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On the spectral radius of bicyclic graphs with n vertices and diameter d ☆

Shu-Guang Guo

Department of Mathematics, Yancheng Teachers College, Yancheng 224002, Jiangsu, PR China

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Abstract

Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. In this paper we determine the graph with the largest spectral radius among all bicyclic graphs with n vertices and diameter d. As an application, we give first three graphs among all bicyclic graphs on n vertices, ordered according to their spectral radii in decreasing order.

AMS classification: 05C50

Keywords: Bicyclic graphs; Eigenvalues; Spectral radius; Diameter

1. Introduction

Let $G = (V(G), E(G))$ be a (simple) graph with n vertices, and let $A(G)$ be a (0, 1)-adjacency matrix of G. Since $A(G)$ is symmetric, its eigenvalues are real. Without loss of generality, we can write them as $\lambda_1(G) \geqslant \lambda_2(G) \geqslant \cdots \geqslant \lambda_n(G)$ and call them the eigenvalues of G. The characteristic polynomial of G is just $\det(\lambda I - A(G))$, and is denoted by $\phi(G; \lambda)$. The largest

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E-mail address: ychgsg@yahoo.com.cn

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eigenvalue $\lambda_1(G)$ is called the spectral radius of G, denoted by $\rho(G)$. If G is connected, then $A(G)$ is irreducible, and by the Perron–Frobenius theory of non-negative matrices, $\rho(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\rho(G)$. We shall refer to such an eigenvector as the Perron vector of G.

The investigation on the spectral radius of graphs is an important topic in the theory of graph spectra. Recently, the problem of finding all graphs with maximal or minimal spectral radius among a given class of graphs has been studied extensively. For related results, one may refer to [1–9,11–13,15–17] and the references therein.

Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. Chang et al. [3] determined graphs with the largest spectral radius among all the bicyclic graphs on n vertices with perfect matching. Yu and Tian [17] determined the graph with the largest spectral radius among all the bicyclic graphs on n vertices with a maximum matching of cardinality m. Guo et al. [7,13] determined the graph with the largest spectral radius among all the bicyclic graphs with n vertices and k pendant vertices. Simić [15] determined the bicyclic graphs on prescribed number of vertices with spectral radius minimal.

The diameter of a connected graph is the maximum distance between pairs of its vertices. Very recently, Guo et al. [9] determined the graphs with the largest and the second largest spectral radius among all trees with n vertices and diameter d. Guo and Shao [6] characterized the first $\lfloor \frac{d}{2} \rfloor + 1$ trees with n vertices and diameter d ordered according to their spectral radii. Guo [8] determined the graph with the largest spectral radius among all unicyclic graphs with n vertices and diameter d.

In this paper, we study the spectral radius of bicyclic graphs with n vertices and diameter d, and determine the graph with the largest spectral radius among all bicyclic graphs with n vertices and diameter d. As an application, we give first three graphs among all bicyclic graphs on n vertices, ordered according to their spectral radii in decreasing order.

2. Preliminaries

Denote by C_n and P_n the cycle and the path, respectively, each on n vertices. Let $G - uv$ denote the graph that arises from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph that arises from G by adding the edge $uv \notin E(G)$, where $u, v \in V(G)$. For $v \in V(G)$, $N(v)$ denotes the set of all neighbors of vertex v in G, and $d(v) = |N(v)|$ denotes the degree of vertex v in G. A pendant vertex of G is a vertex of degree 1. A pendant edge is an edge with which a pendant vertex is incident. For a real number x, we denote by $\lfloor x \rfloor$ the greatest integer $\leqslant x$, and by $\lceil x \rceil$ the least integer $\geqslant x$. We denote by $\mathscr{B}_{n,d}$ the set of all bicyclic graphs with n vertices and diameter d. Let C_p and C_q be two vertex-disjoint cycles. Suppose that a_1 is a vertex of C_p and a_l is a vertex of C_q. Joining a_1 and a_l by a path $a_1a_2 \cdots a_l$ of length $l-1$ results in a graph $B(p, l, q)$ (Fig. 1) to be called an ∞-graph, where $l \geqslant 1$ and $l = 1$ means identifying a_1 with a_l. Let P_{l+1}, P_{p+1} and P_{q+1} be three vertex-disjoint paths, where $l, p, q \geqslant 1$ and at most one of them is 1. Identifying the three initial vertices and terminal vertices of them respectively results in a graph $P(l, p, q)$ (Fig. 2) to be called a θ-graph. Obviously $\mathscr{B}_{n,d}$ consists of two types of graphs: one type, denoted by $\mathscr{B}^{\infty}_{n,d}$, are those graphs each of which is an ∞-graph with trees attached; the other type, denoted by $\mathscr{B}^{\theta}_{n,d}$, are those graphs each of which is a θ-graph with trees attached. Then $\mathscr{B}_{n,d} = \mathscr{B}^{\infty}_{n,d} \cup \mathscr{B}^{\theta}_{n,d}$.

In order to complete the proof of our main result, we need the following lemmas.

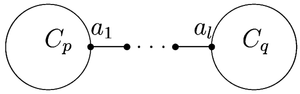

Fig. 1. $B(p, l, q)$.

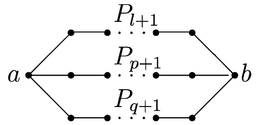

Fig. 2. $P(l, p, q)$.

Lemma 1 [16,12]. *Let G be a connected graph and let $\rho(G)$ be the spectral radius of $A(G)$. Let u, v be two vertices of G. Suppose $v_1, v_2, \ldots, v_s \in N(v)\backslash N(u)(1 \leqslant s \leqslant d(v))$ and $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ is the Perron vector of $A(G)$, where x_i corresponds to the vertex $v_i (1 \leqslant i \leqslant n)$. Let G^* be the graph obtained from G by deleting the edges vv_i and adding the edges uv_i $(1 \leqslant i \leqslant s)$. If $x_u \geqslant x_v$, then $\rho(G) < \rho(G^*)$.*

By Lemma 1, we obtain easily Lemmas 2 and 3 which may be regard as immediate consequences of Lemma 1. Since their proofs are similar, we only give the proof of Lemma 2.

Lemma 2. *Let G be a connected graph and let $e = uv$ be a non-pendant edge of G with $N(u) \cap N(v) = \emptyset$. Let G^* be the graph obtained from G by deleting the edge uv, identifying u with v, and adding a pendant edge to $u(= v)$. Then $\rho(G) < \rho(G^*)$.*

Proof. We use x_u and x_v to denote the components of the Perron vector of G corresponding to u and v respectively. Suppose that $N(u) = \{v, v_1, \ldots, v_s\}$ and $N(v) = \{u, u_1, \ldots, u_t\}$. Since $e = uv$ is a non-pendant edge of G, it follows that $s, t \geqslant 1$. If $x_u \geqslant x_v$, let

$$G' = G - \{vu_1, \ldots, vu_t\} + \{uu_1, \ldots, uu_t\}.$$

If $x_u < x_v$, let

$$G'' = G - \{uv_1, \ldots, uv_s\} + \{vv_1, \ldots, vv_s\}.$$

Obviously, $G^* = G' = G''$. By Lemma 1, we have $\rho(G) < \rho(G^*)$.

This completes the proof. $\square$

Lemma 3. *Let G, G', G'' be three connected graphs disjoint in pairs. Suppose that u, v are two vertices of G, u' is a vertex of G' and u'' is a vertex of G''. Let G_1 be the graph obtained from G, G', G'' by identifying, respectively, u with u' and v with u''. Let G_2 be the graph obtained from G, G', G'' by identifying vertices u, u', u''. Let G_3 be the graph obtained from G, G', G'' by identifying vertices v, u', u''. Then either $\rho(G_1) < \rho(G_2)$ or $\rho(G_1) < \rho(G_3)$.*

Let G be a connected graph, and $uv \in E(G)$. The graph $G_{u,v}$ is obtained from G by subdividing the edge uv, i.e., adding a new vertex w and edges wu, wv in $G - uv$. Hoffman and Smith define an internal path of G as a walk $v_0 v_1 \cdots v_s$ $(s \geqslant 1)$ such that the vertices $v_0, v_1, \ldots, v_s$ are distinct, $d(v_0) > 2$, $d(v_s) > 2$, and $d(v_i) = 2$, whenever $0 < i < s$ (note, s is the length of the path). An internal path is closed if $v_0 = v_s$. They proved the following result.

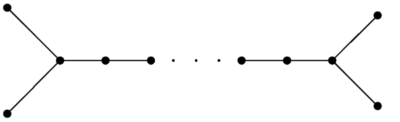

Fig. 3. W_n.

Lemma 4 [10]. *Let uv be an edge of the connected graph G on n vertices.*

(i) *If uv does not belong to an internal path of G, and $G \neq C_n$, then $\rho(G_{u,v}) > \rho(G)$.*
(ii) *If uv belongs to an internal path of G, and $G \neq W_n$, where W_n is shown in Fig. 3, then $\rho(G_{u,v}) < \rho(G)$.*

Lemma 5 [4]. *The characteristic polynomial of P_n satisfies the expression*

$$\phi(P_n; \lambda) = \frac{1}{\sqrt{\lambda^2 - 4}}\left(x_1^{n+1} - x_2^{n+1}\right),$$

where

$$x_1 = \frac{1}{2}\left(\lambda + \sqrt{\lambda^2 - 4}\right) \quad \text{and} \quad x_2 = \frac{1}{2}\left(\lambda - \sqrt{\lambda^2 - 4}\right)$$

are the roots of the equation $x^2 - \lambda x + 1 = 0$.

Lemma 6 [11,6]. *Let u and v be two adjacent vertices of the connected graph G with $d(u) > 1$ and $d(v) > 1$. For non-negative integers k and l, let $G(k, l)$ denote the graph obtained from G by adding pendant paths of length k at u and length l at v. If $k \geqslant l \geqslant 1$, then $\rho(G(k, l)) > \rho(G(k + 1, l - 1))$.*

Lemma 7 [11,6]. *Let G be a connected graph, and G' be a proper spanning subgraph of G. Then $\rho(G) > \rho(G')$ and $\phi(G'; \lambda) > \phi(G; \lambda)$ for all $\lambda \geqslant \rho(G)$.*

The following two results are often used to calculate the characteristic polynomials of graphs.

Lemma 8 [4,14]. *Let $e = uv$ be an edge of G, and $C(e)$ be the set of all cycles containing e. The characteristic polynomial of G satisfies*

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

Lemma 9 [4,14]. *Let u be a vertex of G, and let $C(u)$ be the set of all cycles containing u. The characteristic polynomial of G satisfies*

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

As usual, we assume that the characteristic polynomial of an empty graph is equal to 1. Let $d \geqslant 2$ and $2 \leqslant i \leqslant d$. We denote by $P_{d+1}^*(i)$ the graph obtained from a path $P_{d+1} : v_1 v_2 \cdots v_{d+1}$ and isolated vertices $v_{d+2}, \ldots, v_n$ by adding edges $v_i v_{d+2}, \ldots, v_i v_n$. Denote by $P_{d+1}^{\nabla\nabla}(i)$ the graph obtained from $P_{d+1}^*(i)$ by adding edges $v_{d+2} v_{d+3}$ and $v_{d+4} v_{d+5}$, by $P_{d+1}^{\Delta\nabla}(i)$ the graph obtained from $P^*_{d+1}(i)$ by adding edges $v_{i-1}v_{d+2}$ and $v_{d+3}v_{d+4}$, by $P^{\Delta\Delta}_{d+1}(i)$ the graph obtained from $P^*_{d+1}(i)$ by adding edges $v_{i-1}v_{d+2}$ and $v_{i+1}v_{d+3}$, and by $P^{+}_{d+1}(i)$ the graph (Fig. 7) obtained from $P^*_{d+1}(i)$ by adding edges $v_{i-1}v_n$ and $v_{i+1}v_n$.

Lemma 10. *Let $d \geqslant 3$. Then $\rho(P^{\Delta\Delta}_{d+1}(i)) \geqslant \rho(P^{\Delta\nabla}_{d+1}(i)) \geqslant \rho(P^{\nabla\nabla}_{d+1}(i))$ with the first equality if and only if $i = d$ and the second equality if and only if $i = 2$.*

Proof. Clearly, $P^{\Delta\Delta}_{d+1}(d) = P^{\Delta\nabla}_{d+1}(d)$, $P^{\Delta\nabla}_{d+1}(2) = P^{\nabla\nabla}_{d+1}(2)$. Denote by $P^{\Delta}_{d+1}(i)$ the graph obtained from $P^*_{d+1}(i)$ by adding edge $v_{i-1}v_{d+2}$.

For $2 \leqslant i < d$, applying Lemma 8 to edge $v_{i+1}v_{d+3}$ of $P^{\Delta\Delta}_{d+1}(i)$ and edge $v_{d+3}v_{d+4}$ of $P^{\Delta\nabla}_{d+1}(i)$ respectively, we have

$$\begin{aligned}\phi(P^{\Delta\Delta}_{d+1}(i);\lambda) &= \phi(P^{\Delta}_{d+1}(i);\lambda) - \phi(P^{\Delta\Delta}_{d+1}(i) - v_{i+1} - v_{d+3};\lambda)\\ &\quad - 2\lambda^{n-d-3}\phi(P_i;\lambda)\phi(P_{d-i};\lambda),\\ \phi(P^{\Delta\nabla}_{d+1}(i);\lambda) &= \phi(P^{\Delta}_{d+1}(i);\lambda) - \phi(P^{\Delta\nabla}_{d+1}(i) - v_{d+3} - v_{d+4};\lambda)\\ &\quad - 2\lambda^{n-d-4}\phi(P_i;\lambda)\phi(P_{d-i+1};\lambda).\end{aligned}$$

Note that $P^{\Delta\Delta}_{d+1}(i) - v_{i+1} - v_{d+3}$ is a proper spanning subgraph of $P^{\Delta\nabla}_{d+1}(i) - v_{d+3} - v_{d+4}$, and $K_1 \cup P_{d-i}$ is a proper spanning subgraph of P_{d-i+1}. By Lemma 7 we have

$$\begin{aligned}&\phi(P^{\Delta\nabla}_{d+1}(i);\lambda) - \phi(P^{\Delta\Delta}_{d+1}(i);\lambda)\\ &\quad = \phi(P^{\Delta\Delta}_{d+1}(i) - v_{i+1} - v_{d+3};\lambda) - \phi(P^{\Delta\nabla}_{d+1}(i) - v_{d+3} - v_{d+4};\lambda)\\ &\qquad + 2\lambda^{n-d-4}\phi(P_i;\lambda)[\lambda\phi(P_{d-i};\lambda) - \phi(P_{d-i+1};\lambda)] > 0\end{aligned}$$

for all $\lambda \geqslant \rho(P^{\Delta\nabla}_{d+1}(i))$. Thus $\rho(P^{\Delta\Delta}_{d+1}(i)) > \rho(P^{\Delta\nabla}_{d+1}(i))$.

For $3 \leqslant i \leqslant d$, applying Lemma 8 to edge $v_{i-1}v_{d+2}$ of $P^{\Delta\nabla}_{d+1}(i)$ and edge $v_{d+2}v_{d+3}$ of $P^{\nabla\nabla}_{d+1}(i)$ respectively, by similar reasoning as above, we have

$$\begin{aligned}&\phi(P^{\nabla\nabla}_{d+1}(i);\lambda) - \phi(P^{\Delta\nabla}_{d+1}(i);\lambda)\\ &\quad = \phi(P^{\Delta\nabla}_{d+1}(i) - v_{i-1} - v_{d+2};\lambda) - \phi(P^{\nabla\nabla}_{d+1}(i) - v_{d+2} - v_{d+3};\lambda)\\ &\qquad + 2\lambda^{n-d-5}(\lambda^2 - 1)\phi(P_{d-i+1};\lambda)[\lambda\phi(P_{i-2};\lambda) - \phi(P_{i-1};\lambda)] > 0\end{aligned}$$

for all $\lambda \geqslant \rho(P^{\nabla\nabla}_{d+1}(i))$. Thus $\rho(P^{\Delta\nabla}_{d+1}(i)) > \rho(P^{\nabla\nabla}_{d+1}(i))$.

This completes the proof. $\square$

Lemma 11. *Let $G_1(i)$, $G_2(i)$ and $P^{\theta}_{d+1}(i)$, shown in Figs. 4–6, belong to $\mathscr{B}_{n,d}$. Then*

$$\rho(G_1(i)) < \rho(G_2(i)) \leqslant \rho(P^{\theta}_{d+1}(i)),$$

and the equality holds if and only if $i = 2$.

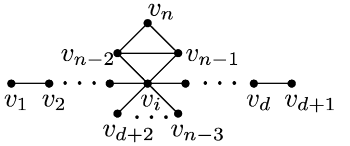

Fig. 4. $G_1(i)$.

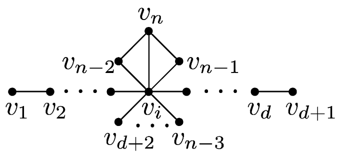

Fig. 5. $G_2(i)$.

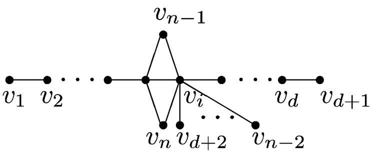

Fig. 6. $P^{\theta}_{d+1}(i)$.

Proof. Applying Lemma 8 to edge $v_{n-2}v_{n-1}$ of $G_1(i)$ and edge v_iv_n of $G_2(i)$ respectively, we have

$$\begin{aligned}\phi(G_1(i);\lambda) &= \phi(G_1(i)-v_{n-2}v_{n-1};\lambda)-\phi(G_1(i)-v_{n-2}-v_{n-1};\lambda)\\ &\quad -2\phi(G_1(i)-v_{n-2}-v_{n-1}-v_i;\lambda)-2\phi(G_1(i)-v_{n-2}-v_{n-1}-v_n;\lambda),\\ \phi(G_2(i);\lambda) &= \phi(G_2(i)-v_iv_n;\lambda)-\phi(G_2(i)-v_i-v_n;\lambda)\\ &\quad -2\phi(G_2(i)-v_i-v_n-v_{n-2};\lambda)-2\phi(G_2(i)-v_i-v_n-v_{n-1};\lambda).\end{aligned}$$

Note that $G_1(i)-v_{n-2}v_{n-1}=G_2(i)-v_iv_n$ and

$$G_1(i)-v_{n-2}-v_{n-1}-v_i=G_2(i)-v_i-v_n-v_{n-2}.$$

Also note that $G_2(i)-v_i-v_n, G_2(i)-v_i-v_n-v_{n-1}$ are proper spanning subgraphs of $G_1(i)-v_{n-2}-v_{n-1}$, $G_1(i)-v_{n-2}-v_{n-1}-v_n$ respectively. By Lemma 7 we have

$$\phi(G_2(i)-v_i-v_n;\lambda)>\phi(G_1(i)-v_{n-2}-v_{n-1};\lambda)$$

for all $\lambda \geqslant \rho(G_1(i)-v_{n-2}-v_{n-1})$ and

$$\phi(G_2(i)-v_i-v_n-v_{n-1};\lambda)>\phi(G_1(i)-v_{n-2}-v_{n-1}-v_n;\lambda)$$

for all $\lambda \geqslant \rho(G_1(i)-v_{n-2}-v_{n-1}-v_n)$. These imply that $\phi(G_1(i);\lambda)>\phi(G_2(i);\lambda)$ for all $\lambda \geqslant \rho(G_1(i))$. Thus $\rho(G_1(i))<\rho(G_2(i))$.

Clearly, $G_2(2)=P^{\theta}_{d+1}(2)$. For $3 \leqslant i \leqslant d$, applying Lemma 8 to edge $v_{n-2}v_n$ of $G_2(i)$ and edge $v_{i-1}v_n$ of $P^{\theta}_{d+1}(i)$ respectively, we have

$$\begin{aligned}\phi(G_2(i);\lambda) &= \phi(G_2(i)-v_{n-2}v_n;\lambda)-\phi(G_2(i)-v_{n-2}-v_n;\lambda)\\ &\quad -2\lambda^{n-d-3}\phi(P_{i-1};\lambda)\phi(P_{d-i+1};\lambda)-2\lambda^{n-d-4}\phi(P_{i-1};\lambda)\phi(P_{d-i+1};\lambda),\\ \phi(P^{\theta}_{d+1}(i);\lambda) &= \phi(P^{\theta}_{d+1}(i)-v_{i-1}v_n;\lambda)-\phi(P^{\theta}_{d+1}(i)-v_{i-1}-v_n;\lambda)\\ &\quad -2\lambda^{n-d-2}\phi(P_{i-2};\lambda)\phi(P_{d-i+1};\lambda)-2\lambda^{n-d-3}\phi(P_{i-2};\lambda)\phi(P_{d-i+1};\lambda).\end{aligned}$$

Applying Lemma 8 to edge $v_{n-1}v_n$ of $G_2(i)-v_{n-2}v_n$ and edge $v_{i-1}v_{n-1}$ of $P^{\theta}_{d+1}(i)-v_{i-1}v_n$ respectively, by similar arguments to the proof of Lemma 10 we can show

$$\phi(G_2(i)-v_{n-2}v_n;\lambda)>\phi(P^{\theta}_{d+1}(i)-v_{i-1}v_n;\lambda)$$

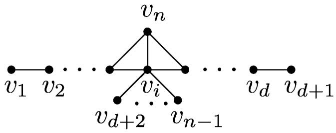

Fig. 7. $P^+_{d+1}(i)$.

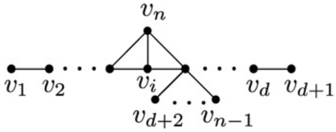

Fig. 8. $G_3(i)$.

for all $\lambda \geqslant \rho(G_2(i))$. Note that $P^\theta_{d+1}(i) - v_{i-1} - v_n$ is proper spanning subgraph of $G_2(i) - v_{n-2} - v_n$. By Lemma 7 we have

$$\phi(P^\theta_{d+1}(i) - v_{i-1} - v_n; \lambda) > \phi(G_2(i) - v_{n-2} - v_n; \lambda)$$

for all $\lambda \geqslant \rho(G_2(i) - v_{n-2} - v_n)$. Moreover, since $\lambda\phi(P_{i-2}; \lambda) - \phi(P_{i-1}; \lambda) = \phi(P_{i-3}; \lambda) > 0$ for all $\lambda \geqslant \rho(G_2(i)) > 2$, it follows that

$$2\lambda^{n-d-2}\phi(P_{i-2}; \lambda)\phi(P_{d-i+1}; \lambda) > 2\lambda^{n-d-3}\phi(P_{i-1}; \lambda)\phi(P_{d-i+1}; \lambda)$$

and

$$2\lambda^{n-d-3}\phi(P_{i-2}; \lambda)\phi(P_{d-i+1}; \lambda) > 2\lambda^{n-d-4}\phi(P_{i-1}; \lambda)\phi(P_{d-i+1}; \lambda)$$

for all $\lambda \geqslant \rho(G_2(i))$. These imply that

$$\phi(G_2(i); \lambda) > \phi(P^\theta_{d+1}(i); \lambda)$$

for all $\lambda \geqslant \rho(G_2(i))$, Thus $\rho(G_2(i)) < \rho(P^\theta_{d+1}(i))$.

This completes the proof. □

Lemma 12. *If $n \geqslant d + 4$ and $d \geqslant 4$ is even, then $\rho\left(P^\theta_{d+1}\left(\frac{d+4}{2}\right)\right) < \rho\left(P^\theta_{d+1}\left(\frac{d+2}{2}\right)\right)$.*

Proof. Let $a = \frac{d-2}{2}$. Denote $P^\theta_{d+1}\left(\frac{d+4}{2}\right)$ by $G(a + 1, a)$, and $P^\theta_{d+1}\left(\frac{d+2}{2}\right)$ by $G(a, a + 1)$. Applying Lemma 9 several times we have

$$\begin{aligned}
&\phi\left(P^\theta_{d+1}\left(\frac{d+4}{2}\right); \lambda\right) - \phi\left(P^\theta_{d+1}\left(\frac{d+2}{2}\right); \lambda\right)\\
&\quad = \phi(G(a + 1, a); \lambda) - \phi(G(a, a + 1); \lambda)\\
&\quad = \lambda\phi(G(a, a); \lambda) - \phi(G(a - 1, a); \lambda) - \lambda\phi(G(a, a); \lambda) + \phi(G(a, a - 1); \lambda)\\
&\quad = \phi(G(a, a - 1); \lambda) - \phi(G(a - 1, a); \lambda) = \cdots = \phi(G(1, 0); \lambda) - \phi(G(0, 1); \lambda)\\
&\quad = \lambda\phi(G(0, 0); \lambda) - \phi(K_{1,n-d-1}; \lambda) - \lambda\phi(G(0, 0); \lambda) + \lambda^{n-d-3}\phi(K_{1,2}; \lambda) > 0
\end{aligned}$$

for all $\lambda \geqslant \rho\left(P^\theta_{d+1}\left(\frac{d+4}{2}\right)\right)$. Thus $\rho\left(P^\theta_{d+1}\left(\frac{d+4}{2}\right)\right) < \rho\left(P^\theta_{d+1}\left(\frac{d+2}{2}\right)\right)$.

This completes the proof. □

Lemma 13. *If $n \geqslant d + 3$ and $2 \leqslant i - 2 \leqslant d - i + 1$, then $\rho\left(P^\theta_{d+1}(i)\right) < \rho\left(P^+_{d+1}(i)\right)$.*

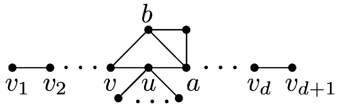

Fig. 9. G^{+}.

Proof. Applying Lemma 8 to edge $v_{i-1}v_n$ of $P_{d+1}^{\theta}(i)$ and edge v_nv_{i+1} of $P_{d+1}^{+}(i)$, and then applying Lemma 9 to the highest degree vertices of $P_{d+1}^{\theta}(i) - v_{i-1} - v_n$ and $P_{d+1}^{+}(i) - v_n - v_{i+1}$ respectively, we have

$$\begin{aligned}&\phi\big(P_{d+1}^{\theta}(i);\lambda\big) - \phi\big(P_{d+1}^{+}(i);\lambda\big)\\&\quad = 2\lambda^{n-d-3}\phi(P_{i-2};\lambda)\phi(P_{d-i-1};\lambda) + \lambda^{n-d-3}[\lambda^2 + 2\lambda - (n-d-2)]\\&\qquad \times [\phi(P_{i-1};\lambda)\phi(P_{d-i};\lambda) - \phi(P_{i-2};\lambda)\phi(P_{d-i+1};\lambda)].\end{aligned}$$

Case 1. $i - 2 < d - i + 1$. Applying Lemma 9 several times, we have further

$$\begin{aligned}&\phi(P_{i-1};\lambda)\phi(P_{d-i};\lambda) - \phi(P_{i-2};\lambda)\phi(P_{d-i+1};\lambda)\\&\quad = [\lambda\phi(P_{i-2};\lambda) - \phi(P_{i-3};\lambda)]\phi(P_{d-i};\lambda) - \phi(P_{i-2};\lambda)[\lambda\phi(P_{d-i};\lambda) - \phi(P_{d-i-1};\lambda)]\\&\quad = \phi(P_{i-2};\lambda)\phi(P_{d-i-1};\lambda) - \phi(P_{i-3};\lambda)\phi(P_{d-i};\lambda)\\&\quad = \cdots = \phi(P_2;\lambda)\phi(P_{d-2i+3};\lambda) - \lambda\phi(P_{d-2i+4};\lambda)\\&\quad = \lambda\phi(P_{d-2i+2};\lambda) - \phi(P_{d-2i+3};\lambda) = \phi(P_{d-2i+1};\lambda) \geqslant 0\end{aligned}$$

for all $\lambda \geqslant \rho(P_{d-2i+3})$. It follows that

$$\phi\big(P_{d+1}^{\theta}(i);\lambda\big) - \phi\big(P_{d+1}^{+}(i);\lambda\big) > 0$$

for all $\lambda \geqslant \rho(P_{d+1}^{\theta}(i)) > \sqrt{n-d+1}$. Thus $\rho(P_{d+1}^{\theta}(i)) < \rho\left(P_{d+1}^{+}(i)\right)$.

Case 2. $i - 2 = d - i + 1$. Then $d - 2i + 3 = 0$. Similarly to Case 1, we have

$$\phi(P_{i-1};\lambda)\phi(P_{d-i};\lambda) - \phi(P_{i-2};\lambda)\phi(P_{d-i+1};\lambda) = \phi(P_2;\lambda) - \lambda^2 = -1.$$

From Lemma 5 we can easily get that $\phi(P_n;\lambda)$ is equal to $\frac{\sinh((n+1)\theta)}{\sinh(\theta)}$ after putting $\lambda = 2\cosh(\theta)$. Making use of this fact, we easily get that $\phi(P_{i-2};\lambda)\phi(P_{d-i-1};\lambda) \geqslant \lambda^2$, for $\lambda \geqslant 2$ and $d - i + 1 \geqslant 3$ (follows from the fact that $\sinh(2x) = 2\sinh(x)\cosh(x)$ and that cosh and sinh are increasing functions in the interval $[0, \infty)$). Combining the above arguments, in this case we have

$$\begin{aligned}&\phi\big(P_{d+1}^{\theta}(i);\lambda\big) - \phi\big(P_{d+1}^{+}(i);\lambda\big)\\&\quad = \lambda^{n-d-3}[2\phi(P_{i-2};\lambda)\phi(P_{d-i-1};\lambda) - \lambda^2 - 2\lambda + n - d - 2]\\&\quad \geqslant \lambda^{n-d-3}[2\lambda^2 - \lambda^2 - 2\lambda + n - d - 2] = \lambda^{n-d-3}(\lambda^2 - 2\lambda + n - d - 2) > 0\end{aligned}$$

for all $\lambda \geqslant \rho(P_{d+1}^{\theta}(i)) > \sqrt{n-d+1} \geqslant 2$. Thus $\rho(P_{d+1}^{\theta}(i)) < \rho\left(P_{d+1}^{+}(i)\right)$.

This completes the proof. □

Lemma 14. *Let $d \geqslant 3$ and $n \geqslant d + 3$. Then $\rho(G_3(i)) < \rho\left(P_{d+1}^{+}(i)\right)$.*

Proof. Let $a = i - 2$, $b = d - i$ and $G_0(i) = G_3(i) - \{v_{d+2}, \ldots, v_{n-1}\}$. Applying Lemma 9 to vertices $v_{d+2}, \ldots, v_{n-1}$ of $G_3(i)$ and to vertices $v_{d+2}, \ldots, v_{n-1}$ of $P_{d+1}^{+}(i)$ respectively, we have

$$\phi(G_3(i);\lambda) = \lambda^{n-d-2}\phi(G_0(i);\lambda) - (n-d-2)\lambda^{n-d-3}\phi(P_b;\lambda)\phi(\Delta - P_a;\lambda),$$
$$\phi\big(P^+_{d+1}(i);\lambda\big) = \lambda^{n-d-2}\phi(G_0(i);\lambda) - (n-d-2)\lambda^{n-d-3}\phi(P_{d+1};\lambda),$$

where $\Delta - P_a$ is the graph obtained from a cycle $C_3 : u_1u_2u_3$ and a path P_a by joining u_3 and an end vertex of P_a. Applying Lemma 9 to v_{a+3} of P_{d+1} and u_1 of $\Delta - P_a$ respectively, we have

$$\begin{aligned}
&\phi(G_3(i);\lambda) - \phi\big(P^+_{d+1}(i);\lambda\big)\\
&\quad = (n-d-2)\lambda^{n-d-3}[\phi(P_{d+1};\lambda) - \phi(P_b;\lambda)\phi(\Delta - P_a;\lambda)]\\
&\quad = (n-d-2)\lambda^{n-d-3}[(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda) - \phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda)].
\end{aligned}$$

From this we can see that it is sufficient to show for all $\lambda \geqslant \rho(G_3(i))$

$$(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda) - \phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda) > 0.$$

By Lemma 5, we have $x_1 + x_2 = \lambda$, $x_1x_2 = 1$ and

$$\begin{aligned}
&(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda) - \phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda)\\
&\quad = \frac{1}{\lambda^2-4}\big[\big(x_1+x_2+2\big)\big(x_1^{a+1} - x_2^{a+1}\big)\big(x_1^{b+1} - x_2^{b+1}\big) - \big(x_1^{a+3} - x_2^{a+3}\big)\big(x_1^{b} - x_2^{b}\big)\big]\\
&\quad = \frac{1}{\lambda^2-4}\big[2x_1^d + 2x_2^d + x_1^{d-1} + x_2^{d-1} + x_1^{a+3}x_2^b + x_1^bx_2^{a+3} - x_1^{a+2}x_2^{b+1} - x_1^{b+1}x_2^{a+2}\\
&\qquad - x_1^{a+1}x_2^{b+2} - x_1^{b+2}x_2^{a+1} - 2x_1^{a+1}x_2^{b+1} - 2x_1^{b+1}x_2^{a+1}\big].
\end{aligned}$$

Since $\rho(G_3(i)) > \sqrt{n-d+1}$, it follows that $x_1 > 1$ and $x_2 > 0$ when $\lambda \geqslant \rho(G_3(i))$. Let $r > 1$. It is easy to see that function $f(x) = r^x + r^{-x}$ is increasing strictly on interval $[0, +\infty)$. We consider the following two cases.

Case 1. $a \geqslant b-1$. Since $a+b = d-2$, it follows that $d-1 \geqslant a-b+1$. For all $\lambda \geqslant \rho(G_3(i))$, by $x_1x_2 = 1$ we have further

$$\begin{aligned}
&(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda) - \phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda)\\
&\quad = \frac{1}{\lambda^2-4}\big[2x_1^d + 2x_2^d + x_1^{d-1} + x_2^{d-1} + x_1^{a-b+3} + x_2^{a-b+3}\\
&\qquad - x_1^{a-b+1} - x_2^{a-b+1} - x_1^{a-b-1} - x_2^{a-b-1} - 2x_1^{a-b} - 2x_2^{a-b}\big]\\
&\quad = \frac{1}{\lambda^2-4}\big[2\big(x_1^d + x_1^{-d}\big) - 2\big(x_1^{a-b} + x_1^{-(a-b)}\big) + \big(x_1^{d-1} + x_1^{-(d-1)}\big)\\
&\qquad - \big(x_1^{a-b+1} + x_1^{-(a-b+1)}\big) + \big(x_1^{a-b+3} + x_1^{-(a-b+3)}\big) - \big(x_1^{a-b-1} + x_1^{-(a-b-1)}\big)\big] > 0.
\end{aligned}$$

Case 2. $a \leqslant b-2$. By $x_1x_2 = 1$ we have further

$$\begin{aligned}
&(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda) - \phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda)\\
&\quad = \frac{1}{\lambda^2-4}\big[2x_1^d + 2x_2^d + x_1^{d-1} + x_2^{d-1} + x_2^{b-a-3} - x_2^{b-a-1} + x_1^{b-a-3} - x_1^{b-a-1}\\
&\qquad - x_2^{b-a+1} - x_1^{b-a+1} - 2x_2^{b-a} - 2x_1^{b-a}\big]\\
&\quad = \frac{1}{\lambda^2-4}\big[2\big[\big(x_1^d + x_1^{-d}\big) - \big(x_1^{b-a} + x_1^{-(b-a)}\big)\big] - \big[\big(x_1^{b-a+1} + x_1^{-(b-a+1)}\big)\\
&\qquad - \big(x_1^{b-a-3} + x_1^{-(b-a-3)}\big)\big] + \big[\big(x_1^{d-1} + x_1^{-(d-1)}\big) - \big(x_1^{b-a-1} + x_1^{-(b-a-1)}\big)\big]\big].
\end{aligned}$$

By $a+b=d-2$, we have $d-(b-a)=2a+2\geqslant 2$. For $r>1$, since $f''(x)=(\ln r)^2(r^x+r^{-x})>0$ for all x in $[0,+\infty)$, it follows that $f(x)$ is concave up on $(0,+\infty)$. Therefore

$$f(d)-f(b-a)>f(b-a+1)-f(b-a-1),$$
$$f(d)-f(b-a)>f(b-a-1)-f(b-a-3)$$

and so

$$2[f(d)-f(b-a)]>f(b-a+1)-f(b-a-3).$$

This implies that

$$2\left[\left(x_1^d+x_1^{-d}\right)-\left(x_1^{b-a}+x_1^{-(b-a)}\right)\right]>\left(x_1^{b-a+1}+x_1^{-(b-a+1)}\right)-\left(x_1^{b-a-3}+x_1^{-(b-a-3)}\right)$$

for $\lambda\geqslant\rho(G_3(i))$. Hence, for all $\lambda\geqslant\rho(G_3(i))$, we have

$$(\lambda+2)\phi(P_a;\lambda)\phi(P_b;\lambda)-\phi(P_{a+2};\lambda)\phi(P_{b-1};\lambda)>0.$$

Combining Cases 1 and 2, the proof follows. □

Lemma 15. *Let $i-2\geqslant d-i+2$. Then $\rho\left(P_{d+1}^+(i)\right)<\rho\left(P_{d+1}^+(i-1)\right)$.*

Proof. Let $a=i-2$ and $b=d-i$. Denote $P_{d+1}^+(i)$ by $G(a,b)$. Similarly, denote $P_{d+1}^+(i-1)$ by $G(a-1,b+1)$. Applying Lemma 9 several times we have

$$\begin{aligned}
&\phi\left(P_{d+1}^+(i);\lambda\right)-\phi\left(P_{d+1}^+(i-1);\lambda\right)\\
&\quad=\phi(G(a,b);\lambda)-\phi(G(a-1,b+1);\lambda)\\
&\quad=\lambda\phi(G(a-1,b);\lambda)-\phi(G(a-2,b);\lambda)-\lambda\phi(G(a-1,b);\lambda)\\
&\qquad+\phi(G(a-1,b-1);\lambda)\\
&\quad=\phi(G(a-1,b-1);\lambda)-\phi(G(a-2,b);\lambda)\\
&\quad=\cdots=\phi(G(a-b,0);\lambda)-\phi(G(a-b-1,1);\lambda)\\
&\quad=\lambda^{n-d-2}(\lambda+1)^2\phi(P_{a-b-2};\lambda)>0
\end{aligned}$$

for all $\lambda\geqslant\rho(P_{d+1}^+(i))$. Thus $\rho\left(P_{d+1}^+(i)\right)<\rho(P_{d+1}^+(i-1))$.

This completes the proof. □

3. Main results

Theorem 1. *Let $n\geqslant d+4$ and $G\in\mathscr{B}_{n,d}$. If $d\geqslant 4$, then*

$$\rho(G)\leqslant\rho\left(P_{d+1}^+\left(\left\lfloor\frac{d+2}{2}\right\rfloor\right)\right)$$

with equality if and only if $G=P_{d+1}^+\left(\left\lfloor\frac{d+2}{2}\right\rfloor\right)$; if $d=3$, then $\rho(G)\leqslant\rho(P_4^\theta(3))$ with equality if and only if $G=P_4^\theta(3)$.

Proof. Choose $G\in\mathscr{B}_{n,d}$ such that the spectral radius of G is as large as possible. Denote the vertex set of G by $\{v_1,v_2,\ldots,v_n\}$ and the Perron vector of G by $\mathbf{x}=(x_1,x_2,\ldots,x_n)$, where x_i corresponds to the vertex v_i $(1\leqslant i\leqslant n)$. We first prove the following fact. □

Fact 1. There is not an internal path of G with length greater than 1 unless the path lies on a cycle of length 3.

Proof. Assume, on the contrary, that $P_{k+1} : v_i v_{i+1} \cdots v_{i+k}$ is an internal path of G with length $k \geqslant 2$ and P_{k+1} does not lie on a cycle of length 3. Let $G' = G - \{v_i v_{i+1}, v_{i+1} v_{i+2}\} + \{v_i v_{i+2}\}$. If the diameter of $G' - v_{i+1}$ is d, it is easy to see that there is $v \in V(G' - v_{i+1})$ such that $G^* = G' + \{v v_{i+1}\} \in \mathscr{B}_{n,d}$. If the diameter of $G' - v_{i+1}$ is $d - 1$, then any shortest path of G between two vertices with length d contains $v_i v_{i+1} \cdots v_{i+k}$ as a part. Let v be an initial vertex of such a path and let $G^* = G' + \{v v_{i+1}\}$, then $G^* \in \mathscr{B}_{n,d}$. By Lemmas 4 and 7, in both cases we have $\rho(G^*) > \rho(G)$, a contradiction. This completes the proof of Fact 1. $\square$

Let P_{d+1} be a shortest path between two vertices of G with length d. Since $\mathscr{B}_{n,d} = \mathscr{B}^{\infty}_{n,d} \cup \mathscr{B}^{\theta}_{n,d}$, it follows that $G \in \mathscr{B}^{\infty}_{n,d}$ or $G \in \mathscr{B}^{\theta}_{n,d}$. Now we distinguish two cases to determine G.

Case 1. Suppose that $G \in \mathscr{B}^{\infty}_{n,d}$. Let $B(p, l, q)$ be the ∞-graph in G. We first prove that $|V(P_{d+1}) \cap V(C_p)| \geqslant 1$ or $|V(P_{d+1}) \cap V(C_q)| \geqslant 1$. Assume, on the contrary, that $|V(P_{d+1}) \cap V(C_p)| = 0$ and $|V(P_{d+1}) \cap V(C_q)| = 0$. Let $P_k : u_1 u_2 \cdots u_k$ be a shortest path such that $u_1 \in V(P_{d+1})$ and $u_k \in V(C_p) \cup V(C_q)$. Then $k \geqslant 2$. Applying Lemma 2 to the edge $u_1 u_2$, we get a graph $G^* \in \mathscr{B}^{\infty}_{n,d}$ with $\rho(G^*) > \rho(G)$, a contradiction. Hence $|V(P_{d+1}) \cap V(C_p)| \geqslant 1$ or $|V(P_{d+1}) \cap V(C_q)| \geqslant 1$.

Let $V' = V(P_{d+1}) \cup V(B(p, l, q))$ and $G' = G[V']$ be the induced subgraph of G. Then G is G' with some trees attached. Applying Lemma 2 to the non-pendant edges, we can similarly prove that all these attached trees are stars with centers in V'. That is to say that G is G' with some pendant edges attached. Applying Lemma 3, we can further prove that all these pendant edges are attached at the same vertex of G'.

From Fact 1, we can see that $p = q = 3$. Let $P_{d+1} : v_1 \cdots v_i \cdots v_{i+s} \cdots v_{d+1}$, where $v_{i+k} \in V(B(p, l, q))$, $k = 0, 1, \ldots, s$. We claim that the path $a_1 \cdots a_l$ in $B(p, l, q)$ lies on P_{d+1}. Otherwise, if $l \geqslant 2$, we may assume $a_1 a_2 \notin E(P_{d+1})$. Applying Lemma 2 to $a_1 a_2$ we get a graph $G^* \in \mathscr{B}^{\infty}_{n,d}$ with $\rho(G^*) > \rho(G)$, a contradiction. If $l = 1$ and $a_1 \notin V(P_{d+1})$, applying Lemma 3 to a_1 and v_i we get a graph $G^* \in \mathscr{B}^{\infty}_{n,d}$ with $\rho(G^*) > \rho(G)$, a contradiction. Hence the path $a_1 \cdots a_l$ lies on P_{d+1}. We distinguish the following four cases.

Subcase 1. $|V(P_{d+1}) \cap V(C_p)| = |V(P_{d+1}) \cap V(C_q)| = 1$. Applying Lemma 3, we have $G = P^{\nabla\nabla}_{d+1}(i)$. This contradicts Lemma 10.

Subcase 2. $|V(P_{d+1}) \cap V(C_p)| = 2$ and $|V(P_{d+1}) \cap V(C_q)| = 1$. We may assume that $v_{i-1} v_i \in E(C_p)$ and $v_j \in V(C_q)$. By Lemma 3, all the pendant edges, not lying on P_{d+1}, of G must be attached at v_j. So we may further assume that $i \leqslant j$. By Fact 1 we have $j \leqslant i + 1$. If $j = i + 1$, applying Lemma 1 to v_i and v_{i+1}, by similar reasoning as the proof of Lemma 2 we can obtain a graph $G^* \in \mathscr{B}^{\infty}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. Thus $j = i$, and so $G = P^{\Delta\nabla}_{d+1}(i)$. This contradicts Lemma 10 when $2 \leqslant i < d$. For $i = d$, it is easy to see that $P^{\Delta\nabla}_{d+1}(d) = P^{\Delta\Delta}_{d+1}(d)$. Applying Lemma 1 to vertices v_{d-1} and v_{d+1} of $P^{\Delta\Delta}_{d+1}(d)$, we have either $\rho(P^{\Delta\Delta}_{d+1}(d)) < \rho(P^{\theta}_{d+1}(2))$ or $\rho(P^{\Delta\Delta}_{d+1}(d)) < \rho(P^{\theta}_{d+1}(d))$, a contradiction.

Subcase 3. $|V(P_{d+1}) \cap V(C_p)| = 1$ and $|V(P_{d+1}) \cap V(C_q)| = 2$. By similar reasoning as Subcase 2, we can obtain a contradiction.

Subcase 4. $|V(P_{d+1}) \cap V(C_p)| = |V(P_{d+1}) \cap V(C_q)| = 2$. We may assume that $v_{i-1} v_i \in C_p$, $v_j v_{j+1} \in C_q$, and $j \geqslant i$. By Fact 1, we have either $j \leqslant i + 1$ or $j = i + 2$, $d(v_{i+1}) > 2$. If $j = i + 1$, or $j = i + 2$, $d(v_{i+1}) > 2$, applying Lemma 1 to vertices v_i and v_{i+1} we can obtain a graph $G^* \in \mathscr{B}^{\infty}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. Thus $j = i$. Applying Lemma 1 to vertices v_{i-1} and v_{i+1} we can obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction.

Case 2. Suppose that $G \in \mathscr{B}^{\theta}_{n,d}$. Let $P(l, p, q)$ be the θ-graph in G. By similar reasoning as Case 1, we can prove that $|V(P_{d+1}) \cap V(P(l, p, q))| \geqslant 1$. Let $V' = V(P_{d+1}) \cup V(P(l, p, q))$ and $G' = G[V']$ be the induced subgraph of G. By similar reasoning as Case 1, we can further prove that G is G' with some pendant edges attached at one vertex. This implies that at most 5 vertices of G have degree greater than 2.

By the definition of $P(l, p, q)$, we have that $l, p, q \geqslant 1$ and at most one of them is 1. Without loss of generality, we may assume that $l \leqslant p \leqslant q$. We claim that $l = 1$ and $p = q = 2$. Indeed, if $l \geqslant 2$, by Fact 1 and the fact that at most 5 vertices of G have degree greater than 2, we have $l = p = q = 2$ and the two vertices of degree 2 of $P(l, p, q)$ lie on P_{d+1}, the third vertex, denoted by w, of degree 2 of $P(l, p, q)$ is attached by some pendant edges. Applying Lemma 2 to aw in G (a is as given in Fig. 2), we obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. So $l = 1$. Similarly, by Fact 1 we can show that $p \leqslant q \leqslant 3$ and that if $q = 3$ then $p = 2$. If $q = 3$, denote $P_{q+1} : auvb$, where a and b are shown in Fig. 2. By Fact 1, we have $d(u) > 2$ and $d(v) > 2$. In the case when neither au nor vb lies on P_{d+1}, applying Lemma 2 to bv, we obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. So we many assume that au lies on P_{d+1}. If neither uv nor ab lies on P_{d+1}, applying Lemma 2 to bv, we obtain similarly a contradiction. Otherwise, G must be the graph G^+ shown in Fig. 9. Apply Lemma 1 to u and v, we obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. So, in further, $l = 1$, $p = q = 2$.

Subcase 1. $|V(P_{d+1}) \cap V(P(l, p, q))| = 1$. Applying Lemma 3, we can prove that $G = G_1(i)$ or $G_2(i)$. By Lemma 11 we have $G = G_2(2) = P^{\theta}_{d+1}(2)$. Since $d \geqslant 3$, by Lemma 6 we have $\rho(G_2(2)) < \rho(P^{\theta}_{d+1}(3))$, a contradiction.

Subcase 2. $|V(P_{d+1}) \cap V(P(l, p, q))| = 2$. If one edge of P_{p+1} or P_{q+1} lies on P_{d+1}, we may assume that $P_{p+1} : aub$ and au lies on P_{d+1}. Applying Lemma 1 (and Lemma 6, if necessary) to u and b we can obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. If P_{l+1} lies on P_{d+1}, by Fact 1, Lemmas 1 and 2 we can similarly prove that all the pendant edges, not lying on P_{d+1}, of G must be at one of a and b. That is to say that $G = P^{\theta}_{d+1}(i)$. For $d \geqslant 5$, by Lemmas 6, 12 and 13, we have further

$$\rho(P^{\theta}_{d+1}(i)) \leqslant \rho\left(P^{\theta}_{d+1}\left(\left\lfloor \frac{d+3}{2} \right\rfloor\right)\right) < \rho\left(P^{+}_{d+1}\left(\left\lfloor \frac{d+3}{2} \right\rfloor\right)\right),$$

a contradiction. For $d = 4$, applying Lemmas 6 and 9, by direct calculation we have $\rho(P^{\theta}_{5}(2)) < \rho(P^{\theta}_{5}(3)) < \rho(P^{+}_{5}(3))$, and by Lemma 13 we have $\rho(P^{\theta}_{5}(4)) < \rho(P^{\theta}_{5}(3)) < \rho(P^{+}_{5}(3))$. That is to say that $\rho(P^{\theta}_{5}(i)) < \rho(P^{+}_{5}(3))$, a contradiction. For $d = 3$, by Lemma 9 we have $\rho(P^{\theta}_{4}(2)) < \rho(P^{\theta}_{4}(3))$. Hence $G = P^{\theta}_{4}(3)$.

Subcase 3. $|V(P_{d+1}) \cap V(P(l, p, q))| = 3$. Then G must be $G_0(i)$ (see Lemma 14) with $n - d - 2$ pendant edges attached at v_j, where $2 \leqslant i, j \leqslant d$. By Fact 1 we may assume that $i \leqslant j \leqslant i + 2$. If $j = i + 2$, applying Lemma 1 to v_j and v_{i-1}, we can obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ such that $\rho(G^*) > \rho(G)$, a contradiction. So G must be $P^{+}_{d+1}(i)$ or $G_3(i)$ for some i. By Lemma 14, we have $G = P^{+}_{d+1}(i)$. By Lemma 15, we have further $G = P^{+}_{d+1}\left(\left\lfloor \frac{d+2}{2} \right\rfloor\right)$. For $d = 3$, applying Lemma 9, by direct calculation we have $\rho(P^{+}_{4}(2)) < \rho(P^{\theta}_{4}(3))$, a contradiction.

Combining Cases 1 and 2, we have $G = P_{d+1}^{+}\left(\left\lfloor \frac{d+2}{2} \right\rfloor\right)$ for $d \geqslant 4$ and $G = P_4^{\theta}(3)$ for $d = 3$.

This completes the proof. □

By Lemma 6, we have $\rho\left(P_{d+1}^{+}\left(\left\lfloor \frac{d+2}{2} \right\rfloor\right)\right) < \rho\left(P_{d}^{+}\left(\left\lfloor \frac{d+1}{2} \right\rfloor\right)\right)$ for $d \geqslant 5$. Moreover, it is easy to see that $P_3^{\nabla\nabla}(2)$ and $P_3^{+}(2)$ are all bicyclic graphs with n vertices and diameter 2. Applying Lemma 9, by direct calculation we can show when $n \geqslant 9$

$$\rho(P_3^{+}(2)) > \rho(P_3^{\nabla\nabla}(2)) > \rho(P_4^{\theta}(3)) > \rho(P_5^{+}(3)).$$

Combining these inequalities and Theorem 1, we have the following two corollaries.

Corollary 1. *Let $d \geqslant 4$, and G be a bicyclic graph on n vertices with diameter not less than d. Then*

$$\rho(G) \leqslant \rho\left(P_{d+1}^{+}\left(\left\lfloor \frac{d+2}{2} \right\rfloor\right)\right),$$

and the equality holds if and only if $G = P_{d+1}^{+}\left(\left\lfloor \frac{d+2}{2} \right\rfloor\right)$.

Corollary 2. *Let $n \geqslant 9$. The first three graphs among all bicyclic graphs on n vertices, ordered according to their spectral radii in decreasing order, are $P_3^{+}(2)$, $P_3^{\nabla\nabla}(2)$ and $P_4^{\theta}(3)$.*

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