

# Minimizing the least eigenvalue of bicyclic graphs with $k$ pendant vertices

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## Abstract

Let  $\mathcal{B}(n, k)$  be the set of bicyclic graphs with  $n$  vertices and  $k$  pendant vertices. In this paper, we determine the unique graph with minimal least eigenvalue among all graphs in  $\mathcal{B}(n, k)$ . This extremal graph is the same as that on the Laplacian spectral radius as done by Ji-Ming Guo [The Laplacian spectral radius of bicyclic graphs with  $n$  vertices and  $k$  pendant vertices, *Science China Mathematics*, 53(8)(2010)2135-2142]. Moreover, the minimal least eigenvalue is a decreasing function on  $k$ .

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## 1 Introduction

All graphs considered in this paper are finite, undirected and simple. Denote by  $V(G)$  the vertex set and  $E(G)$  the edge set of a graph  $G$ . The degree of a vertex  $v$ , written by  $d_G(v)$  or  $d(v)$ , is the number of edges incident with  $v$ . A pendant vertex is a vertex of degree 1. The *girth*  $g(G)$  of a graph  $G$  is the length of the shortest cycle in  $G$ , with the girth of an

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acyclic graph being infinite. Denote by  $C_n$  and  $P_n$  the cycle and the path on  $n$  vertices respectively.

Let  $A$  be the adjacency matrix of a graph  $G$ . Since  $A$  is symmetric and real, the eigenvalue of  $A$ , i.e., the zeros of the characteristic polynomial  $\phi(G; \lambda) = \det(\lambda I - A)$ , can be arranged as follows:  $\lambda_1(G) \geq \lambda_2(G) \geq \dots \geq \lambda_n(G)$ . For connected graph  $G$ , the spectral radius  $\rho(G) = \lambda_1(G)$  is simple and has a unique positive eigenvector up to multiples. We will refer to such an eigenvector as the Perron vector of  $G$ . Denote  $\lambda_n(G)$  by  $\lambda(G)$ . Let  $X$  be a unit vector, by the Rayleigh-Ritz Theorem,  $\lambda(G) = \min X^T A(G) X$ . It is known [2] that  $\lambda(G) = -\rho(G)$  for a bipartite graph  $G$ .

In [1], R.A. Brualdi and E.S. Solheid posed the problem of maximizing the spectral radius and determining the extremal graph for a given class of graphs, which became one of the classic problems of spectral graph theory. Recently, the investigation on minimizing the least eigenvalue of a given class of graphs is of great interest (for example, [3, 6, 7]). Let  $\mathcal{B}(n, k)$  be the set of bicyclic graphs with  $n$  vertices and  $k$  pendant vertices.  $k$  paths  $P_{l_1}, P_{l_2}, \dots, P_{l_k}$  are said to have almost equal lengths if  $l_1, l_2, \dots, l_k$  satisfy  $|l_i - l_j| \leq 1$  for  $1 \leq i, j \leq k$ . Let  $B_1(k)$  denote the bicyclic graph in  $\mathcal{B}(n, k)$  obtained from the graph  $G_1$  (see Fig.1) by attaching  $k$  paths with almost equal lengths to vertex  $v$ . The main result of this paper is as follows:

**Theorem 1.1** *Let  $B^*$  have minimal least eigenvalue in  $\mathcal{B}(n, k)$ , where  $1 \leq k \leq n - 7$ . Then  $B^* \cong B_1(k)$ . Moreover,  $\lambda(B_1(k))$  is a decreasing function on  $k$ .*

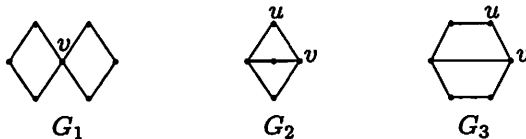


Fig.1. Bicyclic graphs  $G_1, G_2$  and  $G_3$ .

## 2 Preliminaries

Let  $B$  be a bicyclic graph. The base of  $B$ , denoted by  $B_0$ , is the unique bicyclic subgraph of  $B$  containing no pendant vertices, and  $B$  can be obtained from  $B_0$  by planting trees at some vertices of  $B_0$ .

Bicyclic graphs only have two types of bases. Denote by  $B(p, l, q)$  the graph obtained by joining a new path  $P_l : v_0 v_1 \dots v_{l-1}$  between two vertex-disjoint cycles  $C_p$  and  $C_q$ , where  $v_0 \in V(C_p), v_{l-1} \in V(C_q), q \geq p \geq 3$  and  $l \geq 1$ . In particular,  $l = 1$  means identifying  $v_0$  with  $v_{l-1}$ . Denote by  $P(p, q, l)$  the graph consisting of three pairwise internal disjoint paths  $P_{p+1}, P_{q+1}, P_{l+1}$  with common endpoints, where  $l \geq q \geq p \geq 1$  and at most one of them is 1. We introduce two subclasses of  $\mathcal{B}(n, k)$ :  $\mathcal{B}_1(n, k) = \{B \in$

$\mathcal{B}(n, k)|_{B_0} = B(p, l, q)$  and  $\mathcal{B}_2(n, k) = \{B \in \mathcal{B}(n, k) | B_0 = P(p, q, l)\}$ . Then  $\mathcal{B}(n, k) = \mathcal{B}_1(n, k) \cup \mathcal{B}_2(n, k)$ .

Let  $G, H$  be two disjoint connected graphs with  $u \in V(G)$  and  $w \in V(H)$ , we denote by  $GuwH$  the graph obtained from  $G$  and  $H$  by identifying  $u$  with  $w$ .

**Lemma 2.1** ([3]) *Let  $G, H$  be two disjoint nontrivial connected graphs with  $u, v \in V(G)$  and  $w \in V(H)$ . Let  $X$  be a unit eigenvector corresponding to  $\lambda(GuwH)$ . If  $|x_u| \leq |x_v|$ , then  $\lambda(GuwH) \geq \lambda(GvwH)$ , and the equality holds if and only if  $X$  is also an eigenvector corresponding to  $\lambda(GvwH)$ ,  $x_u = x_v$  and  $\sum_{i \in N_H(w)} x_i = 0$ .*

Let  $G$  be a connected graph with  $uv \in E(G)$ . We denote by  $G_{uv}$  the graph obtained from  $G$  by subdividing the edge  $uv$ , that is, introducing a new vertex on the edge  $uv$ . A walk  $v_1v_2 \cdots v_k$  ( $k \geq 2$ ) in a graph  $G$  is called an *internal path*, if these  $k$  vertices are distinct (except possibly  $v_1 = v_k$ ),  $d_G(v_1) > 2$ ,  $d_G(v_k) > 2$  and  $d_G(v_2) = \cdots = d_G(v_{k-1}) = 2$  (unless  $k = 2$ ).

Let  $W_n$  ( $n \geq 6$ ) be the graph obtained from a path  $v_1v_2 \cdots v_{n-4}$  by attaching two pendant vertices to  $v_1$  and another two to  $v_{n-4}$ . Hoffman and Smith showed the following result.

**Lemma 2.2** ([4]) *Let  $G$  be a connected graph with  $uv \in E(G)$ . If  $uv$  belongs to an internal path of  $G$  and  $G \not\cong W_n$ , then  $\rho(G_{uv}) < \rho(G)$ .*

**Lemma 2.3** ([9]) *Let  $u, v$  be two distinct vertices of a connected graph  $G$ ,  $\{v_i | i = 1, 2, \dots, s\} \subseteq N_G(v) \setminus (N_G(u) \cup \{u\})$ , and  $X = (x_1, x_2, \dots, x_n)^T$  be the Perron vector of  $G$ . Let  $G^* = G - \sum_{i=1}^s v_i v + \sum_{i=1}^s v_i u$ . If  $x_u \geq x_v$ , then  $\rho(G) < \rho(G^*)$ .*

**Lemma 2.4** ([6]) *Let  $f_1(x) = x, f_i(x) = x - \frac{1}{f_{i-1}(x)}, i \geq 2$ . For  $x \leq -2$ , then  $f_i(x) < f_{i+1}(x) < -1$ .*

**Lemma 2.5** ([6]) *Let  $v_0$  be a vertex of a connected graph  $G$  with at least two vertices. Let  $G_l$  ( $l \geq 1$ ) be the graph obtained from  $G$  by attaching a new path  $P : v_0v_1 \cdots v_l$  of length  $l$  at  $v_0$ , where  $v_1, \dots, v_l$  are distinct new vertices. Let  $X$  be a unit eigenvector of  $\lambda(G_l)$ . If  $\lambda(G_l) \leq -2$ , then we have (i)  $x_{v_i} = f_{l-i}(\lambda)x_{v_{i+1}}$  ( $0 \leq i \leq l-1$ ), where  $f_i(x)$  is a function on  $x$  defined in Lemma 2.4 and  $\lambda = \lambda(G_l)$ .*

*(ii) For any fixed  $i$  ( $i = 0, 1, \dots, l-1$ ), we have  $|x_{v_{i+1}}| \leq |x_{v_i}|$  and  $x_{v_i}x_{v_{i+1}} \leq 0$ , with equalities if and only if  $x_{v_0} = 0$ .*

**Lemma 2.6** *Let  $g_1(x) = \frac{x}{2}, g_i(x) = x - \frac{1}{g_{i-1}(x)}$  ( $i \geq 2$ ). Let  $h_1(x) = x - 1, h_i(x) = x - \frac{1}{h_{i-1}(x)}$  ( $i \geq 2$ ). If  $x < -2$ , then for any  $i, g_{i+1}(x) < g_i(x) < -1$  and  $h_i(x) < h_{i+1}(x) < -1$ .*

**Proof.** We use induction on  $i$  to show the result. Initially,  $g_1(x) = \frac{x}{2}$  and  $g_2(x) = x - \frac{2}{x}$ . Clearly,  $g_2(x) < g_1(x) < -1$ , since  $x < -2$ . Now suppose that the result holds for  $i > 1$ . Then by the induction hypothesis,  $g_{i+1}(x) = x - \frac{1}{g_i(x)} < x + 1 < -1$  and  $g_{i+2}(x) - g_{i+1}(x) = \frac{1}{g_i(x)} - \frac{1}{g_{i+1}(x)} < 0$ . For  $h_i(x)$ , we can get the result likewise.  $\square$

**Lemma 2.7** ([6]) *Let  $A$  be an  $n \times n$  real symmetric matrix and  $\lambda$  be the least eigenvalue of  $A$ . If  $X \in \mathbb{R}^n$  is a unit vector such that  $\lambda = X^T A X$ , then  $A X = \lambda X$ .*

**Lemma 2.8** *Let  $G$  be a connected graph,  $C_l = v_0 v_1 \cdots v_{l-1} v_0$  be a cycle and  $G v_0 C_l$  be the graph obtained by identifying  $v_0$  with some vertex of  $G$  (see Fig.2). Then there exists an eigenvector  $X$  of  $\lambda(G v_0 C_l)$  such that  $x_{v_i} = x_{v_{l-i}}$ , where  $1 \leq i \leq l-1$ .*

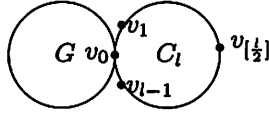


Fig.2.  $G v_0 C_l$ .

**Proof.** Let  $X$  be a unit eigenvector of  $\lambda(G v_0 C_l)$ . Note that there is an automorphism  $\varphi$  of  $G v_0 C_l$  which maps  $v_i$  to  $v_{l-i}$  for  $1 \leq i \leq l-1$  and preserves other vertices. Define a new vector  $\bar{X}$  such that  $\bar{X}_v = x_{\varphi(v)}$  for each vertex  $v \in V(G v_0 C_l)$ .

If  $\bar{X} + X \neq 0$ , then  $\bar{X} + X$  is clearly a desirable eigenvector of  $\lambda(G v_0 C_l)$ . Otherwise  $\bar{X} + X = 0$ , then  $x_v = 0$  for each vertex  $v \in V(G)$ . Note that  $X$  is an eigenvector of  $\lambda(G v_0 C_l)$ , without loss of generality, assume that  $x_{v_k} \neq 0$  for some  $v_k \in V(C_l) \setminus \{v_0\}$ . Let  $\psi$  be a circular permutation of  $C_l$  such that  $\psi(v_i) = v_{i+k(\text{mod } l)}$  ( $0 \leq i \leq l-1$ ) and define a new vector  $Y$  such that  $y_{v_i} = x_{\psi(v_i)}$  for each  $v_i \in V(C_l)$  and  $y_v = x_v$  for each  $v \notin V(C_l)$ . We can observe that  $\lambda(G v_0 C_l) = X^T A X = 2 \sum_{uv \in E(G v_0 C_l)} x_u x_v = Y^T A Y$ , and hence by Lemma 2.7,  $Y$  is also a unit eigenvector of  $\lambda(G v_0 C_l)$  with  $y_{v_0} = x_{v_k} \neq 0$ . Similar to  $\bar{X}$ , define a vector  $\bar{Y}$ , then  $\bar{Y} + Y \neq 0$  is a desirable eigenvector of  $\lambda(G v_0 C_l)$ .  $\square$

**Lemma 2.9** *Let  $X$  be a unit eigenvector of  $G v_0 C_l$  corresponding to  $\lambda(G v_0 C_l)$  such that  $x_{v_i} = x_{v_{l-i}}$ , where  $1 \leq i \leq l-1$ .  $g_i(x)$  and  $h_i(x)$  are two functions on  $x$  defined in Lemma 2.6 and  $\lambda = \lambda(G v_0 C_l)$ . If  $\lambda < -2$ , then*

(i) *For even  $l$ ,  $x_{v_i} = g_{\frac{l}{2}-i}(\lambda)x_{v_{i+1}}$ , and thus  $|x_{v_{i+1}}| \leq |x_{v_i}|$  and  $x_{v_i} x_{v_{i+1}} \leq 0$ , with equalities if and only if  $x_{v_0} = 0$ , where  $0 \leq i \leq \frac{l-2}{2}$ ;*

(ii) *For odd  $l$ ,  $x_{v_i} = h_{\frac{l-1}{2}-i}(\lambda)x_{v_{i+1}}$ , and hence  $|x_{v_{i+1}}| \leq |x_{v_i}|$  and  $x_{v_i} x_{v_{i+1}} \leq 0$ , with equalities if and only if  $x_{v_0} = 0$ , where  $0 \leq i \leq \frac{l-3}{2}$ .*

**Proof.** For even  $l$ . From  $A(Gv_0C_l)X = \lambda X$ , we have  $\lambda x_{v_{\frac{l}{2}}} = x_{v_{\frac{l-2}{2}}} + x_{v_{\frac{l+2}{2}}} = 2x_{v_{\frac{l-2}{2}}}$  and  $\lambda x_{v_i} = x_{v_{i-1}} + x_{v_{i+1}}$ , where  $i = 1, 2, \dots, \frac{l-2}{2}$ . By these two equations, it is easy to show that the first half of (i) holds.

Since  $\lambda < -2$ , then by Lemma 2.6,  $g_i(\lambda) < -1$ . Hence, from the first half of (i), we have if  $x_{v_{i+1}} \neq 0$ , then  $|x_{v_{i+1}}| < |x_{v_i}|$ ,  $x_{v_i}x_{v_{i+1}} < 0$ , where  $i = 0, 1, \dots, \frac{l-2}{2}$ . Also from the first half of (i), we have

$$\begin{aligned} x_{v_0} &= g_{\frac{l}{2}}(\lambda)x_{v_1} = g_{\frac{l}{2}}(\lambda)g_{\frac{l-2}{2}}(\lambda)x_{v_2} \\ &= \dots = g_{\frac{l}{2}}(\lambda)g_{\frac{l-2}{2}}(\lambda) \cdots g_2(\lambda)g_1(\lambda)x_{v_{\frac{l}{2}}}. \end{aligned}$$

Thus  $x_{v_0} = 0$  if and only if  $x_{v_1} = x_{v_2} = \dots = x_{v_{\frac{l}{2}}} = 0$ . Then (i) holds.

Similarly, we can prove that (ii) holds.  $\square$

**Lemma 2.10 ([5])** *Let  $v$  be a vertex in a connected graph  $G$  and suppose that two new paths  $P : vv_1v_2 \cdots v_k$  and  $Q : vv_1u_2 \cdots u_m$  of length  $k, m$  ( $k \geq m \geq 1$ ) are attached to  $G$  at  $v$ , respectively, to form a new graph  $G_{k,m}$ , where  $v_1, v_2, \dots, v_k$  and  $u_1, u_2, \dots, u_m$  are distinct new vertices. Then for any  $\lambda \geq \rho(G_{k,m})$ , we have  $\phi(G_{k+1,m-1}; \lambda) > \phi(G_{k,m}; \lambda)$ . In particular,  $\rho(G_{k,m}) > \rho(G_{k+1,m-1})$ .*

**Lemma 2.11 ([8])** *Let  $v$  be a vertex of  $G$  and  $\mathcal{C}(v)$  be the set of all cycles containing  $v$ . Then*

$$\phi(G; \lambda) = \lambda\phi(G-v; \lambda) - \sum_{u \in N(v)} \phi(G-v-u; \lambda) - 2 \sum_{Z \in \mathcal{C}(v)} \phi(G-V(Z); \lambda).$$

**Lemma 2.12 ([5])** *Let  $G$  and  $H$  be two connected graphs such that  $\phi(G; \lambda) > \phi(H; \lambda)$  for  $\lambda \geq \rho(H)$  or  $\lambda = \rho(G)$ , then  $\rho(G) < \rho(H)$ .*

Let  $B_2(k)$  denote the bicyclic graph in  $\mathcal{B}(n, k)$  obtained from the graph  $G_2$  (see Fig.1) by attaching  $k$  paths with almost equal lengths to vertex  $v$ . Note that both  $B_1(k)$  and  $B_2(k)$  exist if and only if  $k \geq 1, n \geq k+7$ .

**Lemma 2.13** *If both  $B_1(k)$  and  $B_2(k)$  exist, then  $\rho(B_1(k)) > \rho(B_2(k))$ .*

**Proof.** Denote by  $l$  the maximal number of vertices of a path attached to the vertex  $v$  of  $B_2(k)$ . Note that  $k \leq n-7$ , then  $l \geq 2$ . Suppose that the number of such paths is  $t$ .

**Case1.**  $t \geq 2$ .

Let  $B_1$  be the graph analogous to  $B_1(k)$  in which all paths attached to vertex  $v$  have  $l-1$  vertices. Let  $B_2$  be the graph analogous to  $B_2(k)$  in which all paths attached to vertex  $v$  have  $l$  vertices. Evidently,  $B_1$  is

an induced subgraph of  $B_1(k)$  and  $B_2(k)$  is an induced subgraph of  $B_2$ . Therefore,  $\rho(B_1) \leq \rho(B_1(k))$  with equality if and only if  $n = (l-1)k + 7$ . Also,  $\rho(B_2(k)) \leq \rho(B_2)$  with equality if and only if  $n = lk + 5$ . Thus for the proof of Lemma 2.13 it is sufficient to show that  $\rho(B_2) < \rho(B_1)$ . Let  $r = \rho(B_2)$ , by Lemma 2.12, it suffices to show that  $\phi(B_1; r) < 0$ .

By applying Lemma 2.11 to the vertex  $v$  of  $B_1$  and  $B_2$ , respectively,

$$\phi(B_1; \lambda) = \lambda^2(\lambda^2 - 2)\phi(P_{l-1}; \lambda)^{k-1}[(\lambda^3 - 6\lambda)\phi(P_{l-1}; \lambda) - k(\lambda^2 - 2)\phi(P_{l-2}; \lambda)];$$

$$\phi(B_2; \lambda) = \lambda^2\phi(P_l; \lambda)^{k-1}[(\lambda^3 - 6\lambda)\phi(P_l; \lambda) - k(\lambda^2 - 3)\phi(P_{l-1}; \lambda)].$$

Note that  $(r^3 - 6r)\phi(P_l; r) - k(r^2 - 3)\phi(P_{l-1}; r) = 0$ , where  $l \geq 2$ . Then for  $l \geq 3$  we have  $(r^3 - 6r)\phi(P_{l-1}; r) - k(r^2 - 3)\phi(P_{l-2}; r) = 0$ . Hence  $\phi(B_1; r) = -kr^2(r^2 - 2)\phi(P_{l-1}; r)^{k-1}\phi(P_{l-2}; r) < 0$  since  $r > 2$ . When  $l = 2$ ,  $\phi(B_1; r) = r^2(r^2 - 2)\phi(P_1; r)^{k-1}[(r^3 - 6r)\phi(P_1; r) - k(r^2 - 2)\phi(P_0; r)] < 0$  since  $k = \frac{(r^3 - 6r)(r^2 - 1)}{(r^2 - 3)r}$ .

**Case2.**  $t = 1$ .

In this case, it is straightforward to check that the maximal number of vertices of a path attached to the vertex  $v$  of  $B_2(k)$  is  $l$ , while the minimal number of vertices of a path attached to the vertex  $v$  of  $B_1(k)$  is  $l - 2$ , where  $l \geq 3$ . Let  $B'_1$  be the graph analogous to  $B_1(k)$  in which all paths attached to vertex  $v$  have  $l - 2$  vertices and  $B_2$  be the graph analogous to  $B_2(k)$  in which all paths attached to vertex  $v$  have  $l$  vertices. Evidently,  $B'_1$  is an induced subgraph of  $B_1(k)$  and  $B_2(k)$  is an induced subgraph of  $B_2$ . Therefore,  $\rho(B'_1) \leq \rho(B_1(k))$  with equality if and only if  $n = (l-2)k + 7$ . Also,  $\rho(B_2(k)) \leq \rho(B_2)$  with equality if and only if  $n = lk + 5$ . Thus for the proof of Lemma 2.13 it is sufficient to show that  $\rho(B_2) < \rho(B'_1)$ . Let  $r = \rho(B_2)$ , by Lemma 2.12, it suffices to show that  $\phi(B'_1; r) < 0$ . Similar to Case1, we can easily prove the result.  $\square$

Let  $B_3(k)$  denote the bicyclic graph in  $\mathcal{B}(n, k)$  obtained from the graph  $G_3$  (see Fig.1) by attaching  $k$  paths with almost equal lengths to vertex  $v$ . Note that both  $B_1(k)$  and  $B_3(k)$  exist if and only if  $k \geq 1, n \geq k + 7$ .

**Lemma 2.14** *If both  $B_1(k)$  and  $B_3(k)$  exist, then  $\rho(B_1(k)) > \rho(B_3(k))$ .*

**Proof.** Denote by  $l$  the maximal number of vertices of a path attached to the vertex  $v$  of  $B_3(k)$ . Note that  $k \leq n - 7$ , then  $l \geq 2$ .

Let  $B_1$  be the graph analogous to  $B_1(k)$  in which all paths attached to vertex  $v$  have  $l - 1$  vertices. Let  $B_3$  be the graph analogous to  $B_3(k)$  in which all paths attached to vertex  $v$  have  $l$  vertices. Evidently,  $B_1$  is an induced subgraph of  $B_1(k)$  and  $B_3(k)$  is an induced subgraph of  $B_3$ . Therefore,  $\rho(B_1) \leq \rho(B_1(k))$  with equality if and only if  $n = (l-1)k + 7$ . Also,  $\rho(B_3(k)) \leq \rho(B_3)$  with equality if and only if  $n = lk + 6$ . Thus for the proof of Lemma 2.14 it is sufficient to show that  $\rho(B_3) < \rho(B_1)$ . By

Lemma 2.12, it suffices to show that  $\phi(B_1; \rho(B_3)) < 0$ . Similar to Case1 of Lemma 2.13, we can easily get the result.  $\square$

Let  $\bar{B}_2(k)$  denote the bicyclic graph in  $\mathcal{B}(n, k)$  obtained from the graph  $G_2$ (see Fig.1) by attaching  $k$  paths with almost equal lengths to vertex  $u$ . Let  $\bar{B}_3(k)$  denote the bicyclic graph in  $\mathcal{B}(n, k)$  obtained from the graph  $G_3$ (see Fig.1) by attaching  $k$  paths with almost equal lengths to vertex  $u$ .

**Lemma 2.15**  $\rho(B_2(k)) > \rho(\bar{B}_2(k))$  and  $\rho(B_3(k)) > \rho(\bar{B}_3(k))$ .

**Proof.** Assume that  $k(k \geq 1)$  paths in  $B_2(k)$  and  $\bar{B}_2(k)$  are  $P_{i_1}, \dots, P_{i_k}$ . Apply Lemma 2.11 to the vertex  $v$  of  $B_2(k)$  and the vertex  $u$  of  $\bar{B}_2(k)$ ,

$$\begin{aligned} \phi(B_2(k); \lambda) &= (\lambda^5 - 6\lambda^3)\phi(P_{i_1}; \lambda) \cdots \phi(P_{i_k}; \lambda) - (\lambda^4 - 3\lambda^2) \\ &\quad \sum_{i=1}^k \phi(P_{i_1}; \lambda) \cdots \phi(P_{i_{i-1}}; \lambda) \cdots \phi(P_{i_k}; \lambda), \end{aligned}$$

$$\begin{aligned} \phi(\bar{B}_2(k); \lambda) &= (\lambda^5 - 6\lambda^3)\phi(P_{i_1}; \lambda) \cdots \phi(P_{i_k}; \lambda) - (\lambda^4 - 4\lambda^2) \\ &\quad \sum_{i=1}^k \phi(P_{i_1}; \lambda) \cdots \phi(P_{i_{i-1}}; \lambda) \cdots \phi(P_{i_k}; \lambda). \end{aligned}$$

For  $\lambda \geq \rho(B_2(k)) \geq 2.5576$ , we have

$$\phi(\bar{B}_2(k); \lambda) - \phi(B_2(k); \lambda) = \lambda^2 \sum_{i=1}^k \phi(P_{i_1}; \lambda) \cdots \phi(P_{i_{i-1}}; \lambda) \cdots \phi(P_{i_k}; \lambda) > 0.$$

By Lemma 2.12,  $\rho(B_2(k)) > \rho(\bar{B}_2(k))$ . Similarly, we can get  $\rho(B_3(k)) > \rho(\bar{B}_3(k))$ .

### 3 Characterization of the extremal graph

Let  $B^*$  have minimal least eigenvalue in  $\mathcal{B}(n, k)$ , and  $B_1(k) \in \mathcal{B}(n, k)$ . Note that  $B_1(k)$  is a bipartite graph, hence  $\lambda(B^*) \leq \lambda(B_1(k)) = -\rho(B_1(k)) < -\rho(G_1) \approx -2.4495$ . Note that  $B_1(k)$  exists if and only if  $k \geq 1, n \geq k + 7$ . For any  $B \in \mathcal{B}(n, k)$ , we know that  $B \in \mathcal{B}_1(n, k)$  or  $B \in \mathcal{B}_2(n, k)$ .

**Lemma 3.1** For any graph  $B \in \mathcal{B}_1(n, k)$ , there exists a graph  $\bar{B} \in \mathcal{B}_{11}(n, k)$ (see Fig.3) such that  $\lambda(B) \geq \lambda(\bar{B})$ .

**Proof.** For any graph  $B \in \mathcal{B}_1(n, k)$ ,  $B$  can be obtained from  $B(p, l, q)$  by planting trees at a subset  $V_0$  of  $V(B(p, l, q))$ , where  $P_l : v_0 v_1 \cdots v_{l-1}$  is the

unique path between  $C_p$  and  $C_q$ , any  $u \in V_0$  is called the root of tree  $T_u$ , or the root-vertex of  $B$ . Let  $X$  be a unit eigenvector of  $B$  corresponding to  $\lambda(B)$ . Without loss of generality, let  $|x_v| = \max\{|x_u| | u \in V_0\}$ . Let  $B_1$  be the graph obtained from  $B(p, l, q)$  by planting all the trees  $T_u$  at vertex  $u$  to form a new big tree  $T$  with root  $v$ . From a repeated use of Lemma 2.1, we have  $\lambda(B) \geq \lambda(B_1)$ . Consider the graph  $B_1$ . If  $v \notin V(P_l)$ , without loss of generality, we can assume that  $v \in V(C_p) \setminus \{v_0\}$ . Let  $X'$  be a unit eigenvector of  $B_1$  corresponding to  $\lambda(B_1)$ . Denote  $N(v) \cap V(T) = \{z_1, \dots, z_{d_v-2}\}$  and  $N(v_0) \cap V(P_l \cup C_q) = \{w_1, \dots, w_{d_{v_0}-2}\}$ . Define

$$B_2 = \begin{cases} B_1 - \{vz_1, \dots, vz_{d_v-2}\} + \{v_0z_1, \dots, v_0z_{d_v-2}\} & \text{if } |x'_{v_0}| \geq |x'_v| \\ B_1 - \{v_0w_1, \dots, v_0w_{d_{v_0}-2}\} + \{vw_1, \dots, vw_{d_{v_0}-2}\} & \text{if } |x'_{v_0}| < |x'_v| \end{cases}$$

Then in either case, the unique root-vertex  $v = v_0 \in V(P_l)$  in  $B_2$ , and by Lemma 2.1,  $\lambda(B_1) \geq \lambda(B_2)$ . If  $v \in V(P_l)$ , then  $B_2 = B_1$ , and  $\lambda(B_1) = \lambda(B_2)$ . Hence for any graph  $B_1$ , we can always find a graph  $B_2$  with  $\lambda(B_1) \geq \lambda(B_2)$ , and the unique root-vertex  $v = v_i \in V(P_l)$  in  $B_2$ , where  $0 \leq i \leq l-1$ .

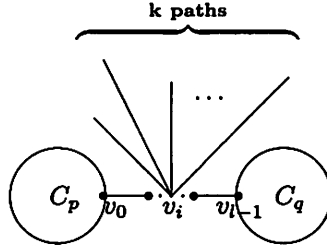


Fig.3.  $\mathcal{B}_{11}(n, k)$ .

Consider the graph  $B_2$ , let  $t$  be the cardinality of the vertices whose degrees are no less than 3 in  $V(T) \setminus \{v_i\}$  and  $X''$  be a unit eigenvector corresponding to  $\lambda(B_2)$ , and now we distinguish the following three cases:

**Case1.**  $t = 0$ . In this case,  $\bar{B} = B_2 \in \mathcal{B}_{11}(n, k)$ , and  $\lambda(B_2) = \lambda(\bar{B})$ .

**Case2.**  $t = 1$ . We can assume that there exists one vertex  $v \in V(T) \setminus \{v_i\}$  with  $d(v) \geq 3$  in  $B_2$ , then there is a unique path with the length at least 1 joining  $v_i$  and  $v$ . Denote  $N(v_i) = \{w_1, w_2, w_3, \dots, w_p\}$  and  $N(v) = \{z_1, z_2, z_3, \dots, z_q\}$ . Assume that  $w_1, z_1$  belong to the path joining  $v_i$  and  $v$ ,  $w_2$  lies on the path from  $v_0$  to  $v_i$ . Define

$$\bar{B} = \begin{cases} B_2 - \{vz_3, \dots, vz_q\} + \{v_i z_3, \dots, v_i z_q\} & \text{if } |x''_{v_i}| \geq |x''_v| \\ B_2 - \{v_i w_3, \dots, v_i w_p\} + \{v w_3, \dots, v w_p\} & \text{if } |x''_{v_i}| < |x''_v|. \end{cases}$$

Then in either case,  $\bar{B} \in \mathcal{B}_{11}(n, k)$  and by Lemma 2.1,  $\lambda(B_2) \geq \lambda(\bar{B})$ .

**Case3.**  $t > 1$ . Suppose that  $u, v \in V(T) \setminus \{v_i\}$  are two vertices of  $B_2$  whose degrees are 3 or greater, and  $|x''_u| \geq |x''_v|$ . Since  $T$  is a tree, there



is a path between  $u$  and  $v$  and only one neighbor of  $v$ , say  $w$ , is on the path. Assume  $\{v_1, v_2, \dots, v_{d_v-2}\} \subset N(v) \setminus \{w\}$ . Delete the edges  $(v, v_j)$  and add the edges  $(u, v_j)$  ( $1 \leq j \leq d_v - 2$ ), then we get a new bicyclic graph  $B'_1$ . Obviously  $B'_1$  still has  $k$  pendant vertices. By Lemma 2.1, we have  $\lambda(B_2) \geq \lambda(B'_1)$  and the cardinality of the vertices of degree 3 or greater decreases to  $t - 1$ . If  $t - 1 > 1$ , to  $B'_1$  repeat the above step until the cardinality is only one. So we get bicyclic graphs  $B'_2, B'_3, \dots, B'_{t-1}$ , and  $\lambda(B'_1) \geq \lambda(B'_2) \geq \dots \geq \lambda(B'_{t-1})$ . Moreover, each  $B'_i$  has  $k$  pendant vertices. Refer to Case2, there exists  $\bar{B} \in \mathcal{B}_{11}(n, k)$  such that  $\lambda(B'_{t-1}) \geq \lambda(\bar{B})$ . By the above cases, we complete the proof.  $\square$

For any graph  $B \in \mathcal{B}_2(n, k)$ ,  $B$  can be obtained from  $P(p, l, q)$  by planting trees at a subset  $V_0$  of  $V(P(p, l, q))$ , where any  $u \in V_0$  is called the root of tree  $T_u$ , or the root-vertex of  $B$ . Similar to the proof of Lemma 3.1, we have the following result.

**Lemma 3.2** For any graph  $B \in \mathcal{B}_2(n, k)$ , there exists a graph  $\bar{B} \in \mathcal{B}_{21}(n, k) \cup \mathcal{B}_{22}(n, k)$  (see Fig.4) such that  $\lambda(B) \geq \lambda(\bar{B})$ .

**Lemma 3.3** Let  $B^*$  have minimal least eigenvalue in  $\mathcal{B}(n, k)$ , where  $1 \leq k \leq n - 7$ . Then  $B^*$  contains no  $C_3$ .

**Proof.** Note that  $\mathcal{B}(n, k) = \mathcal{B}_1(n, k) \cup \mathcal{B}_2(n, k)$ . Suppose that  $B^*$  contains  $C_3$ , then for the proof of Lemma 3.3 it suffices to find a graph  $B \in \mathcal{B}_1(n, k) \cup \mathcal{B}_2(n, k)$  such that  $\lambda(B^*) > \lambda(B)$ .

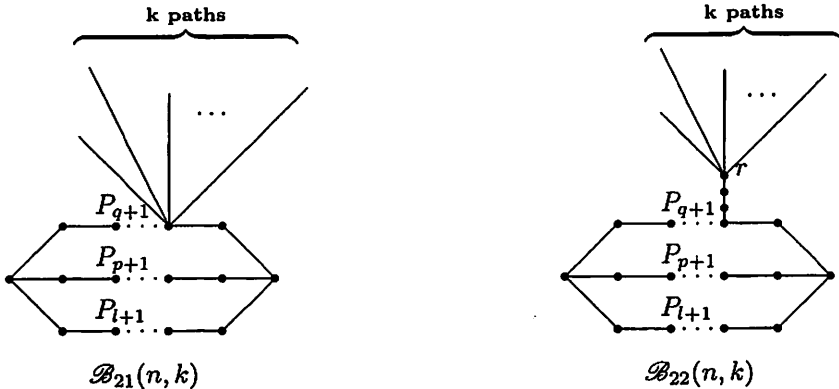


Fig.4. Two classes of graphs in  $\mathcal{B}_2(n, k)$ .

If  $B^* \in \mathcal{B}_1(n, k)$ . By Lemma 3.1, we may assume without loss of generality that  $B^* \in \mathcal{B}_{11}(n, k)$ . By the definition of the graph  $B(p, l, q)$ , we have  $q \geq p \geq 3$  and  $l \geq 1$ . Suppose that  $B^*$  contains  $C_3$ , then  $p = 3$ . Let  $N(v_0) \cap V(C_3) = \{u_1, u_2\}$ ,  $C_q = v_{l-1}w_1w_2 \dots w_{q-1}v_{l-1}$  be the other cycle of  $B^*$ . By Lemma 2.8, there exists a unit eigenvector  $X$  of  $\lambda(B^*)$

such that  $x_{u_1} = x_{u_2}$  and  $x_{w_i} = x_{w_{q-i}}$ , where  $1 \leq i \leq q-1$ . Note that  $\lambda(B^*) < -2.4495$ , by Lemmas 2.5, 2.9 and  $AX = \lambda(B^*)X$ , then  $x_{v_0}, x_{v_{l-1}} \neq 0$  (otherwise  $X = 0$ ). Now we distinguish the following two cases:

**Case1.**  $l = 1$ , then we have  $v_{l-1} = v_l = v_0$ . According to Lemmas 2.5 and 2.9, then each component of  $X$  is not equal to zero.

**Case1.1.**  $q \geq 5$  is odd.

**Case1.1.1.**  $x_{u_1}x_{w_{\frac{q-1}{2}}} < 0$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-1}{2}}w_{\frac{q+1}{2}} + u_1w_{\frac{q-1}{2}} + u_2w_{\frac{q+1}{2}}$ . Clearly  $B \in \mathcal{B}_1(n, k)$ , and

$$\begin{aligned}\lambda(B) - \lambda(B^*) &\leq X^T(A(B) - A(B^*))X \\ &= -2(x_{u_1} - x_{w_{\frac{q-1}{2}}})^2 < 0,\end{aligned}$$

hence  $\lambda(B^*) > \lambda(B)$ .

**Case1.1.2.**  $x_{u_1}x_{w_{\frac{q-1}{2}}} > 0$ , then  $q \geq 7$ . Next, for convenience, let  $\lambda(B^*) = \lambda$ . By Lemma 2.9, we have  $x_{v_0} = h_{\frac{q-1}{2}}(\lambda)h_{\frac{q-3}{2}}(\lambda) \cdots h_1(\lambda)x_{w_{\frac{q-1}{2}}}$  and  $x_{v_0} = (\lambda - 1)x_{u_1}$ . By Lemma 2.6,  $h_i(\lambda) < -1$ , hence

$$\begin{aligned}|x_{v_0}| &= |h_{\frac{q-1}{2}}(\lambda)h_{\frac{q-3}{2}}(\lambda) \cdots h_1(\lambda)||x_{w_{\frac{q-1}{2}}}| \\ &\geq |h_3(\lambda)h_2(\lambda)h_1(\lambda)||x_{w_{\frac{q-1}{2}}}| \\ &= |\lambda^3 - \lambda^2 - 2\lambda + 1||x_{w_{\frac{q-1}{2}}}|.\end{aligned}$$

Since  $\lambda < -2.4495$ , then  $|\lambda^3 - \lambda^2 - 2\lambda + 1| > |\lambda - 1|$ , and we have  $|x_{w_{\frac{q-1}{2}}}| \neq |x_{u_1}|$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-1}{2}}w_{\frac{q+1}{2}} + u_1w_{\frac{q-1}{2}} + u_2w_{\frac{q+1}{2}}$ . Clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ , since  $x_{u_1} = x_{u_1}$  and  $x_{w_{\frac{q-1}{2}}} = x_{w_{\frac{q+1}{2}}}$ .

**Case1.2.**  $q \geq 6$  is even.

**Case1.2.1.**  $\frac{q}{2}$  is odd, then  $x_{u_1}x_{w_{\frac{q}{2}}} > 0$ . By Lemma 2.9, we have  $x_{v_0} = g_{\frac{q}{2}}(\lambda)g_{\frac{q-2}{2}}(\lambda) \cdots g_1(\lambda)x_{w_{\frac{q}{2}}}$  and  $x_{v_0} = (\lambda - 1)x_{u_1}$ . By Lemma 2.6,  $g_i(\lambda) < -1$ , hence

$$\begin{aligned}|x_{v_0}| &= |g_{\frac{q}{2}}(\lambda)g_{\frac{q-2}{2}}(\lambda) \cdots g_1(\lambda)||x_{w_{\frac{q}{2}}}| \\ &\geq |g_3(\lambda)g_2(\lambda)g_1(\lambda)||x_{w_{\frac{q}{2}}}| \\ &= \frac{1}{2}(\lambda^3 - 3\lambda)||x_{w_{\frac{q}{2}}}|.\end{aligned}$$

Since  $\lambda < -2.4495$ , then  $|\frac{1}{2}(\lambda^3 - 3\lambda)| > |\lambda - 1|$ , and we have  $|x_{w_{\frac{q}{2}}}| < |x_{u_1}|$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-2}{2}}w_{\frac{q}{2}} + u_1w_{\frac{q-2}{2}} + u_2w_{\frac{q}{2}}$ . Clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ .

**Case1.2.2.**  $\frac{q}{2}$  is even, then  $q \geq 8$ . Note that  $\frac{q-2}{2} \geq 3$  is odd, hence  $x_{u_1}x_{w_{\frac{q-2}{2}}} > 0$ . Similar to Case1.2.1, we can show that  $|x_{w_{\frac{q-2}{2}}}| < |x_{u_1}|$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-2}{2}}w_{\frac{q}{2}} + u_1w_{\frac{q-2}{2}} + u_2w_{\frac{q}{2}}$ . Clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ .

**Case1.3.**  $q = 3$  or  $4$ . If there exists a pendant vertex  $s$  in  $B^*$  such that  $d_{B^*}(s, v_0)$  is even, then by Lemma 2.5,  $x_{v_0}x_s > 0$ . Note that  $x_{u_1}x_s < 0$ . Let  $B = B^* - u_1u_2 + u_1s$ , clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ . Otherwise for any pendant vertex  $t$  in  $B^*$ ,  $d_{B^*}(t, v_0)$  is odd. Since  $k \leq n - 7$ , then there must exist a pendant path with length  $s \geq 3$ . We have  $x_{u_1}x_s > 0$ . And next we will show that  $|x_s| < |x_{u_2}|$ . By Lemma 2.5, we have  $x_{v_0} = f_s(\lambda)f_{s-1}(\lambda) \cdots f_1(\lambda)x_s$  and  $x_{v_0} = (\lambda - 1)x_{u_2}$ . By Lemma 2.4,  $f_i(\lambda) < -1$ ,

$$\begin{aligned} |x_{v_0}| &= |f_s(\lambda)f_{s-1}(\lambda) \cdots f_1(\lambda)||x_s| \\ &\geq |f_3(\lambda)f_2(\lambda)f_1(\lambda)||x_s| \\ &= |\lambda^3 - 2\lambda||x_s|. \end{aligned}$$

Since  $\lambda < -2.4495$ , then  $|\lambda^3 - 2\lambda| > |\lambda - 1|$ , and we have  $|x_s| < |x_{u_2}|$ . Let  $B = B^* - u_1u_2 + u_1s$ , clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ .

**Case2.**  $l \geq 2$ . We have  $v_0 \neq v_{l-1}$ .

Define a new vector  $Y$  from  $X$  as follows:  $y_i = (-1)^{d_{B^*}(i, v_0)}|x_i|$  for each vertex  $i \in V(B^*)$ , then  $y_{v_0} > 0$ . By Lemma 2.7,  $Y$  is also a unit eigenvector of  $\lambda(B^*)$ .

**Case2.1.**  $i = 0$ , i.e.  $v_i = v_0$ .

Clearly  $|y_{v_0}| > |y_{v_{l-1}}|$ . (Otherwise  $|y_{v_0}| \leq |y_{v_{l-1}}|$ . Let  $B$  be the graph obtained from  $B^*$  by removing all the pendant paths at  $v_0$  to  $v_{l-1}$ , clearly  $B \in \mathcal{B}_1(n, k)$ , and by Lemma 2.1, we have  $\lambda(B^*) \geq \lambda(B)$ . If  $\lambda(B^*) = \lambda(B)$ , then  $y_{v_0} = y_{v_{l-1}} = 0$ , hence  $Y = 0$ , a contradiction. So we have  $\lambda(B^*) > \lambda(B)$ .) When  $q \geq 3$  is odd, by Lemma 2.9,  $|y_{v_0}| = |h_1(\lambda)||y_{u_1}|$  and  $|y_{v_{l-1}}| = |h_{\frac{q-1}{2}}(\lambda)h_{\frac{q-3}{2}}(\lambda) \cdots h_1(\lambda)||y_{w_{\frac{q-1}{2}}}| \geq |h_1(\lambda)||y_{w_{\frac{q-1}{2}}}|$ , hence  $|y_{u_1}| > |y_{w_{\frac{q-1}{2}}}|$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-1}{2}}w_{\frac{q+1}{2}} + u_1w_{\frac{q-1}{2}} + u_2w_{\frac{q+1}{2}}$ . Clearly  $B \in \mathcal{B}_2(n, k)$  and  $\lambda(B^*) > \lambda(B)$ . When  $q \geq 4$  is even. If  $d_{B^*}(v_0, v_{l-1})$  is even, by the definition of  $Y$ ,  $y_{w_1}y_{v_0} < 0$  and  $y_{w_1}y_{v_{l-1}} < 0$ : Let  $B = B^* - w_1v_{l-1} + w_1v_0$ . Clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ . Otherwise  $d_{B^*}(v_0, v_{l-1})$  is odd, then  $y_{v_{l-1}} < 0$ . By Lemma 2.9,  $|y_{u_1}| > |y_{w_{\frac{q-2}{2}}}| > |y_{w_{\frac{q}{2}}}|$ . Let  $B = B^* - u_1u_2 - w_{\frac{q-1}{2}}w_{\frac{q+1}{2}} + u_1w_{\frac{q-1}{2}} + u_2w_{\frac{q+1}{2}}$ . Clearly  $B \in \mathcal{B}_2(n, k)$  and  $\lambda(B^*) > \lambda(B)$ .

**Case2.2.**  $1 \leq i \leq l - 1$ .

Clearly  $|y_{v_0}| < |y_{v_i}|$ . (Otherwise  $|y_{v_0}| \geq |y_{v_i}|$ . Let  $B$  be the graph obtained from  $B^*$  by removing all the pendant paths at  $v_i$  to  $v_0$ , clearly  $B \in \mathcal{B}_1(n, k)$ , and by Lemma 2.1, we have  $\lambda(B^*) \geq \lambda(B)$ . If  $\lambda(B^*) = \lambda(B)$ , then

$y_{v_0} = y_{v_i} = 0$ , hence  $Y = 0$ , a contradiction. So we have  $\lambda(B^*) > \lambda(B)$ . If  $d_{B^*}(v_0, v_i)$  is even, by the definition of  $Y$ ,  $y_{u_1}y_{v_0} < 0$  and  $y_{u_1}y_{v_i} < 0$ . Let  $B = B^* - u_1v_0 + u_1v_i$ . Clearly  $B \in \mathcal{B}_1(n, k)$  and  $\lambda(B^*) > \lambda(B)$ . Otherwise  $d_{B^*}(v_0, v_i)$  is odd. Define a new vector  $Z$  from  $Y$  as follows:  $z_{u_1} = -y_{u_1}$  and  $z_i = y_i, i \in V(B^*) \setminus \{u_1\}$ . Let  $B = B^* - u_1v_0 + u_1v_i$ , clearly  $B \in \mathcal{B}_1(n, k)$ . And

$$\begin{aligned} \lambda(B^*) - \lambda(B) &\geq Y^T A(B^*)Y - Z^T A(B)Z \\ &= 2(y_{u_1}^2 + y_{v_0}y_{u_1} + y_{u_1}^2 + y_{v_i}y_{u_1}) \\ &> 2|y_{u_1}|(|y_{v_i}| - |y_{v_0}|) > 0. \end{aligned}$$

If  $B^* \in \mathcal{B}_2(n, k)$ . By Lemma 3.2, we may assume without loss of generality that  $B^* \in \mathcal{B}_{21}(n, k) \cup \mathcal{B}_{22}(n, k)$ . By the definition of the graph  $P(p, l, q)$ , we have  $l \geq q \geq p \geq 1$  and at most one of them is 1. Suppose that  $B^*$  contains  $C_3$ , then  $p = 1, q = 2, l \geq 2$ .

Let  $X$  be a unit eigenvector of  $B^*$  corresponding to  $\lambda(B^*)$ . Let  $u$  and  $v$  be two common endpoints of  $P_2, P_3, P_{l+1}$ ,  $w$  be the other vertex of  $C_3$ . For even  $l \geq 4$  or odd  $l \geq 3$ . If  $x_u x_v \geq 0$ , without loss of generality letting  $x_u \geq 0, x_v \geq 0$ , then except  $u, v$  the path  $P_{l+1}$  must contain a vertex with negative value given by  $X$ . Deleting  $uv$  and adding edge between  $u$ (or  $v$ ) and the negative vertex, we get a graph  $B \in \mathcal{B}_2(n, k)$  with  $\lambda(B^*) \geq \lambda(B)$ . If  $\lambda(B^*) = \lambda(B)$ , then  $x_u$ (or  $x_v$ ) = 0. Considering the equation  $A(B^*)X = \lambda(B^*)X$  at vertex  $u$ (or  $v$ ), we can deduce that  $X = 0$ , a contradiction. Hence  $\lambda(B^*) > \lambda(B)$ . If  $x_u x_v < 0$ , without loss of generality letting  $x_u > 0, x_v < 0, x_w \geq 0$ , then except  $u, v$  the path  $P_{l+1}$  must contain a negative vertex. Deleting  $wu$  and adding edge between  $w$  and the negative vertex, we get a graph  $B \in \mathcal{B}_2(n, k)$  with  $\lambda(B^*) \geq \lambda(B)$ . If  $\lambda(B^*) = \lambda(B)$ , then  $x_w = 0$ . Considering the equation  $A(B^*)X = \lambda(B^*)X$  at vertex  $w, u, v$ , we can deduce that  $X = 0$ , a contradiction. Hence  $\lambda(B^*) > \lambda(B)$ .

For even  $l = 2$ . When  $v$  is the root-vertex of  $B^*$ . If  $x_u x_v \geq 0$ , without loss of generality letting  $x_u \geq 0, x_v \geq 0$ . Since  $1 \leq k \leq n - 7$ , then there exists a pendant path containing a non-pendant negative vertex  $t$  such that  $d(v, t) = 1$ . Deleting  $uv$  and joining  $ut$ , we get a graph  $B \in \mathcal{B}_2(n, k)$  with  $\lambda(B^*) > \lambda(B)$ . If  $x_u x_v < 0$ , without loss of generality letting  $x_u < 0, x_v > 0$ . If  $x_w \geq 0$ , deleting  $wv$  and joining  $wt$ , we get a graph  $B \in \mathcal{B}_2(n, k)$  with  $\lambda(B^*) > \lambda(B)$ . Otherwise  $x_w < 0$ , there exists a pendant path containing a non-pendant positive vertex  $q$  such that  $d(v, q) = 2$ . Deleting  $wu$  and joining  $wq$ , we get a graph  $B \in \mathcal{B}_1(n, k)$  with  $\lambda(B^*) > \lambda(B)$ . When  $w$  is the root-vertex of  $B^*$ , similar to the above proof, we can find  $B \in \mathcal{B}_1(n, k) \cup \mathcal{B}_2(n, k)$  such that  $\lambda(B^*) > \lambda(B)$ .  $\square$

**Lemma 3.4** *Let  $B^*$  have minimal least eigenvalue in  $\mathcal{B}(n, k)$ , where  $1 \leq k \leq n - 7$ . If  $B^* \in \mathcal{B}_1(n, k)$ , then  $p = q = 4$ . If  $B^* \in \mathcal{B}_2(n, k)$ , then  $B^* \cong B_2(k)$  or  $B_3(k)$ .*

**Proof.** By the Lemma 3.3,  $B^*$  contains no  $C_3$ .

When  $B^* \in \mathcal{B}_1(n, k)$ , by Lemma 3.1, we may assume without loss of generality that  $B^* \in \mathcal{B}_{11}(n, k)$ . By the definition of the graph  $B(p, l, q)$ , we have  $q \geq p \geq 3$ . Note that  $B^*$  contains no  $C_3$ , then  $q \geq p \geq 4$ . If  $q \geq 5$ . Let  $B$  be the graph obtained from  $B^*$  by contracting  $C_q$  to  $C_4$  and adding a pendant path  $P_{q-4}$  to a pendant vertex of  $B^*$ , then  $B \in \mathcal{B}_1(n, k)$  and  $B$  is bipartite. By Lemma 2.2,  $\rho(B^*) < \rho(B)$ . Thus  $\lambda(B^*) \geq -\rho(B^*) > -\rho(B) = \lambda(B)$ . Hence  $p = q = 4$ .

When  $B^* \in \mathcal{B}_2(n, k)$ , by Lemma 3.2, we may assume without loss of generality that  $B^* \in \mathcal{B}_{21}(n, k) \cup \mathcal{B}_{22}(n, k)$ . By the definition of the graph  $P(p, l, q)$ , we have  $l \geq q \geq p \geq 1$  and at most one of them is 1. Note that  $B^*$  contains no  $C_3$ , then we distinguish the following two cases:

**Case1.**  $2 \leq p \leq q \leq l$ .

If  $3 \leq p \leq q \leq l$ . Let  $B$  be the graph obtained from  $B^*$  by contracting  $P(p, l, q)$  to  $P(2, 2, 2)$  and adding a pendant path  $P_{p+q+l-6}$  to a pendant vertex of  $B^*$ , then  $B \in \mathcal{B}_2(n, k)$  and  $B$  is bipartite. By Lemma 2.2,  $\rho(B^*) < \rho(B)$ . Thus  $\lambda(B^*) \geq -\rho(B^*) > -\rho(B) = \lambda(B)$ . If  $p = 2, 3 \leq q \leq l$  or  $p = 2, q = 2, 3 \leq l$ , similar to the above proof, there exists  $B \in \mathcal{B}_2(n, k)$  such that  $\lambda(B^*) > \lambda(B)$ . Hence  $p = q = l = 2$ . Clearly  $P(2, 2, 2) = G_2$  (see Fig.1). Note that at this moment  $B^*$  is bipartite, we consider  $\rho(B^*)$ . If  $v \in G_2$  is the root-vertex of  $B^*$ , by Lemmas 2.2, 2.3 and 2.10, we have  $B^* \cong B_2(k)$ . If  $u \in G_2$  is the root-vertex of  $B^*$ , then  $B^* \cong \bar{B}_2(k)$ . Combining Lemma 2.15,  $\rho(B_2(k)) > \rho(\bar{B}_2(k))$ . Hence  $B^* \cong B_2(k)$ .

**Case2.**  $p = 1, 3 \leq q \leq l$ .

Similar to the proof of Case1, then  $p = 1, q = l = 3$ . Clearly  $P(3, 1, 3) = G_3$  (see Fig.1). Note that at this moment  $B^*$  is bipartite, we consider  $\rho(B^*)$ . If  $v \in G_3$  is the root-vertex of  $B^*$ , by Lemmas 2.2, 2.3 and 2.10, we have  $B^* \cong B_3(k)$ . If  $u \in G_3$  is the root-vertex of  $B^*$ , then  $B^* \cong \bar{B}_3(k)$ . Combining Lemma 2.15,  $\rho(B_3(k)) > \rho(\bar{B}_3(k))$ . Hence  $B^* \cong B_3(k)$ .  $\square$

Let  $B^*$  have minimal least eigenvalue in  $\mathcal{B}(n, k)$ . When  $B^* \in \mathcal{B}_1(n, k)$ , clearly,  $B^*$  have minimal least eigenvalue in  $\mathcal{B}_1(n, k)$ . By Lemma 3.1, we may assume without loss of generality that  $B^* \in \mathcal{B}_{11}(n, k)$ . Let  $\mathcal{B}_{11}^*(n, k)$  be the set of bicyclic graphs in  $\mathcal{B}_{11}(n, k)$  with  $p = q = 4$ . According to Lemma 3.4,  $B^* \in \mathcal{B}_{11}^*(n, k)$ . Note that  $\lambda(G) = -\rho(G)$  for any bipartite graph. Thus the problem minimizing the least eigenvalue in  $\mathcal{B}_1(n, k)$  is equivalent to that of maximizing the spectral radius in  $\mathcal{B}_{11}^*(n, k)$ .

**Theorem 3.5** *Let  $B^*$  have maximal spectral radius in  $\mathcal{B}_{11}^*(n, k)$ , where  $1 \leq k \leq n - 7$ . Then  $B^* \cong B_1(k)$ .*

**Proof.** If  $l = 1$ , then we have  $v_{l-1} = v_i = v_0$ . From a repeated use of Lemma 2.10, we have  $B^* \cong B_1(k)$ . Otherwise  $l \geq 2$ , then  $0 \leq i \leq l-1$ . For any  $B^* \in \mathcal{B}_{11}^*(n, k)$ , by Lemmas 2.2 and 2.3, there exists  $B \in \mathcal{B}_{11}^*(n, k)$  such that  $\rho(B) > \rho(B^*)$ , a contradiction. Hence  $B^* \cong B_1(k)$ .  $\square$

**Proof of Theorem 1.1** According to Theorem 3.5 and Lemma 3.4,  $B^* \cong B_1(k), B_2(k)$  or  $B_3(k)$ . By Lemmas 2.13 and 2.14, we have  $\rho(B_1(k)) > \rho(B_2(k))$  and  $\rho(B_1(k)) > \rho(B_3(k))$ . Note that these three bicyclic graphs are all bipartite, hence  $\lambda(B_1(k)) < \lambda(B_2(k))$  and  $\lambda(B_1(k)) < \lambda(B_3(k))$ . So  $B^* \cong B_1(k)$ .

Let  $1 \leq k < n - 7$ . It follows that there exists a pendant path  $P_l = v_1 v_2 \cdots v_l$  attached to the root vertex  $v_1$  of  $B_1(k)$  such that  $l \geq 3$ . Let  $B = B_1(k) - \{v_{l-1} v_l\} + \{v_1 v_l\}$ . Then  $B \in \mathcal{B}_1(n, k + 1)$ . By Lemma 2.10, we have  $\rho(B_1(k)) < \rho(B)$ . Note that  $B_1(k)$  and  $B$  are bipartite, then  $\lambda(B_1(k)) > \lambda(B)$ . By Theorem 3.5, we have  $\lambda(B) \geq \lambda(B_1(k + 1))$ . Hence  $\lambda(B_1(k)) > \lambda(B_1(k + 1))$ . Hence  $\lambda(B_1(k))$  is a decreasing function on  $k$ . This completes the proof of Theorem 1.1.  $\square$

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