|N_{G^*_\rho}(S^*)|}{|S^*|} = \frac{t_1}{s+1} < \frac{t_1}{s} = b(G^*_\rho)$, a contradiction. Hence $t_2 \geqslant 2$. $\Diamond$

Claim 19. $s = rt_1 + 1$.

Proof. Note that $b(K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)) \leqslant \frac{t_1}{rt_1+1} < \frac{1}{r}$. Then $K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1) \in \mathcal{G}_{n,r}$. By (3), $s \geqslant rt_1+1$. If $s \geqslant rt_1+2$, then G^*_ρ is a spanning subgraph of $K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)$. By Lemma 11, $\rho(K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)) > \rho(G^*_\rho)$. This contradicts the maximality of G^*_ρ. Hence $s = rt_1+1$. $\Diamond$

By Claim 19, $G^*_\rho \cong K_{t_1} \vee (K_{n-(r+1)t_1-1} \cup (rt_1+1)K_1)$. Combining $s + t_1 + t_2 = n$, Claim 18 and Claim 19, we deduce that $1 \leqslant t_1 \leqslant \left\lfloor \frac{n-3}{r+1} \right\rfloor$. Next our goal is to prove that $t_1 = 1$. Suppose to the contrary that $2 \leqslant t_1 \leqslant \left\lfloor \frac{n-3}{r+1} \right\rfloor$. Note that $A(G^*_\rho)$ has an equitable quotient matrix

$$R(A(G^*_\rho)) = \begin{bmatrix} t_1-1 & n-(r+1)t_1-1 & rt_1+1 \\ t_1 & n-(r+1)t_1-2 & 0 \\ t_1 & 0 & 0 \end{bmatrix}.$$

Then the characteristic polynomial of $R(A(G^*_\rho))$ is

$$f_3(x) = x^3-(n-rt_1-3)x^2-(rt_1^2-(r-1)t_1+n-2)x-(r^2+r)t_1^3+((n-3)r-1)t_1^2+(n-2)t_1.$$

Let $G''' = K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$. Note that $A(G''')$ has an equitable quotient matrix

$$R(A(G''')) = \begin{bmatrix} 0 & n-r-2 & r+1 \\ 1 & n-r-3 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

Its characteristic polynomial is

$$f_4(x) = x^3 - (n-r-3)x^2 - (n-1)x + (r+1)(n-r-3).$$

By (4), $\rho(K_1 \vee (K_{n-r-2} \cup (r+1)K_1)) > n-r-2$. Next we prove that $f_3(x) - f_4(x) > 0$ for $x \geqslant n-r-2$. Let $f_5(x) = rx^2-(rt_1+1)x-(t_1^2+t_1+1)r^2+(nt_1-t_1^2+n-4t_1-4)r+n-t_1-3$.

Then $f_3(x) - f_4(x) = (t_1 - 1)f_5(x)$. Since $n \geqslant 2r + 15$, the axis of symmetry of $f_5(x)$ is $x = \frac{rt_1+1}{2r} < n - r - 2$, which implies that $f_5(x)$ is increasing for $x \geqslant n - r - 2$. Then $f_5(x) \geqslant f_5(n-r-2) = -((r^2+r)t_1^2 + (2r+1)t_1 - r^3 + (2n-3)r^2 - (n^2-3n+1)r + 1) \geqslant \frac{n^2r^2-(2r^3+5r^2-r+1)n+r^4+4r^3+4r^2-3r+2}{r+1} > 0$ for $x \geqslant n - r - 2$. Hence $f_3(x) - f_4(x) > 0$ for $x \geqslant n - r - 2$. By Lemma 10, we have

$$\rho(K_1 \vee (K_{n-r-2} \cup (r+1)K_1)) = \lambda_1(R(A(G'''))) > \lambda_1(R(A(G^*_\rho))) = \rho(G^*_\rho),$$

which contradicts (4). Hence $t_1 = 1$, and so $G^*_\rho \cong K_1 \vee (K_{n-r-2} \cup (r+1)K_1)$. □

3 Proof of Theorem 8

Before proceeding with the proof, we first state several useful lemmas.

Lemma 20. *Let $G = (X, Y)$ be a bipartite graph, and let S be a binding set of G. If $S \cap X \neq \emptyset$ and $S \cap Y \neq \emptyset$, then $S \cap X$ and $S \cap Y$ are also binding sets.*

Proof. Let $S_1 = S \cap X$ and $S_2 = S \cap Y$. Since S is a binding set of G, $b(G) = \frac{|N_G(S)|}{|S|} = \frac{|N_G(S_1)|+|N_G(S_2)|}{|S_1|+|S_2|}$. For short, let $b(G) = b$. By the definition of binding number, we have $\frac{|N_G(S_1)|}{|S_1|} \geqslant b$ and $\frac{|N_G(S_2)|}{|S_2|} \geqslant b$. We claim that $\frac{|N_G(S_1)|}{|S_1|} = \frac{|N_G(S_2)|}{|S_2|} = b$. In fact, if $\frac{|N_G(S_1)|}{|S_1|} > b$ or $\frac{|N_G(S_2)|}{|S_2|} > b$, then $|N_G(S_1)| + |N_G(S_2)| > b(|S_1| + |S_2|)$, and hence

$$b = b(G) = \frac{|N_G(S_1)| + |N_G(S_2)|}{|S_1| + |S_2|} > b,$$

a contradiction. This implies that $S \cap X$ and $S \cap Y$ are binding sets. □

Lemma 21. *Let p, q, r, n be four positive integers. Then $b(D(p - r(q-1) - 1, r(q-1) + 1; q-1, 1)) < \frac{1}{r}$, $b(D(p-r-1, r+1; 1, q-1)) < \frac{1}{r}$ and $b(K_{n-\lfloor\frac{n-1}{r+1}\rfloor, \lfloor\frac{n-1}{r+1}\rfloor}) < \frac{1}{r}$.*

Proof. Let $G_1 = D(p - r(q-1) - 1, r(q-1) + 1; q-1, 1)$, $G_2 = D(p - r - 1, r + 1; 1, q-1)$ and $G_3 = K_{n-\lfloor\frac{n-1}{r+1}\rfloor, \lfloor\frac{n-1}{r+1}\rfloor}$. The vertex set of G_1 can be partitioned as $V(G_1) = V((p - r(q-1) - 1)K_1) \cup V((r(q-1) + 1)K_1) \cup V((q-1)K_1) \cup V(K_1)$. Take $S_1 = V((r(q-1)+1)K_1)$. Then $b(G_1) \leqslant \frac{|N_{G_1}(S_1)|}{|S_1|} = \frac{q-1}{r(q-1)+1} < \frac{1}{r}$. The vertex set of G_2 can be partitioned as $V(G_2) = V((p-r-1)K_1) \cup V((r+1)K_1) \cup V(K_1) \cup V((q-1)K_1)$. Take $S_2 = V((r+1)K_1)$. Then $b(G_2) \leqslant \frac{|N_{G_2}(S_2)|}{|S_2|} = \frac{1}{r+1} < \frac{1}{r}$. The vertex set of G_3 can be partitioned as $V(G_3) = V((n - \lfloor\frac{n-1}{r+1}\rfloor)K_1) \cup V((\lfloor\frac{n-1}{r+1}\rfloor)K_1)$. Take $S_3 = V((n - \lfloor\frac{n-1}{r+1}\rfloor)K_1)$. Then $b(G_3) \leqslant \frac{|N_{G_3}(S_3)|}{|S_3|} = \frac{\lfloor\frac{n-1}{r+1}\rfloor}{n-\lfloor\frac{n-1}{r+1}\rfloor} \leqslant \frac{n-1}{rn+1} < \frac{1}{r}$. □

Next we prove a technical lemma which is very important to our main result. Let $\mathcal{B}_{p,q,r}$ be the family of n-vertex bipartite graphs with the bipartition (X, Y) that contain no isolated vertices and satisfy $b(G) < \frac{1}{r}$ for each $G \in \mathcal{B}_{p,q,r}$, where $r \geqslant 1$ is an integer. Without loss of generality, assume that $|X| = p \geqslant |Y| = q$.

Lemma 22. *Let $r \geqslant 1$ be an integer, and let $G \in \mathcal{B}_{p,q,r}$. Each of the following holds.*

(i) If $p \geqslant rq+1$, then $e(G) \leqslant pq$ with equality if and only if $G \cong K_{p,q}$.

(ii) If $r(q-1)+2 \leqslant p \leqslant rq$, then $e(G) \leqslant pq - r(q-1) - 1$ with equality if and only if $G \cong D(p-r(q-1)-1, r(q-1)+1; q-1, 1)$.

(iii) If $p \leqslant r(q-1)+1$, then $e(G) \leqslant pq-(r+1)(q-1)$ with equality if and only if $G \cong D(p-r-1, r+1; 1, q-1)$.

Proof. Let B_e^* be the graph with the maximum size in $\mathcal{B}_{p,q,r}$. Note that $b(B_e^*) < \frac{1}{r}$ for integer $r \geqslant 1$. By Lemma 20, we can choose a binding set S such that $S \subseteq X$ or $S \subseteq Y$. Then $b(B_e^*) = \frac{|N_{B_e^*}(S)|}{|S|} < \frac{1}{r}$ and $N_{B_e^*}(S) \neq V(B_e^*)$. Let $|S| = s$ and $|N_{B_e^*}(S)| = t$. Then we have

$$s \geqslant rt+1. \tag{6}$$

Claim 23. *If $S \subseteq X$, then $B_e^*[(X \setminus S) \cup Y] \cong K_{p-s,q}$ and $B_e^*[S \cup N_{B_e^*}(S)] \cong K_{s,t}$.*

Proof. Suppose to the contrary that $B_e^*[(X \setminus S) \cup Y] \ncong K_{p-s,q}$. Then there exist two vertices u, v such that $uv \notin E(B_e^*)$, where $u \in X \setminus S$ and $v \in Y$. Let $B' = B_e^* + uv$. Then $b(B') \leqslant \frac{|N_{B'}(S)|}{|S|} = \frac{|N_{B_e^*}(S)|}{|S|} < \frac{1}{r}$, which implies that $B' \in \mathcal{B}_{p,q,r}$. However, $e(B') > e(B_e^*)$, which contradicts the maximality of B_e^*. So $B_e^*[(X \setminus S) \cup Y] \cong K_{p-s,q}$. Similarly, we can prove that $B_e^*[S \cup N_{B_e^*}(S)] \cong K_{s,t}$. $\lozenge$

Similar to the analysis of Claim 23, one can immediately obtain the following result.

Claim 24. *If $S \subseteq Y$, then $B_e^*[X \cup (Y \setminus S)] \cong K_{p,q-s}$ and $B_e^*[S \cup N_{B_e^*}(S)] \cong K_{t,s}$.*

By Claim 23 and Claim 24, $B_e^* \cong D(p-s, s; t, q-t)$ for $S \subseteq X$ and $B_e^* \cong D(t, p-t; q-s, s)$ for $S \subseteq Y$. Hence B_e^* is connected.

Claim 25. *$s = rt+1$.*

Proof. We first consider $S \subseteq X$. Note that $b(D(p-rt-1, rt+1; t, q-t)) \leqslant \frac{t}{rt+1} < \frac{1}{r}$. Then $D(p-rt-1, rt+1; t, q-t) \in \mathcal{B}_{p,q,r}$. By (6), $s \geqslant rt+1$. If $s \geqslant rt+2$, then B_e^* is a proper subgraph of $D(p-rt-1, rt+1; t, q-t)$. It follows that $e(D(p-rt-1, rt+1; t, q-t)) > e(B_e^*)$, which contradicts the maximality of B_e^*. Therefore, $s = rt+1$. By the same analysis, the result holds for $S \subseteq Y$. $\lozenge$

By Claim 25, $B_e^* \cong D(p-rt-1, rt+1; t, q-t)$ for $S \subseteq X$ and $B_e^* \cong D(t, p-t; q-rt-1, rt+1)$ for $S \subseteq Y$.

Claim 26. *If $S \subseteq Y$ and $p \leqslant rq$, then $t = 1$.*

Proof. Note that $S \subseteq Y$. Then $s \leqslant q$. By Claim 25, we have $t < s \leqslant q \leqslant p$, and hence $t \leqslant p-1$. If $s = q$, then B_e^* is disconnected, a contradiction. So $s \leqslant q-1$. Recall that $s = rt+1$. Then $1 \leqslant t \leqslant \left\lfloor \frac{q-2}{r} \right\rfloor$. Note that $b(D(1, p-1; q-r-1, r+1)) \leqslant \frac{1}{r+1} < \frac{1}{r}$. Then

$D(1,p-1;q-r-1,r+1) \in \mathcal{B}_{p,q,r}$, and hence $e(B_e^*) \geqslant e(D(1,p-1;q-r-1,r+1)) = pq-(r+1)(p-1)$. If $1 < t \leqslant \left\lfloor \frac{q-2}{r} \right\rfloor$, then

$$\begin{array}{rcl} pq-(r+1)(p-1) \leqslant e(B_e^*) & = & e(D(t,p-t;q-rt-1,rt+1)) \\ & = & pq+rt^2+(1-rp)t-p \\ & < & pq-(r+1)(p-1), \end{array}$$

a contradiction. Hence $t=1$. $\Diamond$

Claim 27. *If $S \subseteq X$ and $p \leqslant rq$, then $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$.*

Proof. Since $S \subseteq X$, we have $N_{B_e^*}(S) \subseteq Y$, and hence $t \leqslant q$. By $p \leqslant rq$, Claim 25 and $s \leqslant p$, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-1}{r} \right\rfloor$. If $q=t<s=p$, then $b(B_e^*) = \frac{|N_{B_e^*}(S)|}{|S|} = \frac{t}{s} = \frac{q}{p} \geqslant \frac{1}{r}$, a contradiction. If $t \leqslant q-1 < s = p$, then B_e^* is disconnected, a contradiction. Hence $s \leqslant p-1$. Since $s = rt+1$, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$. $\Diamond$

(i) Since $p \geqslant rq+1$, $b(K_{p,q}) = \frac{q}{p} \leqslant \frac{q}{rq+1} < \frac{1}{r}$, and hence $K_{p,q} \in \mathcal{B}_{p,q,r}$. So we have $e(B_e^*) \geqslant e(K_{p,q}) = pq$. Note that B_e^* is a subgraph of $K_{p,q}$. Then $B_e^* \cong K_{p,q}$.

(ii) By Lemma 21, $D(p-r(q-1)-1, r(q-1)+1; q-1, 1) \in \mathcal{B}_{p,q,r}$. Therefore,

$$e(B_e^*) \geqslant e(D(p-r(q-1)-1, r(q-1)+1; q-1,1)) = pq-r(q-1)-1. \tag{7}$$

Next we will prove that $S \subseteq X$. If $S \subseteq Y$, by Claim 26 and $B_e^* \cong D(t,p-t;q-rt-1,rt+1)$, we have

$$e(B_e^*) = pq-(r+1)(p-1) < pq-r(q-1)-1,$$

which contradicts (7). Hence $S \subseteq X$. Since $r(q-1)+2 \leqslant p \leqslant rq$, we have $r \geqslant 2$ and $q-1 \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$. Moreover, as $r \geqslant 2$ and $p \leqslant rq$, we obtain that $q-1 \geqslant \left\lfloor \frac{p-2}{r} \right\rfloor$. Hence $q-1 = \left\lfloor \frac{p-2}{r} \right\rfloor$. By Claim 27, we have $1 \leqslant t \leqslant q-1$. Next we claim that $t = q-1$. In fact, if $t < q-1$, then

$$\begin{array}{rcl} e(B_e^*) & = & e(D(p-rt-1,rt+1;t,q-t)) \\ & = & pq+rt^2+(1-rq)t-q \\ & < & pq-r(q-1)-1, \end{array}$$

which contradicts (7). Hence $t = q-1$. Then we have $B_e^* \cong D(p-r(q-1)-1, r(q-1)+1; q-1, 1)$.

(iii) By Lemma 21, $D(p-r-1, r+1; 1, q-1) \in \mathcal{B}_{p,q,r}$, and hence

$$e(B_e^*) \geqslant e(D(p-r-1,r+1;1,q-1)) = pq-(r+1)(q-1). \tag{8}$$

We distinguish our proof into the following two cases.

Case 1. $S \subseteq X$.

By $p \leqslant r(q-1)+1 \leqslant rq$ and Claim 27, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor \leqslant q-2$. Note that $B_e^* \cong D(p-rt-1, rt+1; t, q-t)$. If $1 < t \leqslant q-2$, then

$$\begin{aligned} e(B_e^*) &= e(D(p-rt-1, rt+1; t, q-t)) \\ &= pq + rt^2 + (1-rq)t - q \\ &< pq - (r+1)(q-1), \end{aligned}$$

which contradicts (8). Hence $t = 1$. Then we have $B_e^* \cong D(p-r-1, r+1; 1, q-1)$.

Case 2. $S \subseteq Y$.

By $q \leqslant p \leqslant r(q-1)+1 \leqslant rq$, Claim 26 and $B_e^* \cong D(t, p-t; q-rt-1, rt+1)$, we have $e(B_e^*) = pq - (r+1)(p-1) \leqslant pq - (r+1)(q-1)$. If $p > q$, then $e(B_e^*) = pq - (r+1)(p-1) < pq - (r+1)(q-1)$, which contradicts (8). Hence $p = q$. Then $B_e^* \cong D(p-r-1, r+1; 1, q-1)$. □

Recall that $f(n,r) = \left\lfloor \frac{n-1}{r+1} \right\rfloor \left(n - \left\lfloor \frac{n-1}{r+1} \right\rfloor\right)$ and $g(n,r) = \left\lfloor \frac{n-r-1}{2} \right\rfloor \left\lceil \frac{n-r-1}{2} \right\rceil + r + 1$.

Proof of Theorem 8. Let $\tilde{B}_e^* = (X, Y)$ be the bipartite graph with the maximum size in $\mathcal{B}_{n,r}$. Without loss of generality, we assume that $|X| \geqslant |Y|$. Let $|Y| = q$. Then $|X| = n-q$ and $q \leqslant \left\lfloor \frac{n}{2} \right\rfloor$.

(i) Note that $r = 1$. We claim that $|X| = n-q \geqslant q+1$. In fact, if $n-q \leqslant q$, then $n = 2q$, which implies that n is even. By Lemma 22 (iii), we have $\tilde{B}_e^* \cong D(\frac{n}{2}-2, 2; 1, \frac{n}{2}-1)$. Then $e(\tilde{B}_e^*) = e(D(\frac{n}{2}-2, 2; 1, \frac{n}{2}-1)) = \frac{n^2}{4} - n + 2$. According to Lemma 21, $K_{n-\left\lfloor \frac{n-1}{2} \right\rfloor, \left\lfloor \frac{n-1}{2} \right\rfloor} \in \mathcal{B}_{n,1}$ and $e(K_{n-\left\lfloor \frac{n-1}{2} \right\rfloor, \left\lfloor \frac{n-1}{2} \right\rfloor}) = \left(n - \left\lfloor \frac{n-1}{2} \right\rfloor\right) \left\lfloor \frac{n-1}{2} \right\rfloor$. Note that n is even. Then

$$\left(n - \left\lfloor \frac{n-1}{2} \right\rfloor\right) \left\lfloor \frac{n-1}{2} \right\rfloor \leqslant e(\tilde{B}_e^*) = \frac{n^2}{4} - n + 2 < \frac{n^2-4}{4} = \left(n - \left\lfloor \frac{n-1}{2} \right\rfloor\right) \left\lfloor \frac{n-1}{2} \right\rfloor,$$

a contradiction. Hence $n-q \geqslant q+1$, and $q \leqslant \left\lfloor \frac{n-1}{2} \right\rfloor$. By Lemma 22 (i), we have $\tilde{B}_e^* \cong K_{n-q,q}$. Since $q \leqslant \left\lfloor \frac{n-1}{2} \right\rfloor$, $\tilde{B}_e^* \cong K_{n-\left\lfloor \frac{n-1}{2} \right\rfloor, \left\lfloor \frac{n-1}{2} \right\rfloor}$.

(ii) Note that $r \geqslant 2$. We first prove that $n-q \geqslant rq+1$. Suppose to the contrary that $n-q \leqslant rq$. If $r(q-1)+2 \leqslant n-q \leqslant rq$, then $\left\lceil \frac{n}{r+1} \right\rceil \leqslant q \leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor$. By Lemma 22 (ii), we have $\tilde{B}_e^* \cong D(n-(r+1)q+r-1, r(q-1)+1; q-1, 1)$. Note that $K_{n-\left\lfloor \frac{n-1}{r+1} \right\rfloor, \left\lfloor \frac{n-1}{r+1} \right\rfloor} \in \mathcal{B}_{n,r}$ and $e(K_{n-\left\lfloor \frac{n-1}{r+1} \right\rfloor, \left\lfloor \frac{n-1}{r+1} \right\rfloor}) = (n - \left\lfloor \frac{n-1}{r+1} \right\rfloor) \left\lfloor \frac{n-1}{r+1} \right\rfloor$. Then $e(\tilde{B}_e^*) \geqslant (n - \left\lfloor \frac{n-1}{r+1} \right\rfloor) \left\lfloor \frac{n-1}{r+1} \right\rfloor = f(n,r)$. By $\left\lceil \frac{n}{r+1} \right\rceil \leqslant q \leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor$ and $n \geqslant r^2+r+1$, we have

$$\begin{aligned} f(n,r) &\leqslant e(\tilde{B}_e^*) = (n-q)q - r(q-1) - 1 \\ &\leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor \left(n - r - \left\lfloor \frac{n+r-2}{r+1} \right\rfloor\right) + r - 1 \\ &< f(n,r), \end{aligned}$$

a contradiction. If $n-q \leqslant r(q-1)+1$, then $\left\lfloor \frac{n+r-1}{r+1} \right\rfloor \leqslant q \leqslant \lfloor \frac{n}{2} \rfloor$. By Lemma 22 (iii), we have $\tilde{B_e^*} \cong D(n-q-r-1, r+1; 1, q-1)$. By $f(n,r) > g(n,r)$ and $\left\lfloor \frac{n+r-1}{r+1} \right\rfloor \leqslant q \leqslant \lfloor \frac{n}{2} \rfloor$, we can obtain that

$$\begin{aligned} f(n,r) \leqslant e(\tilde{B_e^*}) &= (n-q)q-(r+1)(q-1) \\ &\leqslant \left\lfloor \frac{n-r-1}{2} \right\rfloor \left\lceil \frac{n-r-1}{2} \right\rceil + r + 1 < f(n,r), \end{aligned}$$

a contradiction. Hence $n-q \geqslant rq+1$, and $1 \leqslant q \leqslant \left\lfloor \frac{n-1}{r+1} \right\rfloor$. By Lemma 22 (i), we have $\tilde{B_e^*} \cong K_{n-q,q}$. If $q < \left\lfloor \frac{n-1}{r+1} \right\rfloor$, then

$$f(n,r) \leqslant e(\tilde{B_e^*}) = e(K_{n-q,q}) = (n-q)q < f(n,r),$$

a contradiction. Therefore, $q = \left\lfloor \frac{n-1}{r+1} \right\rfloor$, which implies that $\tilde{B_e^*} \cong K_{n-\left\lfloor \frac{n-1}{r+1} \right\rfloor, \left\lfloor \frac{n-1}{r+1} \right\rfloor}$.

(iii) Note that $r \geqslant 2$. We claim that $n-q \leqslant r(q-1)+1$. By contradiction, assume that $n-q \geqslant r(q-1)+2$. If $r(q-1)+2 \leqslant n-q \leqslant rq$, then $\left\lceil \frac{n}{r+1} \right\rceil \leqslant q \leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor$. Combining Lemma 22 (ii), we have $\tilde{B_e^*} \cong D(n-(r+1)q+r-1, r(q-1)+1; q-1, 1)$. Note that $D\big(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\big) \in \mathcal{B}_{n,r}$ and $e\big(D\big(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\big)\big) = g(n,r)$. Then $e(\tilde{B_e^*}) \geqslant g(n,r)$. By $\left\lceil \frac{n}{r+1} \right\rceil \leqslant q \leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor$ and $n \geqslant r^2+r+1$, we have

$$\begin{aligned} g(n,r) &\leqslant e(\tilde{B_e^*}) = (n-q)q - r(q-1) - 1 \\ &\leqslant \left\lfloor \frac{n+r-2}{r+1} \right\rfloor \left(n - r - \left\lfloor \frac{n+r-2}{r+1} \right\rfloor \right) + r - 1 \\ &< g(n,r), \end{aligned}$$

a contradiction. If $n-q \geqslant rq+1$, then $1 \leqslant q \leqslant \left\lfloor \frac{n-1}{r+1} \right\rfloor$. By Lemma 22 (i), we have $\tilde{B_e^*} \cong K_{n-q,q}$. By $1 \leqslant q \leqslant \left\lfloor \frac{n-1}{r+1} \right\rfloor$ and $f(n,r) < g(n,r)$, we have

$$g(n,r) \leqslant e(\tilde{B_e^*}) = (n-q)q \leqslant \left(n - \left\lfloor \frac{n-1}{r+1} \right\rfloor \right) \left\lfloor \frac{n-1}{r+1} \right\rfloor = f(n,r) < g(n,r),$$

a contradiction. Hence $n-q \leqslant r(q-1)+1$, and $\left\lfloor \frac{n+r-1}{r+1} \right\rfloor \leqslant q \leqslant \lfloor \frac{n}{2} \rfloor$. By Lemma 22 (iii), we have $\tilde{B_e^*} \cong D(n-q-r-1, r+1; 1, q-1)$. If $q \neq \left\lfloor \frac{n-r-1}{2} \right\rfloor$ and $q \neq \left\lceil \frac{n-r-1}{2} \right\rceil$, then

$$\begin{aligned} g(n,r) \leqslant e(\tilde{B_e^*}) &= (n-q)q-(r+1)(q-1) \\ &< \left\lfloor \frac{n-r-1}{2} \right\rfloor \left\lceil \frac{n-r-1}{2} \right\rceil + r + 1 = g(n,r), \end{aligned}$$

a contradiction. Hence we have $q = \left\lfloor \frac{n-r-1}{2} \right\rfloor$ or $q = \left\lceil \frac{n-r-1}{2} \right\rceil$, which implies that $\tilde{B_e^*} \cong D\Big(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\Big)$ or $\tilde{B_e^*} \cong D\Big(\left\lfloor \frac{n-r-1}{2} \right\rfloor, r+1; 1, \left\lceil \frac{n-r-1}{2} \right\rceil - 1\Big)$.

(iv) Based on the proofs of (ii) and (iii), (iv) directly follows. □

4 Proof of Theorem 9

Before presenting the proof, we state some necessary lemmas.

Lemma 28 (Bhattacharya et al.[1]). *If G is a bipartite graph, then $\rho(G) \leqslant \sqrt{e(G)}$ with equality if and only if G is a complete bipartite graph.*

Recall that $\mathcal{B}_{p,q,r}$ is the family of n-vertex bipartite graphs with the bipartition (X, Y) that contain no isolated vertices and satisfy $b(G) < \frac{1}{r}$ for each $G \in \mathcal{B}_{p,q,r}$, where $r \geqslant 1$ is an integer and $|X| = p \geqslant |Y| = q$.

Lemma 29. *Let $2 \leqslant t \leqslant \lfloor \frac{p-2}{r} \rfloor$ be an integer. If $\lfloor \frac{p-2}{r} \rfloor \leqslant q-3$, then $\rho(D(p-rt-1, rt+1; t, q-t)) < \rho(D(p-r-1, r+1; 1, q-1))$.*

Proof. Since $\lfloor \frac{p-2}{r} \rfloor \leqslant q-3$, $p \leqslant r(q-2)+1$. Define $G_1 = D(p-rt-1, rt+1; t, q-t)$. Then the vertex set of G_1 can be partitioned as $V(G_1) = V(X_1) \cup V(X_2) \cup V(Y_1) \cup V(Y_2)$, where $V(X_1) = \{u_1, u_2, \ldots, u_{p-rt-1}\}$, $V(X_2) = \{v_1, v_2, \ldots, v_{rt+1}\}$, $V(Y_1) = \{w_1, w_2, \ldots, w_t\}$ and $V(Y_2) = \{z_1, z_2, \ldots, z_{q-t}\}$. Let x be the Perron vector of $A(G_1)$, and let $\rho = \rho(G_1)$. By symmetry, x takes the same value (say x_1, x_2, x_3, x_4) on the vertices of $V(X_1)$, $V(X_2)$, $V(Y_1)$, $V(Y_2)$, respectively. By $A(G_1)x = \rho x$, we have

$$\begin{aligned}
\rho x_1 &= t x_3 + (q-t) x_4, \\
\rho x_2 &= t x_3, \\
\rho x_3 &= (p-rt-1) x_1 + (rt+1) x_2, \\
\rho x_4 &= (p-rt-1) x_1,
\end{aligned}$$

which leads to

$$x_2 = \frac{t}{\rho} x_3, \ \ x_4 = \left(1 - \frac{t(rt+1)}{\rho^2}\right) x_3.$$

Let $G_2 = D(p-r-1, r+1; 1, q-1)$. Then the vertex set of G_2 can be partitioned as $V(G_2) = V(X_1') \cup V(X_2') \cup V(Y_1') \cup V(Y_2')$. Let y be the Perron vector of $A(G_2)$, and let $\rho' = \rho(G_2)$. By symmetry, y takes the same value (say y_1, y_2, y_3, y_4) on the vertices of $V(X_1')$, $V(X_2')$, $V(Y_1')$, $V(Y_2')$, respectively. Then, by $A(G_2)y = \rho' y$, we have

$$\begin{aligned}
\rho' y_1 &= y_3 + (q-1) y_4, \\
\rho' y_2 &= y_3, \\
\rho' y_3 &= (p-r-1) y_1 + (r+1) y_2, \\
\rho' y_4 &= (p-r-1) y_1,
\end{aligned}$$

which leads to

$$y_2 = \left(1 - \frac{(p-r-1)(q-1)}{\rho'^2}\right) y_1, \ \ y_4 = \frac{p-r-1}{\rho'} y_1.$$

Let $E_1 = \{v_i z_j \mid r+2 \leqslant i \leqslant rt+1, 1 \leqslant j \leqslant q-t\}$ and $E_2 = \{v_i w_j \mid 1 \leqslant i \leqslant r+1, 1 \leqslant j \leqslant t-1\}$. Note that $G_2 = G_1 + E_1 - E_2$. Then

$$\begin{aligned}
& x^T(\rho' - \rho)y \\
= \ & x^T(A(G_2) - A(G_1))y \\
= \ & \sum_{v_i z_j \in E_1} (x_{v_i} y_{z_j} + x_{z_j} y_{v_i}) - \sum_{v_i w_j \in E_2} (x_{v_i} y_{w_j} + x_{w_j} y_{v_i}) \\
= \ & r(t-1)(q-t)(x_2 y_4 + x_4 y_1) - (r+1)(t-1)(x_2 y_4 + x_3 y_2) \\
= \ & (t-1)\left((r(q-t-1)-1)x_2 y_4 + r(q-t)x_4 y_1 - (r+1)x_3 y_2\right) \\
= \ & (t-1)x_3 y_1 \left((r(q-t-1)-1)\Big(\frac{t(p-r-1)}{\rho\rho'} + 1\Big) + \frac{(r+1)(q-1)(p-r-1)}{\rho'^2} \right. \\
& \left. - \frac{rt(q-t)(rt+1)}{\rho^2} \right) \triangleq (t-1)x_3 y_1 (*).
\end{aligned}$$

Suppose to the contrary that $\rho \geqslant \rho'$. Then we have $\frac{1}{\rho'} \geqslant \frac{1}{\rho}$. Note that $\rho' = \rho(D(p-r-1, r+1; 1, q-1)) > \rho(K_{p-r-1,q}) = \sqrt{(p-r-1)q}$. Then $\rho > \sqrt{(p-r-1)q}$. It follows that

$$\begin{aligned}
(*) \ \geqslant \ & (r(q-t-1)-1)\left(\frac{t(p-r-1)}{\rho^2} + 1\right) + \frac{(r+1)(q-1)(p-r-1)}{\rho^2} \\
& - \frac{rt(q-t)(rt+1)}{\rho^2} \\
\geqslant \ & (r(q-t-1)-1)\left(\frac{t(p-r-1)}{\rho^2} + \frac{(p-r-1)q}{\rho^2}\right) + \frac{(r+1)(q-1)(p-r-1)}{\rho^2} \\
& - \frac{rt(q-t)(rt+1)}{\rho^2} \\
\triangleq \ & \frac{g(t)}{\rho^2},
\end{aligned}$$

where $g(t) = r^2t^3 + [(1-q)r^2 + (2-p)r]t^2 + [r^2 - (p+q-2)r - p + 1]t + (1-q^2)r^2 + (pq^2 - q^2 - p + 2)r - p + 1$. Observe that $g'(t) = 3r^2t^2 + 2[(1-q)r^2 + (2-p)r]t + r^2 + (2-p-q)r - p + 1$. A direct computation gives $g'(2) = (17-4q)r^2 + (10-5p-q)r - p + 1 < 0$ and

$$\begin{aligned}
g'\left(\frac{p-2}{r}\right) \ &= \ p^2 + [(1-2q)r - 5]p + r^2 + (3q-2)r + 5 \\
&\leqslant \ q^2 + [(1-2q)r - 5]q + r^2 + (3q-2)r + 5 \\
&= \ (1-2r)q^2 + (4r-5)q + r^2 - 2r + 5 \\
&< \ 0.
\end{aligned}$$

This implies that $g(t)$ is decreasing for $2 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor \leqslant \frac{p-2}{r}$. Together with the condition

$p \leqslant r(q-2)+1$, we deduce that

$$\begin{aligned} g(t) &\geqslant g\left(\frac{p-2}{r}\right) \\ &= \frac{(-qr-1)p^2+(q^2r^2+3qr-r+3)p-q^2r^3-q^2r^2+r^3-2qr+r-2}{r} \\ &\geqslant \frac{q^2r^3+r(-4r^2+r+1)q+r(r^2-2r-2)}{r} \\ &> 0. \end{aligned}$$

Hence $x^T(\rho'-\rho)y > 0$, which implies that $\rho < \rho'$, a contradiction. Hence $\rho(D(p-rt-1, rt+1; t, q-t)) < \rho(D(p-r-1, r+1; 1, q-1))$. □

Next we will prove a technical lemma which is crucial to our main result.

Lemma 30. *Let $r \geqslant 1$ be an integer, and let $G \in \mathcal{B}_{p,q,r}$. Each of the following holds.*

(i) If $p \geqslant rq+1$, then $\rho(G) \leqslant \sqrt{pq}$ with equality if and only if $G \cong K_{p,q}$.

(ii) If $r(q-1)+2 \leqslant p \leqslant rq$, then $\rho(G) \leqslant \rho(D(p-r(q-1)-1, r(q-1)+1; q-1, 1))$ with equality if and only if $G \cong D(p-r(q-1)-1, r(q-1)+1; q-1, 1)$.

(iii) If $p \leqslant r(q-1)+1$, then $\rho(G) \leqslant \rho(D(p-r-1, r+1; 1, q-1))$ with equality if and only if $G \cong D(p-r-1, r+1; 1, q-1)$.

Proof. Let B_ρ^* be the graph with the maximum spectral radius in $\mathcal{B}_{p,q,r}$. Note that $b(B_\rho^*) < \frac{1}{r}$ for integer $r \geqslant 1$. By Lemma 20, we can select a binding set S satisfying $S \subseteq X$ or $S \subseteq Y$. Then $b(B_\rho^*) = \frac{|N_{B_\rho^*}(S)|}{|S|} < \frac{1}{r}$ and $N_{B_\rho^*}(S) \neq V(B_\rho^*)$. Define $|S| = s$ and $|N_{B_\rho^*}(S)| = t$. Then we can obtain that

$$s \geqslant rt+1. \tag{9}$$

Claim 31. *B_ρ^* is connected.*

Proof. Suppose to the contrary that B_ρ^* is disconnected. Let $B_1, B_2, \ldots, B_c$ be the connected components of B_ρ^*, where $B_i = (X_i, Y_i)$ for each $1 \leqslant i \leqslant c$. Hence there exists a connected component B_i such that $S \cap V(B_i) \neq \emptyset$. Without loss of generality, assume that $S \cap V(B_1) = S_1 \neq \emptyset$. We first consider the case $S \subseteq X$. Note that B_ρ^* contains no isolated vertices. Then $N_{B_1}(S_1) \neq \emptyset$ and $|X_i| \geqslant 1$ for $2 \leqslant i \leqslant c$. Define $B' = B_\rho^* + uv_2 + uv_3 + \cdots + uv_c$, where $u \in V(N_{B_1}(S_1))$ and $v_i \in X_i$ for $2 \leqslant i \leqslant c$. One can check that $b(B') \leqslant \frac{|N_{B'}(S)|}{|S|} = \frac{|N_{B_\rho^*}(S)|}{|S|} < \frac{1}{r}$. Then $B' \in \mathcal{B}_{p,q,r}$. Note that B' is connected and B_ρ^* is a proper subgraph of B'. By Lemma 11, we have $\rho(B') > \rho(B_\rho^*)$, which contradicts the maximality of B_ρ^*. Hence B_ρ^* is connected. From the above analysis, we can still conclude that B_ρ^* is connected for $S \subseteq Y$. ♢

Claim 32. *If $S \subseteq X$, then $B_\rho^*[(X \setminus S) \cup Y] \cong K_{p-s,q}$ and $B_\rho^*[S \cup N_{B_\rho^*}(S)] \cong K_{s,t}$.*

Proof. Suppose to the contrary that $B^*_\rho[(X \setminus S) \cup Y] \not\cong K_{p-s,q}$. Then there exist two vertices u, v such that $uv \notin E(B^*_\rho)$, where $u \in X \setminus S$ and $v \in Y$. Let $B' = B^*_\rho + uv$. Then $b(B') \leqslant \frac{|N_{B'}(S)|}{|S|} = \frac{|N_{B^*_\rho}(S)|}{|S|} < \frac{1}{r}$, which implies that $B' \in \mathcal{B}_{p,q,r}$. By Claim 31 and Lemma 11, we have $\rho(B') > \rho(B^*_\rho)$, a contradiction. Hence $B^*_\rho[(X \setminus S) \cup Y] \cong K_{p-s,q}$. Similarly, $B^*_\rho[S \cup N_{B^*_\rho}(S)] \cong K_{s,t}$. $\diamondsuit$

By a similar argument to Claim 32, we obtain the following result.

Claim 33. *If $S \subseteq Y$, then $B^*_\rho[X \cup (Y \setminus S)] \cong K_{p,q-s}$ and $B^*_\rho[S \cup N_{B^*_\rho}(S)] \cong K_{t,s}$.*

By Claim 32 and Claim 33, $B^*_\rho \cong D(p-s, s; t, q-t)$ for $S \subseteq X$ and $B^*_\rho \cong D(t, p-t; q-s, s)$ for $S \subseteq Y$.

Claim 34. $s = rt + 1$.

Proof. We first consider $S \subseteq X$. Note that $b(D(p-rt-1, rt+1; t, q-t)) \leqslant \frac{t}{rt+1} < \frac{1}{r}$. Then $D(p-rt-1, rt+1; t, q-t) \in \mathcal{B}_{p,q,r}$. By (9), $s \geqslant rt+1$. If $s \geqslant rt+2$, then B^*_ρ is a proper subgraph of $D(p-rt-1, rt+1; t, q-t)$. By Lemma 11, $\rho(D(p-rt-1, rt+1; t, q-t)) > \rho(B^*_\rho)$, which contradicts the maximality of B^*_ρ. Hence $s = rt+1$. Following the same analysis, the result holds for $S \subseteq Y$. $\diamondsuit$

By Claim 34, $B^*_\rho \cong D(p-rt-1, rt+1; t, q-t)$ for $S \subseteq X$ and $B^*_\rho \cong D(t, p-t; q-rt-1, rt+1)$ for $S \subseteq Y$.

Claim 35. *If $S \subseteq Y$ and $p \leqslant rq$, then $t = 1$.*

Proof. Note that $S \subseteq Y$. Then $s \leqslant q$. By Claim 34, we have $t < s \leqslant q \leqslant p$, and hence $t \leqslant p-1$. If $s = q$, then B^*_ρ is disconnected, a contradiction. So $s \leqslant q-1$. Since $s = rt+1$, we have $1 \leqslant t \leqslant \left\lfloor \frac{q-2}{r} \right\rfloor$. Note that $A(B^*_\rho)$ has an equitable quotient matrix

$$R(A(B^*_\rho)) = \begin{bmatrix} 0 & 0 & q-rt-1 & rt+1 \\ 0 & 0 & q-rt-1 & 0 \\ t & p-t & 0 & 0 \\ t & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(B^*_\rho))$ is

$$g_1(x) = x^4 + [(p-t)(rt+1) - pq]x^2 + t(rt+1)(q-rt-1)(p-t).$$

Note that $A(D(1, p-1; q-r-1, r+1))$ has an equitable quotient matrix

$$R(A(D(1, p-1; q-r-1, r+1))) = \begin{bmatrix} 0 & 0 & q-r-1 & r+1 \\ 0 & 0 & q-r-1 & 0 \\ 1 & p-1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(D(1, p-1; q-r-1, r+1)))$ is

$$g_2(x) = x^4 + ((r+1)(p-1) - pq)x^2 + (r+1)(q-r-1)(p-1).$$

Observe that $D(1,p-1;q-r-1,r+1)$ contains $K_{p,q-r-1}$ as a proper subgraph. Combining Lemma 11, we have

$$\rho(D(1,p-1;q-r-1,r+1)) > \rho(K_{p,q-r-1}) = \sqrt{p(q-r-1)}.$$

Let $g_3(x) = (r(p-t)-(r+1))x^2 + r^2t^3 - r(pr+q-r-2)t^2 + ((1-p)r^2 + (q-2)(p-1)r - q + 1)t + (r+1)(q-r-1)(p-1)$. Then we have $g_1(x) - g_2(x) = (t-1)g_3(x)$. Suppose that $2 \leqslant t \leqslant \left\lfloor \frac{q-2}{r} \right\rfloor$. Then $r(p-t)-(r+1) \geqslant 0$. The symmetry axis of $g_3(x)$ is $x = 0 < \sqrt{p(q-r-1)}$, which implies that $g_3(x)$ is increasing for $x \geqslant \sqrt{p(q-r-1)}$. By calculation, we have

$$g_3(x) \quad \geqslant \quad g_3(\sqrt{p(q-r-1)}) \geqslant \frac{(2r^3+3r^2+3r)(q-1)(r-1)}{r} > 0.$$

Then $\lambda_1(R(A(B_\rho^*))) < \lambda_1(R(A(D(1,p-1;q-r-1,r+1))))$. According to Lemma 10, we conclude that $\rho(B_\rho^*) < \rho(D(1,p-1;q-r-1,r+1))$ for $2 \leqslant t \leqslant \left\lfloor \frac{q-2}{r} \right\rfloor$. Note that $D(1,p-1;q-r-1,r+1) \in \mathcal{B}_{p,q,r}$. This contradicts the maximality of B_ρ^*. Hence $t=1$. $\Diamond$

Claim 36. *If $S \subseteq X$ and $p \leqslant rq$, then $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$.*

Proof. Since $S \subseteq X$, we have $N_{B_\rho^*}(S) \subseteq Y$, and hence $t \leqslant q$. By $p \leqslant rq$, Claim 34 and $s \leqslant p$, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-1}{r} \right\rfloor$. If $q = t < s = p$, then $b(B_\rho^*) = \frac{|N_{B_\rho^*}(S)|}{|S|} = \frac{t}{s} = \frac{q}{p} \geqslant \frac{1}{r}$, a contradiction. If $t \leqslant q-1 < s = p$, then B_ρ^* is disconnected, a contradiction. Hence $s \leqslant p-1$. Since $s = rt+1$, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$. $\Diamond$

Claim 37. $\rho(D(p-r-1,r+1;1,q-1)) \geqslant \rho(D(1,p-1;q-r-1,r+1))$ *with equality if and only if $p=q$.*

Proof. Let $G_1 = D(p-r-1,r+1;1,q-1)$. Then $A(G_1)$ has an equitable quotient matrix

$$R(A(G_1)) = \begin{bmatrix} 0 & 0 & 1 & q-1 \\ 0 & 0 & 1 & 0 \\ p-r-1 & r+1 & 0 & 0 \\ p-r-1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(G_1))$ is

$$g_4(x) = x^4 + ((r+1)(q-1)-pq)x^2 + (r+1)(q-1)(p-r-1).$$

Recall that the characteristic polynomial of $R(A(D(1,p-1;q-r-1,r+1)))$ is

$$g_2(x) = x^4 + ((r+1)(p-1)-pq)x^2 + (r+1)(p-1)(q-r-1).$$

Observe that G_1 contains $K_{r+1,1}$ as a proper subgraph. By Lemma 11, we have $\rho(G_1) > \rho(K_{r+1,1}) = \sqrt{r+1}$. Since $g_2(x) - g_4(x) = (r+1)(x^2-r)(p-q) \geqslant 0$ for $x \geqslant \sqrt{r+1}$, $\lambda_1(G_1) \geqslant \lambda_1(R(A(D(1,p-1;q-r-1,r+1))))$ with equality if and only if $p=q$. By Lemma 10, we have $\rho(D(p-r-1,r+1;1,q-1)) \geqslant \rho(D(1,p-1;q-r-1,r+1))$ with equality if and only if $p=q$. $\Diamond$

(i) Since $p \geqslant rq+1$, $K_{p,q} \in \mathcal{B}_{p,q,r}$. Then $\rho(B^*_\rho) \geqslant \rho(K_{p,q}) = \sqrt{pq}$. Note that B^*_ρ is a subgraph of $K_{p,q}$. Then $B^*_\rho \cong K_{p,q}$.

(ii) Note that $r(q-1)+2 \leqslant p \leqslant rq$. Then $r \geqslant 2$ and $p > q$. Recall that $D(p-r-1, r+1; 1, q-1) \in \mathcal{B}_{p,q,r}$. If $S \subseteq Y$, then $B^*_\rho \cong D(t, p-t; q-rt-1, rt+1)$. By Claim 35 and Claim 37, we obtain that $\rho(D(p-r-1, r+1; 1, q-1)) > \rho(D(1, p-1; q-r-1, r+1)) = \rho(B^*_\rho)$, a contradiction. Hence $S \subseteq X$ and $B^*_\rho \cong D(p-rt-1, rt+1; t, q-t)$. Since $r(q-1)+2 \leqslant p \leqslant rq$ and $r \geqslant 2$, $q-1 = \left\lfloor \frac{p-2}{r} \right\rfloor$. By Claim 36, we have $1 \leqslant t \leqslant q-1$. Observe that $A(B^*_\rho)$ has an equitable quotient matrix

$$R(A(B^*_\rho)) = \begin{bmatrix} 0 & 0 & t & q-t \\ 0 & 0 & t & 0 \\ p-rt-1 & rt+1 & 0 & 0 \\ p-rt-1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(B^*_\rho))$ is given by

$$g_5(x) = x^4 + ((rt+1)(q-t) - pq)x^2 + t(rt+1)(q-t)(p-rt-1).$$

Let $G_2 = D(p-r(q-1)-1, r(q-1)+1; q-1, 1)$. Note that $A(G_2)$ has an equitable quotient matrix

$$R(A(G_2)) = \begin{bmatrix} 0 & 0 & q-1 & 1 \\ 0 & 0 & q-1 & 0 \\ p-r(q-1)-1 & r(q-1)+1 & 0 & 0 \\ p-r(q-1)-1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(G_2))$ is

$$g_6(x) = x^4 + (r(q-1) - pq + 1)x^2 + (q-1)(qr-r+1)(p-rq+r-1).$$

Observe that G_2 contains $K_{p,q-1}$ as a proper subgraph. By Lemma 11, we have

$$\rho(G_2) > \rho(K_{p,q-1}) = \sqrt{p(q-1)}.$$

Let $g_7(x) = (rt-r+1)x^2 + (t(rt-r+1) - r(q-1) - 1)p - r^2t^3 + r(r-2)t^2 + (qr^2 - (r-1)^2)t + (q^2+1)r^2 - 2r(r-1)q - 2r + 1$. Then $g_5(x) - g_6(x) = (q-t-1)g_7(x)$. The symmetry axis of $g_7(x)$ is $x = 0 < \sqrt{p(q-1)}$, which implies that $g_7(x)$ is increasing for $x \geqslant \sqrt{p(q-1)}$. If $1 \leqslant t \leqslant q-2$, then combining $p \leqslant rq$, we have

$$g_7(x) \geqslant g_7(\sqrt{p(q-1)}) \geqslant (q-1)(qr^2 - (p-2)r + p) \geqslant (q^2+q-2)r > 0.$$

Then $\lambda_1(R(A(B^*_\rho))) < \lambda_1(R(A(G_2)))$. By Lemma 10, we have

$$\rho(B^*_\rho) < \rho(G_2),$$

a contradiction. Hence $t = q-1$, so $B^*_\rho \cong D(p-r(q-1)-1, r(q-1)+1; q-1, 1)$.

(iii) By Lemma 21, $D(p-r-1,r+1;1,q-1) \in \mathcal{B}_{p,q,r}$. Then

$$\rho(B^*_\rho) \geqslant \rho(D(p-r-1,r+1;1,q-1)). \tag{10}$$

Now we divide our argument into the following two cases.

Case 1. $S \subseteq X$.

By $p \leqslant r(q-1)+1 \leqslant rq$ and Claim 36, we have $1 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor \leqslant q-2$. Note that $B^*_\rho \cong D(p-rt-1,rt+1;t,q-t)$. Recall that the characteristic polynomial of $R(A(B^*_\rho))$ is

$$g_5(x) = x^4 + ((rt+1)(q-t)-pq)x^2 + t(rt+1)(q-t)(p-rt-1).$$

Since $D(p-r-1,r+1;1,q-1)$ contains $K_{p-r-1,q}$ as a proper subgraph, we have

$$\rho(D(p-r-1,r+1;1,q-1)) > \rho(K_{p-r-1,q}) = \sqrt{(p-r-1)q}.$$

Recall that the characteristic polynomial of $R(A(D(p-r-1,r+1;1,q-1)))$ is

$$g_4(x) = x^4 + ((r+1)(q-1)-pq)x^2 + (r+1)(q-1)(p-r-1).$$

Let $g_8(x) = ((q-t-1)r-1)x^2 + (t^3-(t^2+t+1)(q-1))r^2 + ((t+1)(q-t)-1)(p-2)r + (q-t-1)(p-1)$. Then $g_5(x) - g_4(x) = (t-1)g_8(x)$. The symmetry axis of $g_8(x)$ is $x = 0 < \sqrt{(p-r-1)q}$, which implies that $g_8(x)$ is increasing with respect to $x \geqslant \sqrt{(p-r-1)q}$.

Next we claim that $t=1$. Suppose that $2 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor$. If $2 \leqslant t \leqslant \left\lfloor \frac{p-2}{r} \right\rfloor - 1$, then

$$\begin{aligned}
g_8(x) &\geqslant g_8(\sqrt{(p-r-1)q}) \\
&\geqslant \frac{(p-r-1)((-qr-r-1)p+q^2r^2+r^2q+2rq+2r+2)}{r} \\
&\geqslant \frac{(p-r-1)(1+(q+1)r^2+2r)}{r} \\
&> 0,
\end{aligned}$$

implying $\lambda_1(R(A(B^*_\rho)) < \lambda_1(R(A(D(p-r-1,r+1;1,q-1))))$. By Lemma 10, we have $\rho(B^*_\rho) < \rho(D(p-r-1,r+1;1,q-1))$, a contradiction. Hence $t = \left\lfloor \frac{p-2}{r} \right\rfloor \leqslant q-2$. If $t = \left\lfloor \frac{p-2}{r} \right\rfloor = q-2$, then $r(q-2)+2 \leqslant p \leqslant r(q-1)+1$, and

$$g_8(x) \geqslant g_8(\sqrt{(p-r-1)q}) \geqslant (r-1)((q^2-4q+1)r+q-1) > 0.$$

Hence $\rho(B^*_\rho) < \rho(D(p-r-1,r+1;1,q-1))$, a contradiction. If $t = \left\lfloor \frac{p-2}{r} \right\rfloor \leqslant q-3$, then by Lemma 29, we have $\rho(B^*_\rho) < \rho(D(p-r-1,r+1;1,q-1))$, a contradiction. Hence $t=1$ and $B^*_\rho \cong D(p-r-1,r+1;1,q-1)$.

Case 2. $S \subseteq Y$.

Note that $B^*_\rho \cong D(t,p-t;q-rt-1,rt+1)$ and $q \leqslant p \leqslant r(q-1)+1 \leqslant rq$. Combining (10), Claim 35 and Claim 37, we have $\rho(D(p-r-1,r+1;1,q-1)) \leqslant \rho(B^*_\rho) = \rho(D(1,p-1;q-r-1,r+1)) \leqslant \rho(D(p-r-1,r+1;1,q-1))$. Then $p=q$ and $B^*_\rho \cong D(p-r-1,r+1;1,q-1)$. $\square$

Lemma 38. *If $n-q \leqslant r(q-1)+1$ and $r \geqslant 2$, then $\rho(D(n-q-r-1, r+1; 1, q-1)) \leqslant \rho\left(D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)\right)$ with equality if and only if $q = \left\lfloor \frac{n-r-1}{2} \right\rfloor$.*

Proof. Since $n-q \leqslant r(q-1)+1$ and $q \leqslant \lfloor \frac{n}{2} \rfloor$, $\left\lfloor \frac{n+r-1}{r+1} \right\rfloor \leqslant q \leqslant \lfloor \frac{n}{2} \rfloor$. Let $G_1 = D(n-q-r-1, r+1; 1, q-1)$. For short, let $\beta = \left\lfloor \frac{n-r-1}{2} \right\rfloor$. Then $\left\lfloor \frac{n+r-1}{r+1} \right\rfloor \leqslant \beta \leqslant \lfloor \frac{n}{2} \rfloor$. If $q = \beta$, then $\rho(G_1) = \rho(D(n-\beta-r-1, r+1; 1, \beta-1))$. Next we will prove that $\rho(G_1) < \rho(D(n-\beta-r-1, r+1; 1, \beta-1))$ for $q \neq \beta$. Note that $A(G_1)$ has an equitable quotient matrix

$$R(A(G_1)) = \begin{bmatrix} 0 & 0 & 1 & q-1 \\ 0 & 0 & 1 & 0 \\ n-q-r-1 & r+1 & 0 & 0 \\ n-q-r-1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(G_1))$ is

$$h_1(x) = x^4 + (q^2 - nq + rq + q - r - 1)x^2 + (r+1)(q-1)(n-q-r-1).$$

Let $G_2 = D(n-\beta-r-1, r+1; 1, \beta-1)$. Then $A(G_2)$ has an equitable quotient matrix

$$R(A(G_2)) = \begin{bmatrix} 0 & 0 & 1 & \beta-1 \\ 0 & 0 & 1 & 0 \\ n-\beta-r-1 & r+1 & 0 & 0 \\ n-\beta-r-1 & 0 & 0 & 0 \end{bmatrix}.$$

The characteristic polynomial of $R(A(G_2))$ is

$$h_2(x) = x^4 + (\beta^2 - n\beta + r\beta + \beta - r - 1)x^2 + (r+1)(\beta-1)(n-\beta-r-1).$$

Note that G_2 contains $K_{n-\beta-r-1,\beta}$ as a proper subgraph. Combining Lemma 11, we have

$$\rho(G_2) > \rho(K_{n-\beta-r-1,\beta}) = \sqrt{(n-\beta-r-1)\beta}.$$

Let $h_3(x) = h_1(x) - h_2(x) = (\beta-q)((n-r-\beta-q-1)x^2 + r^2 + (\beta+q+1-n)r + \beta + q - n)$.

If $q \leqslant \beta - 1$, then $\beta - q \geqslant 1$ and $n-r-\beta-q-1 > 0$, which implies that $h_3(x)$ is increasing on $x \geqslant \sqrt{(n-\beta-r-1)\beta}$. Combining $n \geqslant r^2+r+2$ and $\frac{n-r-2}{2} \leqslant \beta \leqslant \frac{n-r-1}{2}$, we obtain that $h_3(x) \geqslant h_3(\sqrt{(n-\beta-r-1)\beta}) \geqslant \frac{r^4}{4} + \frac{r^2}{2} - 2r - \frac{7}{4} > 0$. By Lemma 10, we have $\rho(G_1) < \rho\left(D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)\right)$.

If $q \geqslant \beta + 1$, then $\beta - q < 0$ and $n-r-\beta-q-1 \leqslant 0$. It follows that $h_3(x)$ is increasing for $x \geqslant \sqrt{(n-\beta-r-1)\beta}$. By $n \geqslant r^2+r+2$ and $\frac{n-r-2}{2} \leqslant \beta \leqslant \frac{n-r-1}{2}$, we deduce that $h_3(x) \geqslant h_3(\sqrt{(n-\beta-r-1)\beta}) \geqslant r+1 > 0$. By Lemma 10, we have $\rho(G_1) < \rho\left(D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)\right)$. □

Recall that $\rho' = \rho\left(K_{n-\left\lfloor \frac{n-1}{r+1} \right\rfloor, \left\lfloor \frac{n-1}{r+1} \right\rfloor}\right)$ and $\rho'' = \rho\left(D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)\right)$.

Proof of Theorem 9. Let $\tilde{B_\rho^*}=(X,Y)$ be the bipartite graph with the maximum spectral radius in $\mathcal{B}_{n,r}$. Without loss of generality, we assume that $|X|\geqslant|Y|$. Let $|Y|=q$. Then $|X|=n-q$ and $q\leqslant\left\lfloor\frac{n}{2}\right\rfloor$.

(i) Note that $r=1$. We claim that $|X|=n-q\geqslant q+1$. In fact, if $n-q\leqslant q$, then $n=2q$, which implies that n is even. By Lemma 30 (iii), we have $\tilde{B_\rho^*}\cong D(\frac{n}{2}-2,2;1,\frac{n}{2}-1)$. Note that $K_{n-\left\lfloor\frac{n-1}{2}\right\rfloor,\left\lfloor\frac{n-1}{2}\right\rfloor}\in\mathcal{B}_{n,1}$. Combining Lemma 28, we obtain that

$$\begin{aligned}\rho(\tilde{B_\rho^*})&=\rho\Big(D\Big(\frac{n}{2}-2,2;1,\frac{n}{2}-1\Big)\Big)\\&\leqslant\sqrt{e\Big(D\Big(\frac{n}{2}-2,2;1,\frac{n}{2}-1\Big)\Big)}<\rho\left(K_{n-\left\lfloor\frac{n-1}{2}\right\rfloor,\left\lfloor\frac{n-1}{2}\right\rfloor}\right),\end{aligned}$$

which contradicts the maximality of $\tilde{B_\rho^*}$. Hence $n-q\geqslant q+1$, and $q\leqslant\left\lfloor\frac{n-1}{2}\right\rfloor$. By Lemma 30 (i), we have $\tilde{B_\rho^*}\cong K_{n-q,q}$. Since $q\leqslant\left\lfloor\frac{n-1}{2}\right\rfloor$, $\tilde{B_\rho^*}\cong K_{n-\left\lfloor\frac{n-1}{2}\right\rfloor,\left\lfloor\frac{n-1}{2}\right\rfloor}$.

(ii) Note that $r\geqslant 2$. We first prove that $n-q\geqslant rq+1$. Suppose to the contrary that $n-q\leqslant rq$. If $r(q-1)+2\leqslant n-q\leqslant rq$, then $\left\lceil\frac{n}{r+1}\right\rceil\leqslant q\leqslant\left\lfloor\frac{n+r-2}{r+1}\right\rfloor$. By Lemma 30 (ii), we have $\tilde{B_\rho^*}\cong D(n-(r+1)q+r-1,r(q-1)+1;q-1,1)$. Note that $K_{n-\left\lfloor\frac{n-1}{r+1}\right\rfloor,\left\lfloor\frac{n-1}{r+1}\right\rfloor}\in\mathcal{B}_{n,r}$. Combining Lemma 28 and $n\geqslant r^2+r+2$,

$$\begin{aligned}\rho(\tilde{B_\rho^*})&\leqslant\sqrt{(n-q)q-r(q-1)-1}\\&\leqslant\sqrt{\left\lfloor\frac{n+r-2}{r+1}\right\rfloor\left(n-r-\left\lfloor\frac{n+r-2}{r+1}\right\rfloor\right)+r-1}<\rho',\end{aligned}$$

which contradicts the maximality of $\tilde{B_\rho^*}$. If $n-q\leqslant r(q-1)+1$, then by Lemma 30 (iii), we have $\tilde{B_\rho^*}\cong D(n-q-r-1,r+1;1,q-1)$. By $\rho'>\rho''$ and Lemma 38, we have

$$\rho(\tilde{B_\rho^*})=\rho(D(n-q-r-1,r+1;1,q-1))\leqslant\rho''<\rho',$$

which contradicts the maximality of $\tilde{B_\rho^*}$. Hence $n-q\geqslant rq+1$, and $1\leqslant q\leqslant\left\lfloor\frac{n-1}{r+1}\right\rfloor$. By Lemma 30 (i), we have $\tilde{B_\rho^*}\cong K_{n-q,q}$. Since $q\leqslant\left\lfloor\frac{n-1}{r+1}\right\rfloor$, $\tilde{B_\rho^*}\cong K_{n-\left\lfloor\frac{n-1}{r+1}\right\rfloor,\left\lfloor\frac{n-1}{r+1}\right\rfloor}$.

(iii) Note that $r\geqslant 2$. We claim that $n-q\leqslant r(q-1)+1$. By contradiction, assume that $n-q\geqslant r(q-1)+2$. If $r(q-1)+2\leqslant n-q\leqslant rq$, then by Lemma 30 (ii), we have $\tilde{B_\rho^*}\cong D(n-(r+1)q+r-1,r(q-1)+1;q-1,1)$. Note that $D\left(\left\lceil\frac{n-r-1}{2}\right\rceil,r+1;1,\left\lfloor\frac{n-r-1}{2}\right\rfloor-1\right)\in\mathcal{B}_{n,r}$. Combining Lemma 28, $n\geqslant r^2+r+2$ and $\rho'<\rho''$, we can obtain that

$$\begin{aligned}\rho(\tilde{B_\rho^*})&\leqslant\sqrt{(n-q)q-r(q-1)-1}\\&\leqslant\sqrt{\left\lfloor\frac{n+r-2}{r+1}\right\rfloor\left(n-r-\left\lfloor\frac{n+r-2}{r+1}\right\rfloor\right)+r-1}<\rho'<\rho'',\end{aligned}$$

which contradicts the maximality of $\tilde{B}_{\rho}^{*}$. If $n-q \geqslant rq+1$, then $1 \leqslant q \leqslant \left\lfloor \frac{n-1}{r+1} \right\rfloor$. By Lemma 30 (i), we have $\tilde{B}_{\rho}^{*} \cong K_{n-q,q}$. By $\rho' < \rho''$ and $q \leqslant \left\lfloor \frac{n-1}{r+1} \right\rfloor$, we have

$$\rho(\tilde{B}_{\rho}^{*}) \leqslant \rho(K_{n-\left\lfloor \frac{n-1}{r+1} \right\rfloor, \left\lfloor \frac{n-1}{r+1} \right\rfloor}) = \rho' < \rho'',$$

which contradicts the maximality of $\tilde{B}_{\rho}^{*}$. Hence $n-q \leqslant r(q-1)+1$. By Lemma 30 (iii), we have $\tilde{B}_{\rho}^{*} \cong D(n-q-r-1, r+1; 1, q-1)$. If $q \neq \left\lfloor \frac{n-r-1}{2} \right\rfloor$, then by Lemma 38, we have $\rho(\tilde{B}_{\rho}^{*}) < \rho''$, a contradiction. Hence $q = \left\lfloor \frac{n-r-1}{2} \right\rfloor$, which implies that $\tilde{B}_{\rho}^{*} \cong D\left(\left\lceil \frac{n-r-1}{2} \right\rceil, r+1; 1, \left\lfloor \frac{n-r-1}{2} \right\rfloor - 1\right)$.

(iv) Based on the proofs of (ii) and (iii), (iv) directly follows. □

5 Concluding remarks

The bipartite binding number was introduced in [18, 13] to characterize structural properties of bipartite graphs. For a bipartite graph $G = (X, Y)$, its *bipartite binding number* $b^B(G)$ is defined as follows. If $G = K_{|X|,|Y|}$, then $b^B(G) = \min\{|X|, |Y|\}$. Otherwise,

$$b^B(G) = \min\left\{ \min_{\substack{\emptyset \neq S \subseteq X \\ N_G(S) \subsetneq Y}} \frac{|N_G(S)|}{|S|}, \min_{\substack{\emptyset \neq T \subseteq Y \\ N_G(T) \subsetneq X}} \frac{|N_G(T)|}{|T|} \right\}.$$

Hao et al.[12] characterized the extremal graphs with the maximum size (spectral radius) among all connected balanced bipartite graphs with $b^B(G) < r$, where $r \geqslant 1$ is an integer.

Theorem 39 (Hao et al.[12])**.** *Let r be a positive integer, and let G be a connected balanced bipartite graph of order $2n$ such that $b^B(G) < r$. Each of the following holds.*
(i) If $r = 1$ and $n \geqslant 3$, then $e(G) \leqslant n^2 - 2n + 2$ with equality if and only if $G \cong D(n-2, 2; 1, n-1)$.
(ii) If $r \geqslant 2$, $n \geqslant r+1$ and $n \equiv 0 \pmod r$, then $e(G) \leqslant n^2 - \frac{n}{r}$ with equality if and only if $G \cong D(n - \frac{n}{r}, \frac{n}{r}; n-1, 1)$.
(iii) If $r \geqslant 2$, $n \geqslant r+1$ and $n \not\equiv 0 \pmod r$, then $e(G) \leqslant n^2 - \left\lceil \frac{n+1}{r} \right\rceil$ with equality if and only if $G \cong D(n - \left\lceil \frac{n+1}{r} \right\rceil, \left\lceil \frac{n+1}{r} \right\rceil; n-1, 1)$.

Theorem 40 (Hao et al.[12])**.** *Let r be a positive integer, and let G be a connected balanced bipartite graph of order $2n$ such that $b^B(G) < r$. Each of the following holds.*
(i) If $r = 1$ and $n \geqslant 3$, then $\rho(G) \leqslant \rho(D(n-2, 2; 1, n-1))$ with equality if and only if $G \cong D(n-2, 2; 1, n-1)$.
(ii) If $r \geqslant 2$, $n \geqslant r+1$ and $n \equiv 0 \pmod r$, then $\rho(G) \leqslant \rho(D(n - \frac{n}{r}, \frac{n}{r}; n-1, 1))$ with equality if and only if $G \cong D(n - \frac{n}{r}, \frac{n}{r}; n-1, 1)$.
(iii) If $r \geqslant 2$, $n \geqslant r+1$ and $n \not\equiv 0 \pmod r$, then $\rho(G) \leqslant \rho(D(n - \left\lceil \frac{n+1}{r} \right\rceil, \left\lceil \frac{n+1}{r} \right\rceil; n-1, 1))$ with equality if and only if $G \cong D(n - \left\lceil \frac{n+1}{r} \right\rceil, \left\lceil \frac{n+1}{r} \right\rceil; n-1, 1)$.

With the above characterization on connected balanced bipartite graphs, one may ask the following problem: What is the maximum size (spectral radius) among bipartite graphs satisfying $b^B(G) < r$, where $r \geqslant 1$ is an integer? The methods and techniques developed in our work offer a viable and insightful approach to tackling this problem.

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