Minimizing the least eigenvalue of bicyclic graphs with fixed diameter*

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Abstract

Let $\mathscr{B}(n,d)$ be the set of bicyclic graphs with both n vertices and diameter d, and let θ^* consist of three paths $u_0w_1v_0$, $u_0w_2v_0$ and $u_0w_3v_0$. For four nonnegative integers n,d,k,j satisfying $n \geq d+3, d = k+j+2$, we let $B(n,d;k,j)$ denote the bicyclic graph obtained from θ^* by attaching a path of length k to u_0, attaching a path of length j to vertex v_0 and $n-d-3$ pedant edges to v_0, and let $\mathscr{B}(n,d;k,j) = \{B(n,d;k,j) | k+j \geq 1\}$. In this paper, the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d;k,j)$ are well characterized, some structural characterizations about the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d)$ are presented as well.

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1 Introduction

All graphs considered here are simple and undirected. Denote by $V(G)$ and $E(G)$ the vertex set and edge set of a graph G respectively. $|V(G)|$ is always called the order of G. For $S \subseteq V(G)$, let $G[S]$ denote the subgraph induced by S. For a vertex set $\{v_1, v_2, \ldots, v_k\}$, we denote by $G[v_1, v_2, \ldots, v_k]$ simply for $G[\{v_1, v_2, \ldots, v_k\}]$ sometimes. Let $N_G(v)$ denote the set of the vertices adjacent to v in G. The degree of v in G, denoted by $d_G(v)$, $d(v)$ or $deg(v)$, is equal to $|N_G(v)|$.

Let $W = v_0e_1v_1e_2 \cdots e_kv_k$ ($e_i = v_{i-1}v_i$ for $1 \leq i \leq k$) denote a walk in a graph G. A walk is also denoted simply by $W = (v_0, v_1, \ldots, v_k)$, $W = v_0v_1 \cdots v_k$ or $W = e_1e_2 \cdots e_k$ if there is no ambiguity; the positive integer k is called the length of the walk W, denoted by $L(W)$. A cycle with length k is always called k-cycle, denoted by C_k. A path with order n is denoted by P_n. In a graph G, the length of the shortest path from v_i to v_j is called the distance between v_i and v_j, denoted by $d_G(v_i, v_j)$ or $d(v_i, v_j)$. $d(G) = \max\{d(v_i, v_j) | v_i, v_j \in V(G)\}$ is called the *diameter* of the graph G.

Definition 1.1 *Let A be a nonnegative irreducible square matrix. The spectral radius, denoted by $\rho(A)$, is the maximum of the moduli of its eigenvalues.*

Theorem 1.2 (Perron-Frobenius [9]) *Let A be a nonnegative irreducible square real matrix with order n. Suppose $\lambda_1, \lambda_2, \ldots, \lambda_n$ are all the eigenvalues of A. Then*

(i) $\rho(A)$ is a simple eigenvalue of A and $|\lambda_i| \leq \rho(A)$ for any eigenvalue λ_i $(1 \leq i \leq n)$;

(ii) there exists a positive unit eigenvector corresponding to $\rho(A)$, which is called the Perron vector of A.

Let $A(G)$ be the adjacency matrix of a graph G. The characteristic polynomial of $A(G)$ is called the characteristic polynomial of graph G, denoted by $P(G)$ (or $P(G, \lambda)$). Suppose $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of $A(G)$. The largest eigenvalue of $A(G)$ is called the *spectral radius* of G, denoted by $\rho(G)$. The *Perron vector* $X = (x_{v_1}, x_{v_2}, \ldots, x_{v_n})^T$ is the non-negative unit eigenvector corresponding to $\rho(G)$, where x_{v_i} corresponds to the vertex v_i. By the Perron-Frobenius theorem, the Perron vector is a positive vector for a connected graph. The least eigenvalue

$\lambda_n(G)$ of graph G can be denoted by $\lambda(G)$ simply. It is well known that $\lambda(G) = -\rho(G)$ for a bipartite graph (see [3]).

Definition 1.3 *A connected graph G with order n is called a bicyclic graph if $|E(G)| = n+1$. Let $\mathscr{B}(n,d) = \{G|\ G$ be a bicyclic graph with both order n and diameter $d\}$ and $\lambda_B = \min\{\lambda_n(G)|\ G \in \mathscr{B}(n,d),\ n \geq d+3,\ d \geq 3\}$.*

Definition 1.4 *Let θ^* consist of three paths $u_0w_1v_0$, $u_0w_2v_0$ and $u_0w_3v_0$. For four nonnegative integers n, d, k, j satisfying $n \geq d+3, d = k+j+2$, we let $B(n,d;k,j)$ denote the bicyclic graph obtained from θ^* by attaching a path of length k to u_0, attaching a path of length j to vertex v_0 and $n-d-3$ pedant edges to v_0 (see Fig. 1.1). Let $\mathscr{B}(n,d;k,j) = \{B(n,d;k,j)|d \geq 3\}$ and let $\lambda_{\mathbb{B}} = \min\{\lambda_n(G)|G \in \mathscr{B}(n,d;k,j)\}$.*

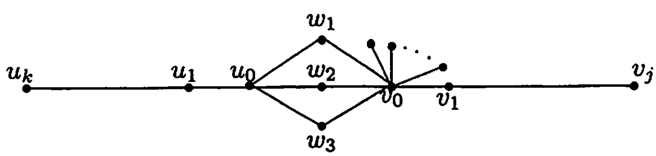


Fig. 1.1. $B(n,d;k,j)$

The investigation on the lower bound of the least eigenvalue of a graph is of great significance and interest (see [1], [2], [4], [7], etc.). In 2008, M. Petrović [10] characterized the bicyclic graphs with the minimal least eigenvalue among all the graphs with given order. In this paper, we consider the bicyclic graphs with the minimal least eigenvalue λ_B among $\mathscr{B}(n,d)$ $(n \geq d+3, d \geq 3)$. The paper is organized as follows: Section 1 introduces the basic ideas of spectra of graphs and their supports; Section 2 introduces series of working lemmas; Section 3 presents some basic results; Section 4 presents some structural characterizations about the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d)$; Section 5 characterizes the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d;k,j)$; Section 6 conjectures that the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d;k,j)$ are also the extremal graphs with the minimal least eigenvalue among all graphs in $\mathscr{B}(n,d)$.

2 Preliminaries

Lemma 2.1 ([12]) *Let A be an $n \times n$ real symmetric irreducible nonnegative matrix and $X \in R^n$ be an unit vector. If $\rho(A) = X^TAX$, then $AX = \rho(A)X$.*

Lemma 2.2 ([14]) *Let G be a connected bipartite graph with order n. Let $X = (x_1, x_2, \dots, x_n)^T$ be a real unit vector such that $\lambda(G) = X^T AX$. Then $x_i \neq 0$ for each $1 \leq i \leq n$.*

Let $\mathscr{U}(n, d)$ denote the set of unicyclic graphs with both order n and diameter d.

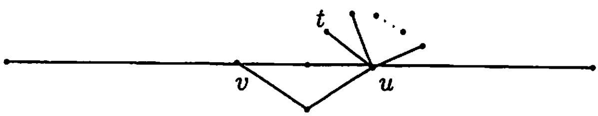


Fig. 2.1. $U^k_{p,q}$

Lemma 2.3 ([14]) *For every pair of positive integers n, d with $3 \leq d \leq n-2$, there is (up to isomorphism) an unique graph in $\mathscr{U}_{n,d}$ that has the minimal least eigenvalue among all graphs in $\mathscr{U}_{n,d}$, namely, $U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil}$ for $3 \leq d \leq n-6$ and $U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil}$ for $n-5 \leq d \leq n-2$, where $U^k_{p,q}$ (see Fig. 2.1) denotes the graph obtained from a 4-cycle by attaching k pendant edges and a path with length q to a vertex u, and attaching a path with length p to the vertex not adjacent to u.*

Lemma 2.4 ([8]) *Let the connected graph $G^m_{k,l}$ be obtained from G by attaching two pendant paths P_{k+1} and P_{l+1} at vertices u and v respectively, $d(u,v) = m$. If $k \geq l \geq 1$, then $\rho(G^m_{k,l}) > \rho(G^m_{k+1,l-1})$ if $G^m_{k,l}$ satisfies one of the following conditions:*

(1) $m = 0, \deg_G(u) \geq 1$ and $k \geq l \geq 1$;

(2) $m = 1, \deg_G(u) \geq 2, \deg_G(v) \geq 2$, and $k \geq l \geq 1$;

(3) $m > 1, \deg_G(u) \geq 2, \deg_G(v) \geq 2$, and $k - l \geq m, l \geq 1$.

Lemma 2.5 ([13]) *Let u, v be two vertices of a connected graph G. Suppose $v_1, v_2, \dots, v_s$ $(1 \leq s \leq d_v)$ are some vertices of $N_G(v) \backslash N_G(u)$ and $X = (x_1, x_2, \dots, x_n)^T$ is the Perron vector of G, where x_i corresponds to the vertex v_i $(1 \leq i \leq n)$. Let G^* be the graph obtained from G by deleting the edges (v, v_i) and adding the edges (u, v_i) $(1 \leq i \leq s)$. If $x_u \geq x_v$, then $\rho(G) < \rho(G^*)$.*

Lemma 2.6 ([13]) *Let graphs G and G^* be as in Lemma 2.5. If G^* is also connected, suppose $X = (x_1, x_2, x_3, \dots, x_{n-1}, x_n)^T$ is the Perron vector of G^* where x_i corresponds to vertex v_i, $\| X \| = 1$, then $x_u \geq x_v$.*

Let G, H be two disjoint connected graphs with $u \in V(G)$ and $w \in V(H)$. We denote by $G\underline{uw}H$ the graph obtained from G and H by identifying u with w (See Fig. 2.2).

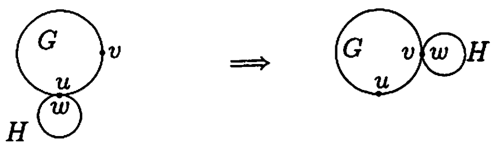


Fig. 2.2 $G\underline{uw}H$ and $G\underline{vw}H$.

Lemma 2.7 ([4]) *Let G, H be two disjoint nontrivial connected graphs with $u, v \in V(G)$ and $w \in V(H)$. Let X be an unit eigenvector corresponding to $\lambda(G\underline{uw}H)$. If $|x_u| \leq |x_v|$, then $\lambda(G\underline{uw}H) \geq \lambda(G\underline{vw}H)$. The equality holds if and only if X is also an eigenvector corresponding to $\lambda(G\underline{vw}H)$, $x_u = x_v$ and $\sum_{i \in N_H(w)} x_i = 0$.*

Lemma 2.8 ([6, 8]) *Let G_1 and G_2 be two graphs. If G_2 is a proper subgraph of G_1. Then $\rho(G_2) < \rho(G_1)$ and for $\lambda \geq \rho(G_1)$, $P(G_2, \lambda) > P(G_1, \lambda)$.*

Lemma 2.9 ([8]) *Let G and H be two connected graphs such that $P(G, \lambda) > P(H, \lambda)$ for $\lambda \geq \rho(H)$ or $\lambda = \rho(G)$, then $\rho(G) < \rho(H)$.*

Let G be a connected simple graph with $uv \in E(G)$. The graph G_{uv} is obtained from G by subdividing the edge uv, that is, introducing a new vertex on the edge uv; while the graph G^{uv} is obtained by contracting uv, that is, deleting the edge uv, deleting possible multiple edge and identifying the two vertices u, v. Suppose $G[v_1, v_2, \ldots, v_k]$ $(k \geq 1)$ is a path of graph G, $d_G(v_i) = 2$ $(2 \leq i \leq k-1)$ and $d_G(v_i) \geq 3$ $(i = 1, k)$ (or $G[v_1, v_2, \ldots, v_k]$ is a cycle if $k \geq 3$, $d_G(v_i) = 2$ $(2 \leq i \leq k)$ and $d_G(v_1) \geq 3$), then the induced graph $G[v_1, v_2, \ldots, v_k]$ $(k \geq 2)$ can be called an internal path of G. Let $\mathcal{T}_n$ $(n \geq 6)$ be the graph obtained from a path $v_1 v_2 \cdots v_{n-4}$ by attaching two pendant edges to v_1 and another two to v_{n-4}. Hoffman and Smith showed the following result.

Lemma 2.10 ([5]) *Let G be a connected graph and $G \not\cong \mathcal{T}_n, G \not\cong C_n$. If the edge uv belongs to an internal path of G, then $\rho(G_{uv}) < \rho(G)$.*

Lemma 2.11 ([11]) *Let v be a vertex of graph G and $C(v)$ be the set of* *cycles containing v. Then*

$$P(G,\lambda)=\lambda P(G-v,\lambda)-\sum_{u\in N_G(v)}P(G-v-u,\lambda)-2\sum_{C\in \mathcal{C}(v)}P(G-V(C),\lambda). \quad (1)$$

Let u be a pendant vertex of a graph G and v be its neighbor. It follows from Lemma 2.9 that

$$P(G,\lambda)=\lambda P(G-u,\lambda)-P(G-u-v,\lambda). \quad (2)$$

3 Some basic results

Let $G=G_1v_0v_1P_k$ denote the graph obtained from graph G_1 and path P_k by adding an edge v_0v_1 between the vertex v_0 of G_1 and a pedant vertex v_1 of P_k (see Fig. 3.1).

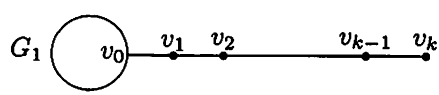


Fig. 3.1. $G_1v_0v_1P_{k+1}$

Lemma 3.1 *Let A be the adjacency matrix of the graph $G=G_1v_0v_1P_k$ (see Fig. 3.1) with order n, λ_i $(1\le i\le n)$ be the ith largest eigenvalue of A. Suppose $X_i=(x_{i,0},\ x_{i,1},\ x_{i,2},\ \dots,\ x_{i,k},\ x_{i,k+1},\ \dots,\ x_{i,n-1})^T$ is an eigenvector corresponding to eigenvalue λ_i and $x_{i,s}$ $(0\le s\le n-1)$ corresponds to vertex v_s. Let $f_1=\lambda_i$ and $f_{j+1}=\lambda_i-\frac{1}{f_j}$. Then $x_{i,k-j}=f_jx_{i,k-j+1}$ for $1\le j\le k$ and we have*

(i)

$$\begin{cases}\dfrac{\lambda_i}{2}\le f_j\le \lambda_i, & if\ \lambda_i\ge 2;\\[2ex] \dfrac{\lambda_i}{2}\ge f_j\ge \lambda_i, & if\ \lambda_i\le -2;\end{cases}$$

(ii) $|f_{j+1}|<|f_j|$ *if* $|\lambda_i|\ge 2$;

(iii) $f_{j+1}f_j\ge|\lambda_i|$ $(1\le j\le k-1)$ *if* $|\lambda_i|\ge 2.2$;

In particular,

$$\begin{cases} f_{j+1}f_j \geq 3 \ (1 \leq j \leq k-1) & \textit{if } |\lambda_i| \geq 2.3095; \\ f_{j+1}f_j \geq 3|\lambda_i| \ (1 \leq j \leq k-1) & \textit{if } |\lambda_i| \geq 4. \end{cases}$$

Proof. (i) Noting that $x_{i,k-1} = \lambda_i x_{i,k} = f_1 x_{i,k}$ and $x_{i,k-2} + x_{i,k} = \lambda_i x_{i,k-1}$, we get

$$x_{i,k-2} = (\lambda_i - \frac{1}{\lambda_i})x_{i,k-1} = (\lambda_i - \frac{1}{f_1})x_{i,k-1} = f_2 x_{i,k-1}.$$

So, by induction, $f_{j+1} = \lambda_i - \frac{1}{f_j}$ and $x_{i,k-j} = f_j x_{i,k-j+1}$ for $1 \leq j \leq k$.

We prove that $\frac{\lambda_i}{2} \leq f_j \leq \lambda_i$ if $\lambda_i \geq 2$ firstly. It is easy to check that $\frac{\lambda_i}{2} \leq f_2$ if $\lambda_i \geq 2$. Suppose that $\frac{\lambda_i}{2} \leq f_j \leq \lambda_i$ for $j < N$. Because $f_N = \lambda_i - \frac{1}{f_{N-1}}$, so $-\frac{2}{\lambda_i} \leq -\frac{1}{f_{N-1}} \leq -\frac{1}{\lambda_i}, \lambda_i - \frac{2}{\lambda_i} \leq f_N \leq \lambda_i - \frac{1}{\lambda_i}$. Note that if $\lambda_i \geq 2$, then $\lambda_i - \frac{2}{\lambda_i} \geq \frac{\lambda_i}{2}$. Therefore, $\frac{\lambda_i}{2} \leq f_N \leq \lambda_i$. By induction, we get $\frac{\lambda_i}{2} \leq f_j \leq \lambda_i$ if $\lambda_i \geq 2$. If $\lambda_i \leq -2$, $\frac{\lambda_i}{2} \geq f_j \geq \lambda_i$ can be similarly proved.

Same as (i), (ii) and (iii) can be proved. □

Let $G = G_1 v_0 G_2$ denote the graph obtained from graph G_1 by attaching graph G_2 to the vertex v_0 of G_1.

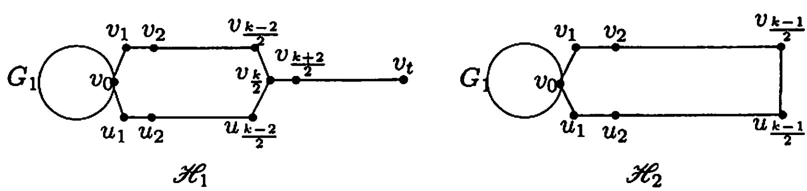


Fig. 3.2 $\mathscr{H}_1, \mathscr{H}_2$

Let $\mathscr{H}_1 = G_1 v_0 C_k v_{\frac{k}{2}} P_{t-\frac{k}{2}+1}$ where k is even and $d_{G_1}(v_0) \geq 2$ (see Fig. 3.2), $V(C_k) = \{v_0, v_1, v_2, \ldots, v_{\frac{k-4}{2}}, v_{\frac{k-2}{2}}, v_{\frac{k}{2}}, u_1, u_2, \ldots, u_{\frac{k-2}{2}}\}$, $V(P_{t-\frac{k}{2}+1}) = (v_{\frac{k}{2}}, v_{\frac{k}{2}+1}, \ldots, v_t)$ and $V(G_1) = \{v_0, s_1, s_2, \ldots, s_{n-t-\frac{k-2}{2}-1}\}$. Let graph $\mathscr{H}_2 = G_1 v_0 C_k$ where k is odd (see Fig. 3.2), $V(G_1) = \{v_0, s_1, s_2, \ldots, s_{n-k}\}$, $V(C_k) = \{v_0, v_1, v_2, \ldots, v_{\frac{k-1}{2}}, u_1, u_2, \ldots, u_{\frac{k-1}{2}}\}$.

Lemma 3.2 (i) *For the graph* $\mathscr{H}_1$ *(see Fig. 3.2), there must be a nonzero eigenvector* $X_i = (x_{i,v_0}, x_{i,s_1}, x_{i,s_2}, \ldots, x_{i,s_{n-t-\frac{k-2}{2}-1}}, x_{i,v_1}, x_{i,v_2}, \ldots, x_{i,v_{\frac{k-2}{2}}}, x_{i,v_{\frac{k}{2}}}, x_{i,u_1}, x_{i,u_2}, \ldots, x_{i,u_{\frac{k-2}{2}}}, x_{i,v_{\frac{k+2}{2}}}, x_{i,v_{\frac{k+4}{2}}}, \ldots, x_{i,v_t})^T$ *corresponding to eigenvalue* λ_i *where* $x_{i,v}$ *corresponds to vertex* v *satisfying the following:*

1° $x_{i,v_j} = x_{i,u_j}$ $(1 \le j \le \frac{k-2}{2})$;

2° $x_{i,v_{t-j}} = f_j x_{i,v_{t-j+1}}$ $(1 \le j \le t,\ t \ne \dfrac{k-2}{2})$, $2x_{i,v_{\frac{k-2}{2}}} = f_{t-\frac{k-2}{2}} x_{i,v_{\frac{k}{2}}}$, *where* $f_1 = \lambda_i$, $f_{j+1} = \lambda_i - \frac{1}{f_j}$;

3° f_j $(1 \le j \le t)$ *satisfies (i), (ii), (iii) in Lemma 3.1.*

(ii) *For the graph* $\mathscr{H}_2$ *(see Fig. 3.2), there must be a nonzero eigenvector* $X_i = (x_{i,v_0}, x_{i,s_1}, x_{i,s_2}, \ldots, x_{i,s_{n-k}}, x_{i,v_1}, x_{i,v_2}, \ldots, x_{i,v_{\frac{k-1}{2}}}, x_{i,u_1}, x_{i,u_2}, \ldots, x_{i,u_{\frac{k-1}{2}}})^T$ *corresponding to eigenvalue* λ_i *where* $x_{i,v}$ *corresponds to vertex* v *satisfying the following:*

1° $x_{i,v_j} = x_{i,u_j}$ $(1 \le j \le \frac{k-1}{2})$;

2° $x_{i,v_{t-j}} = f_j x_{i,v_{t-j+1}}$ $(1 \le j \le \frac{k-1}{2})$, *where* $f_1 = \lambda_i - 1$, $f_{j+1} = \lambda_i - \frac{1}{f_j}$;

3° f_j $(1 \le j \le \frac{k-1}{2})$ *satisfies (i), (ii) in Lemma 3.1;*

5° $f_{j+1} f_j \ge |\lambda_i|$ $(1 \le j \le \frac{k-3}{2})$ if $|\lambda_i| \ge 2$.

Proof. (i) For $\mathscr{H}_1$, suppose X_i does not satisfy 1°. Then there exists $x_{i,v_j} \ne x_{i,u_j} (1 \le j \le \frac{k-4}{2})$. Let $S_1 = \{x_{i,v_0}, x_{i,s_1}, x_{i,s_2}, \ldots, x_{i,s_{n-t-\frac{k-2}{2}-1}}, x_{i,v_{\frac{k}{2}}}, x_{i,v_{\frac{k+2}{2}}}, x_{i,v_{\frac{k+4}{2}}}, \ldots, x_{i,v_t}\}$, $V_1 = \{v_0, s_1, s_2, \ldots, s_{n-t-\frac{k-2}{2}-1}, v_{\frac{k}{2}}, v_{\frac{k+2}{2}}, v_{\frac{k+4}{2}}, \ldots, v_t\}$, $S_2 = \{x_{i,v_1}, x_{i,v_2}, \ldots, x_{i,v_{\frac{k-2}{2}}}, x_{i,u_1}, x_{i,u_2}, \ldots, x_{i,u_{\frac{k-2}{2}}}\}$, and let $X_i' = (x'_{i,v_0}, x'_{i,s_1}, x'_{i,s_2}, \ldots, x'_{i,s_{n-t-\frac{k-2}{2}-1}}, x'_{i,v_1}, x'_{i,v_2}, \ldots, x'_{i,v_{\frac{k-2}{2}}}, x'_{i,v_{\frac{k}{2}}}, x'_{i,u_1}, x'_{i,u_2}, \ldots, x'_{i,u_{\frac{k-2}{2}}}, x'_{i,v_{\frac{k+2}{2}}}, x'_{i,v_{\frac{k}{2}+2}}, \ldots, x'_{i,v_t})^T$ satisfy

$$\begin{cases} x'_{i,v} = x_{i,v} & v \in V_1; \\ x'_{i,v_j} = x_{i,u_j},\ x'_{i,u_j} = x_{i,v_j} & 1 \le j \le \frac{k-2}{2}. \end{cases}$$

Then X_i' is also an eigenvector corresponding to λ_i.

Let $S_3 = \{x'_{i,v_1} + x_{i,v_1}, x'_{i,v_2} + x_{i,v_2}, \ldots, x'_{i,v_{\frac{k-2}{2}}} + x_{i,v_{\frac{k-2}{2}}}\}$. If there exists one element in $S_1 \bigcup S_3$ is nonzero, then $Y = X_i + X'_i$ is also a nonzero eigenvector corresponding to λ_i and satisfies 1°. If each element in $S_1 \bigcup S_3$ is zero. Note that X_i is nonzero, so there exists at least one element in S_2 is nonzero. Suppose $x_{i,v_j} \neq 0$ $(1 \leq j \leq \frac{k-2}{2})$ and $x_{i,v_l} = 0$ $(1 \leq l \leq j)$. By a rotation, then we obtain a nonzero vector Y_i corresponding to λ_i, where

$$\begin{cases} y_{i,v_0} = x_{i,v_l},\ y_{i,v_1} = x_{i,v_{l+1}},\ \ldots,\ y_{i,v_{\frac{k}{2}-l}} = x_{i,v_{\frac{k}{2}}}, \\ y_{i,v_{\frac{k}{2}-l+1}} = x_{i,u_{\frac{k-2}{2}}},\ y_{i,v_{\frac{k}{2}-l+2}} = x_{i,u_{\frac{k-4}{2}}},\ \ldots, y_{i,v_{\frac{k}{2}}} = x_{i,u_{\frac{k-2}{2}-(l-1)}}, \\ y_{i,u_{\frac{k-2}{2}}} = x_{i,u_{\frac{k-2}{2}-l}},\ y_{i,u_{\frac{k-2}{2}-1}} = x_{i,u_{\frac{k-2}{2}-l-1}},\ \ldots,\ y_{i,u_{l+1}} = x_{i,u_1} \\ y_{i,u_l} = x_{i,v_0},\ y_{i,u_{l-1}} = x_{i,v_1},\ \ldots,\ y_{i,u_1} = x_{i,v_{l-1}}; \\ y_{i,v} = x_{i,v}, \quad v \in V_1. \end{cases}$$

As X'_i, we can construct an eigenvector Y'_i corresponding to λ_i such that $Z = Y_i + Y'_i$ is also a nonzero eigenvector corresponding to λ_i satisfying 1°.

Similar to the proof of Lemma 3.1, we can prove 2°, 3° of (i).

In a same way, we can prove that (ii) holds. □

4 Structural characterizations of the extremal graphs with the minimal least eigenvalue in $\mathscr{B}(n,d)$

Definition 4.1 *Let $G \in \mathscr{B}(n,d)$. We call the shortest path $P_{i,j}$ from vertex v_i to v_j a diameter-path in G if the length of $P_{i,j}$ is equal to d, where v_i and v_j are called the end vertices of $P_{i,j}$.*

Definition 4.2 *Let G consist of connected graph G_1 and tree T_i $(1 \leq i \leq k)$ (see Fig. 4.1) with order t_i $(t_i \geq 2)$, where $V(T_i) \bigcap V(G_1) = \{v_i\}$. Vertex v_i is called the root of the tree T_i on G_1; T_i is called nontrivial attaching tree to G_1 with root v_i (or rooted at v_i). We say a path P pass through T_j if $|V(P) \bigcap V(T_j)| \geq 1$.*

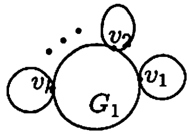


Fig. 4.1. attaching tree

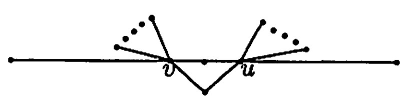


Fig. 4.2. $U^{s,t}_{p,q}$

Let $U^{s,t}_{p,q}$ (see Fig. 4.2) denote the graph obtained from a 4-cycle by attaching t pendant edges and a path with length q to a vertex u, and attaching s pendant edges and a path with length p to the vertex v not adjacent to u.

Lemma 4.3 *Let $G \in \mathscr{B}(n,d)$ $(n \geq d+3, d \geq 3)$ and $\lambda_n(G) = \lambda_B$. Then there G is a bipartite graph.*

Proof. Suppose the lemma does not hold. Then there exist an odd cycle in G. Suppose that C_1 is an odd cycle, and suppose that $X = (x_1, x_2, x_3, \ldots, x_{n-1}, x_n)^T$ is an unit eigenvector corresponding to eigenvalue $\lambda(G)$ in which x_i corresponds to vertex v_i. There must be an edge $e_1 = v_s v_{s+1}$ on C_1 such that $x_s x_{s+1} > 0$ or $x_s x_{s+1} = 0$. Let $\mathcal{H}_1 = G - e_1$, $d' = d(H_1)$. Then $d' \geq d$, $\lambda(\mathcal{H}_1) \leq \lambda(G)$, and $\lambda(\mathcal{H}_1)$ is an unicyclic graph. By Lemma 2.3, we have $\lambda(\mathcal{H}_1) \geq \lambda(U^{n-d'-2}_{\lfloor \frac{d'-3}{2} \rfloor, \lceil \frac{d'-1}{2} \rceil})$ or $\lambda(\mathcal{H}_1) \geq \lambda(U^{n-d'-2}_{\lfloor \frac{d'-2}{2} \rfloor, \lceil \frac{d'-2}{2} \rceil})$. By Lemmas 2.4 and 2.3, there exists an $U^{s,t}_{p,q}$ $(p+q+2 = d, s+t+p+q+4 = n)$ such that $\rho(U^{s,t}_{p,q}) > \rho(U^{n-d'-2}_{\lfloor \frac{d'-3}{2} \rfloor, \lceil \frac{d'-1}{2} \rceil})$ or $\rho(U^{s,t}_{p,q}) > \rho(U^{n-d'-2}_{\lfloor \frac{d'-2}{2} \rfloor, \lceil \frac{d'-2}{2} \rceil})$. Note that $U^{s,t}_{p,q}$, $U^{n-d'-2}_{\lfloor \frac{d'-3}{2} \rfloor, \lceil \frac{d'-1}{2} \rceil}$ and $U^{n-d'-2}_{\lfloor \frac{d'-2}{2} \rfloor, \lceil \frac{d'-2}{2} \rceil}$ are all bipartite. Therefore, $\lambda(U^{s,t}_{p,q}) < \lambda(U^{n-d'-2}_{\lfloor \frac{d'-3}{2} \rfloor, \lceil \frac{d'-1}{2} \rceil})$ or $\lambda(U^{s,t}_{p,q}) < \lambda(U^{n-d'-2}_{\lfloor \frac{d'-2}{2} \rfloor, \lceil \frac{d'-2}{2} \rceil})$. By Lemma 2.3, we have $\lambda(U^{s,t}_{p,q}) > \lambda(U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil})$ or $\lambda(U^{s,t}_{p,q}) > \lambda(U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil})$.

For $U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil}$ or $U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil}$ (see Fig. 2.1), let $\mathcal{H}_2 = U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil} + tv$, $\mathcal{H}_3 = U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil} + tv$. Then $\rho(\mathcal{H}_2) > \rho(U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil})$, $\rho(\mathcal{H}_3) > \rho(U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil})$. Note that $U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil}$, $U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil}$, $\mathcal{H}_2$ and $\mathcal{H}_3$ are all bipartite. Therefore, $\lambda(U^{n-d-2}_{\lfloor \frac{d-3}{2} \rfloor, \lceil \frac{d-1}{2} \rceil}) > \lambda(\mathcal{H}_2)$, $\lambda(U^{n-d-2}_{\lfloor \frac{d-2}{2} \rfloor, \lceil \frac{d-2}{2} \rceil}) > \lambda(\mathcal{H}_3)$. Hence $\lambda(G) > \lambda(\mathcal{H}_2)$ or $\lambda(G) > \lambda(\mathcal{H}_3)$, which contradicts $\lambda_n(G) = \lambda_B$. Then the lemma follows. □

Definition 4.4 *The union of simple graphs H and G is the simple graph $G \bigcup H$ with vertex set $V(G) \bigcup V(H)$ and edge set $E(G) \bigcup E(H)$. The intersection $G \bigcap H$ of simple graphs H and G is defined analogously.*

Lemma 4.5 *Let $G \in \mathscr{B}(n,d)$ $(n \geq d+3, d \geq 3)$ and $\lambda_n(G) = \lambda_B$. Suppose C_1 and C_2 are two different cycles in G. Let $\mathscr{D} = C_1 \bigcup C_2$. Then*

(i) *C_1 and C_2 have common vertices in G;*

(ii) *in fact, $\mathscr{D}$ is the union of two 4-cycles;*

(iii) *$\mathscr{D}$ have common vertices with a diameter-path P_d, and all the vertices in $V(G) \backslash V(\mathscr{D} \bigcup P_d)$ are pendant vertices attaching to one vertex of $\mathscr{D}$.*

Proof. Suppose the Lemma does not hold. By Lemma 4.3, we know that $L(C_1) \geq 4, L(C_2) \geq 4$.

Case 1 $C_1 \bigcap C_2 = \phi$.

Subcase 1.1 Both C_1, C_2 have common vertices with a diameter-path P_d.

Suppose $C_1 \bigcap P_d = P_1, C_2 \bigcap P_d = P_2$ and $C_1 = P_1 \bigcup P_1', C_2 = P_2 \bigcup P_2'$. Then $L(P_1) \leq [\frac{L(C_1)}{2}], L(P_2) \leq [\frac{L(C_2)}{2}]$. Suppose the path between C_1 and C_2 on diameter-path P_d are path P_3 and $P_3 \bigcap C_1 = v_a, P_3 \bigcap C_2 = v_b$. Let $\mathscr{E} = C_1 \bigcup C_2 \bigcup P_d$ and $P_d = P_e \bigcup P_1 \bigcup P_3 \bigcup P_2 \bigcup P_f$, $(P_1' \bigcap P_d) \backslash \{v_a\} = \{v_e\} = P_e \bigcap C_1, (P_2' \bigcap P_d) \backslash \{v_b\} = \{v_f\} = P_f \bigcap C_2$ (see Fig. 4.3).

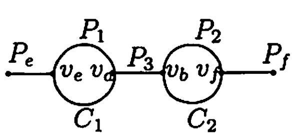


Fig. 4.3. G

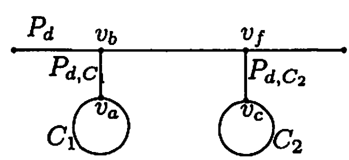


Fig. 4.4. G

Denote by $T_{\mathscr{E},i_l}$ $(v_{i_l} \in V(\mathscr{E}), 1 \leq l \leq k)$ the nontrivial attaching tree to $\mathscr{E}$ rooted at vertex v_{i_l}. Suppose $Y = (y_1, y_2, y_3, \dots, y_{n-1}, y_n)^T$ is the Perron vector of G and y_i corresponds to vertex v_i. Suppose $y_{i_s} = \max\{y_{i_l} | 1 \leq l \leq k\}$. Let

$$H = G - \sum_{1 \leq l \leq k} \sum_{v_g \in N_{T_{\mathscr{E},i_l}}(v_{i_l})} v_{i_l} v_g + \sum_{1 \leq l \leq k} \sum_{v_g \in N_{T_{\mathscr{E},i_l}}(v_{i_l})} v_{i_s} v_g.$$

Then $\rho(H) > \rho(G)$ by Lemma 2.4. Denote by $T^H_{\mathscr{E},i_s}$ the nontrivial attaching tree to $\mathscr{E}$ rooted at v_{i_s} in H. Let H_1 be the graph obtained from H by transforming $T^H_{\mathscr{E},i_s}$ into a star with center v_{i_s}. Then $\rho(H_1) \geq \rho(H) \geq \rho(G)$ by Lemmas 2.4, 2.5 and $d(H_1) = d(G)$. Suppose $v_{i_s} \in V(P_f)$, and suppose $Z = (z_1, z_2, z_3, \ldots, z_{n-1}, z_n)^T$ is the Perron vector of H_1 and z_i corresponds to vertex v_i, $z_b = \max\{z_a, z_b\}$, $z_{i_s} = \max\{z_{i_s}, z_f\}$. Suppose $N_{P_1'}(v_a) = \{v_c\}$, $N_{P_2'}(v_f) = \{v_d\}$. Let $H_2 = H_1 - v_a v_c + v_b v_c - v_d v_f + v_d v_{i_s}$. Then $\rho(H_2) > \rho(H_1)$ by Lemmas 2.5. Denote by $C_{2,1}, C_{2,2}$ the two cycles which have common vertex v_b in H_2. If $L(C_{2,1}) \geq 5$ or $L(C_{2,2}) \geq 5$, We can get graph H_3 from H_2 by contracting an edge of an internal path with length $l \geq 2$ on $C_{2,1}$ or $C_{2,2}$ in H_2 . Denote by C_{1,H_3}, C_{2,H_3} the two cycles in H_3. Proceeding like this, we can get graph $\mathcal{H}$ such that the two cycles $C_{2,\mathcal{H}}, C_{2,\mathcal{H}}$ in $\mathcal{H}$ are both with length 4. Let $P_{d,H}$ be a diameter-path with length $d(\mathcal{H})$ in $\mathcal{H}$. We can obtain graph $\mathcal{H}_1$ from $\mathcal{H}$ by attaching a pendant path with length $d(G) - d(\mathcal{H})$ to one end vertex of $P_{d,H}$ and $n - (|V(\mathcal{H})| + d(G) - d(\mathcal{H}))$ pendant vertices to vertex v_{i_s}. By Lemmas 2.5, 2.4, then $\rho(\mathcal{H}_1) > \rho(G)$, $d(\mathcal{H}_1) = d(G)$. Note that $\mathcal{H}_1$ is bipartite. So $\lambda(\mathcal{H}_1) < \lambda(G)$, which contradicts $\lambda_n(G) = \lambda_B$.

In a same way, for the cases that $v_{i_s} \in V(P_3)$, or $v_{i_s} \in V(C_1)$, or $v_{i_s} \in V(C_2)$, or $v_{i_s} \in V(P_e)$, we can get the same conclusion as $v_{i_s} \in V(P_f)$.

Subcase 1.2 There exists no diameter-path such that both C_1, C_2 have common vertices with it.

Denote by P_d a diameter-path in G. Denote by P_{d,C_1} the path from C_1 to P_d, P_{d,C_2} the path from C_2 to P_d. Suppose $P_{d,C_2} \bigcap P_{d,C_1} = \phi$ (see Fig. 4.4), and suppose $P_{d,C_1} \bigcap C_1 = v_a, P_{d,C_1} \bigcap P_d = v_b$, $P_{d,C_2} \bigcap C_2 = v_c, P_{d,C_2} \bigcap P_d = v_f$. Suppose $Y = (y_1, y_2, y_3, \ldots, y_{n-1}, y_n)^T$ is the Perron vector of G and y_i corresponds to vertex v_i. Suppose $y_b \geq y_a$, $y_f \geq y_c$. Let

$$H = G - \sum_{v_g \in N_{C_1}(v_a)} v_a v_g + \sum_{v_g \in N_{C_1}(v_a)} v_b v_g - \sum_{v_g \in N_{C_2}(v_c)} v_c v_g + \sum_{v_g \in N_{C_2}(v_c)} v_f v_g.$$

Then $\rho(H) > \rho(G)$ by Lemma 2.4, and $d(H) = d(G)$. Now P_d is still a diameter-path in H. Denote by C_1' the cycle having common vertex v_b with P_d and C_2' the cycle having common vertex v_f with P_d in H. As Subcase 1.1, we can prove that there exists a bipartite bicyclic graph $\mathcal{H}$, denote by $\mathscr{D}'$ the union of the cycles in $\mathcal{H}$, such that $\rho(\mathcal{H}) > \rho(G)$, $d(\mathcal{H}) = d(G)$, $\mathscr{D}'$ consists of the two different 4-cycles, but $\lambda(\mathcal{H}) < \lambda(G)$.

Similarly, we can get the same conclusion for the cases that $y_b < y_a$, $y_f < y_c$; $y_b \geq y_a$, $y_f < y_c$; $y_b < y_a$, $y_f \geq y_c$. As the case that $P_{d,C_2} \bigcap P_{d,C_1} = \phi$, for the case that $P_{d,C_2} \bigcap P_{d,C_1} \neq \phi$, we can get the same conclusion.

Case 2 $C_1 \bigcap C_2 \neq \phi$.

As Case 1, we can prove that there exists a bipartite bicyclic graph $\mathcal{H}$, denote by $\mathscr{D}'$ the union of the cycles in $\mathcal{H}$, such that $\rho(\mathcal{H}) > \rho(G)$, $d(\mathcal{H}) = d(G)$, $\mathscr{D}'$ consists of the two different 4-cycles, but $\lambda(\mathcal{H}) < \lambda(G)$.

This completes the proof of this lemma. □

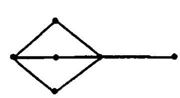
5 Extremal graphs with the minimal least eigenvalue in $\mathscr{B}(n, d; k, j)$

Theorem 5.1 *If $G \in \mathscr{B}(n, d; k, j)$ and $\lambda_n(G) = \lambda_{\mathbf{B}}$, then G satisfies that $j - 2 \le k \le j + 1$ and*

(1) if d is even, let $S_1 = B(n, d; s, s)$, $S_2 = B(n, d; s-1, s+1)$. Then

$$\begin{cases} G \cong S_1, & if\ \rho(S_1) \ge \dfrac{\sqrt{6(n-d-3)}}{2}; \\[2ex] G \cong S_2, & if\ \rho(S_1) < \dfrac{\sqrt{6(n-d-3)}}{2}; \end{cases}$$

(2) if d is odd, then $G \cong B(n, d; s, s+1)$.



H

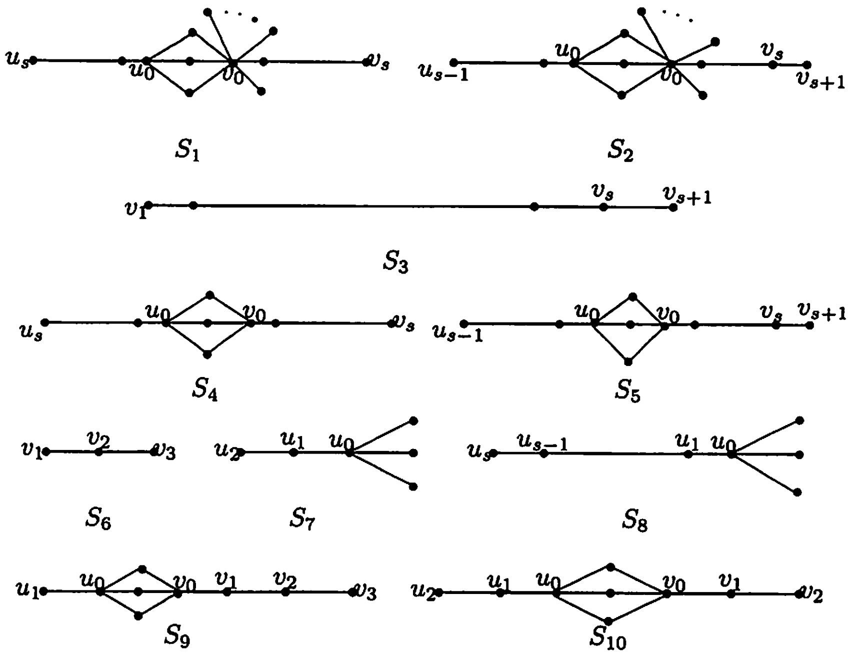


Fig. 5.1. S_1-S_{10}

Proof. Because $d \geq 3$, then $H \subseteq G$ (see Fig. 5.1). By computation, we get $\rho(H) \approx 2.5576$, so $\rho(G) \geq 2.5576$. Suppose $X = (x_{u_0}, x_{u_1}, x_{u_2}, \ldots, x_{w_1}, x_{w_2}, x_{w_3}, \ldots, x_{v_0}, x_{v_1}, x_{v_2}, \ldots)^T$ is the Perron vector of G, in which x_s corresponds to vertex s, $x_{v_0} \geq x_{u_0}$. By symmetry, then $x_{w_1} = x_{w_2} = x_{w_3}$. As Lemmas 3.1, 3.2, we get $x_{u_k} f_1 f_2 \cdots f_{k+1} f_{k+2} = 3x_{v_0} = 3f_j f_{j-1} \cdots f_1 x_{v_j}$, where f_i ($1 \leq i \leq \max\{k+2, j\}$) satisfies that $f_1 = \rho(G)$, $f_{i+1} = \rho(G) - \frac{1}{f_i}$, $x_{u_{k-i}} = f_i x_{u_{k-i+1}}$ ($1 \leq i \leq k$), $3x_{w_1} = f_{k+1} x_{u_0}$, $3x_{v_0} = f_{k+2} 3x_{w_1}$, $x_{v_{j-i}} = f_i x_{v_{j-i+1}}$ ($1 \leq i \leq j$), and f_i satisfies the (i), (ii), (iii) in Lemma 3.1.

If $k \geq j+2$, then

$$x_{u_{k-1}} f_2 \cdots f_j f_{j+1} f_{j+2} f_{j+3} \cdots f_{k+2} = 3x_{v_0} = 3f_j f_{j-1} \cdots f_1 x_{v_j}.$$

By Lemma 3.1, we get that $f_{j+1} f_{j+2} f_{j+3} \cdots f_{k+2} \geq 3\rho(G)$, then $x_{v_j} \geq x_{u_{k-1}}$. Let $G_1 = G - u_{k-1}u_k + u_k v_j$. By Lemma 2.5, then $\rho(G_1) > \rho(G)$. Note that both G_1, G are bipartite. So $\lambda_n(G_1) < \lambda_n(G)$, which contradicts that $\lambda_n(G) = \lambda_{\mathbf{B}}$. Hence $k \leq j+1$. If $k \leq j-3$, then $x_{u_k} f_1 f_2 \cdots f_{k+1} f_{k+2} = 3x_{v_0} = 3f_j f_{j-1} \cdots f_2 x_{v_{j-1}}$. By Lemma 3.1, we have $3f_j f_{j-1} \cdots f_{k+3} \geq \frac{3\rho}{2} > \rho(G)$. So $x_{u_k} > x_{v_{j-1}}$. Let $G_1 = G - v_j v_{j-1} + u_k v_j$.

By Lemma 2.5, then $\rho(G_1) > \rho(G)$. Note that both G_1, G are bipartite. So $\lambda_n(G_1) < \lambda_n(G)$, which contradicts that $\lambda_n(G) = \lambda_{\mathbb{B}}$. Hence $k \geq j-2$.

Note that $d = k+j+2$. If d is even, then $k+j$ is even. Note that $j-2 \leq k \leq j+1$. So there are only two possible cases for G, namely $j = k$ or $k = j-2$. Hence, for G, there are only two cases that $G \cong S_1$ or $G \cong S_2$ (S_1-S_{10} are as shown in Fig. 5.1). Let $r = n-d-3$. By Lemma 2.11,

$$P(S_1,\lambda) = \lambda^r P(S_4,\lambda) - r\lambda^{r-1}P(S_8,\lambda)P(S_3-v_{s+1},\lambda)$$

$$= \lambda^{r+1}P(S_5-v_{s+1},\lambda) - \lambda^r P(S_4-u_s-u_{s-1},\lambda)$$

$$-r\lambda^r P(S_8-u_s,\lambda)P(S_3-v_{s+1},\lambda) + r\lambda^{r-1}P(S_8-u_s-u_{s-1},\lambda)P(S_3-v_{s+1},\lambda),$$

$$P(S_2,\lambda) = \lambda^r P(S_5,\lambda) - r\lambda^{r-1}P(S_8-u_s,\lambda)P(S_3,\lambda)$$

$$= \lambda^{r+1}P(S_5-v_{s+1},\lambda) - \lambda^r P(S_4-v_s-u_s,\lambda) - r\lambda^r P(S_8-u_s,\lambda)P(S_3-v_{s+1},\lambda)$$

$$+r\lambda^{r-1}P(S_8-u_s,\lambda)P(S_3-v_{s+1}-v_s,\lambda).$$

So

$$P(S_2,\lambda) - P(S_1,\lambda) = \lambda^r[P(S_4-u_s-u_{s-1},\lambda) - P(S_4-v_s-u_s,\lambda)] +$$

$$r\lambda^{r-1}[P(S_8-u_s,\lambda)P(S_3-v_{s+1}-v_s,\lambda) - P(S_8-u_s-u_{s-1},\lambda)P(S_3-v_{s+1},\lambda)]$$

$$= \lambda^r[P(S_4-u_s-u_{s-1}-v_s-u_{s-2},\lambda) - P(S_4-v_s-u_s-v_{s-1}-u_{s-1},\lambda)]$$

$$+r\lambda^{r-1}[P(S_8-u_s-u_{s-1},\lambda)P(S_3-v_{s+1}-v_s-v_{s-1},\lambda) -$$

$$P(S_8-u_s-u_{s-1}-u_{s-2},\lambda)P(S_3-v_{s+1}-v_s,\lambda)] = \cdots$$

$$= \lambda^r[P(S_9,\lambda) - P(S_{10},\lambda)] + r\lambda^{r-1}[P(S_7,\lambda)P(S_6-v_3,\lambda)$$

$$-P(S_7-u_2,\lambda)P(S_6,\lambda)]$$

$$= \lambda^r[P(S_9-v_3-u_1,\lambda) - P(S_{10}-v_2-u_2,\lambda)] + r\lambda^{r-1}[3\lambda^3 P(S_6,\lambda)$$

$$-3\lambda^2(P(S_6-v_3,\lambda))^2]$$

$$= \lambda^r[P(S_7-u_2,\lambda) - P(S_{10}-u_2-u_1-v_1-v_2,\lambda)] - 3r\lambda^{r+1}$$

$$= 2\lambda^{r+3} - 3r\lambda^{r+1} = \lambda^{r+1}(2\lambda^2 - 3r).$$

Therefore, by Lemma 2.9, we have $\begin{cases} \rho(S_2) \leq \rho(S_1), & if\ \rho(S_1) \geq \dfrac{\sqrt{6r}}{2}; \\ \rho(S_2) > \rho(S_1), & if\ \rho(S_1) < \dfrac{\sqrt{6r}}{2}. \end{cases}$

Note that G is bipartite. Then $\lambda_n(G) = -\rho(G)$. So (1) is proved.

In a same way, (2) can be proved. □

6 Conjecture about the extremal graphs with the minimal least eigenvalue in $\mathscr{B}(n, d)$

By many computations and comparisons with computer, we find the trend that G is isomorphic to a $B(n, d; k, j)$ if $\lambda_n(G) = \lambda_B$ for a graph $G \in \mathscr{B}(n, d)$ $(n \geq d+3, d \geq 3)$.

Conjecture 6.1 *When $n \to \infty$, if $\lambda_n(G) = \lambda_B$ for a graph $G \in \mathscr{B}(n, d)$ $(n \geq d+3, d \geq 3)$, then $G \in \mathscr{B}(n, d; k, j)$ $(k+j \geq 1)$ and G satisfies the conclusions in Theorem 5.1.*

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