On the signless Laplacian spectral radius of bicyclic graphs with fixed diameter

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Abstract Let G be a bicyclic graph. Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. In the paper, we determine the graph with the maximal signless Laplacian spectral radius among all the bicyclic graphs with n vertices and diameter d.
Keywords signless Laplacian spectral; bicyclic graph; diameter
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1 Introduction

In this paper, all graphs are undirected finite graphs without loops and multiple edges. Let $G = (V, E)$ be a graph with vertex set $V(G) = \{v_1, v_2, \cdots, v_n\}$ and edge set $E(G)$. Denote by $d(v_i)$ the degree of the graph G, $N(v_i)$ the set of vertices which are adjacent to vertex v_i. Let $A(G)$ be the adjacency matrix and $Q(G) = D(G) + A(G)$ be the signless Laplacian matrix of the graph G, where $D(G) = diag(d(v_1), d(v_2), \cdots, d(v_n))$ denotes the diagonal matrix of vertex degrees of G. The characteristic polynomial $\Phi(G, x)$ of G is defined as $\Psi(G, x) = det(xI - A(G))$. The signless laplacian characteristic polynomial $\Psi(G, x)$ of G is defined as $\Psi(G, x) = det(xI -$

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$Q(G)$). The spectrum of $Q(G)$ is also called the signless Laplacian spectrum of G.

The matrix Q is real symmetric and positive semidefinite, the eigenvalues of Q can be arranged as

$$q_1(Q) \geq q_2(Q) \geq \cdots \geq q_n(Q) \geq 0$$

where the largest eigenvalue $q_1(Q)$ is called Q- index of graph G. When G is connected, $Q(G)$ is irreducible and by the Perron-Frobenius Theorem, the signless Laplacian spectral radius is simple and there is a unique positive unit eigenvector corresponding to $q_1(G)$. We shall refer to such an eigenvector as the Perron vector of G.

Bicyclic graphs are connected graphs in which the number of edges equals the number of vertices plus one. The diameter of a connected graph is the maximum distance between pairs of its vertices. Recently, the problem concerning graphs with maximal spectral radius or the Laplacian spectral radius of a given class of graphs has been studied by many authors.

Guo [3] determined the spectral radius of trees with fixed diameter. Tan [4] determined the largest eigenvalue of signless laplacian matrix of a graph. Geng and Li [5] determind the graph with the largest spectral radius among all the tricyclic graphs with n vertices and diameter d. Guo [6] determind the laplacian spectral radius of trees with fixed diameter. He and Li [19] identified graphs with the maximal signless Laplacian spectral radius among all the unicyclic graphs with n vertices of diameter d. In this paper, we determine the unique graph with the largest signless Laplacian spectral radius among all the bicyclic graphs with n vertices and diameter d.

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 $l \geq 1$ 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 $l, p, q \geq 1$ 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. 1) 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 an θ-graph with trees attached. Then $\mathscr{B}_{n,d} = \mathscr{B}^{\infty}_{n,d} \bigcup \mathscr{B}^{\theta}_{n,d}$.

Let C_n and P_n the cycle and the path, on n vertices, respectively. Let $G-u$ or $G-uv$ denote the graph obtained from G by deleting the vertex $u \in V(G)$ or the edge $uv \in E(G)$. Similarly, $G+uv$ is a graph obtained from G by adding an edge uv, where $u, v \in V(G)$ and $uv \notin E(G)$. For two

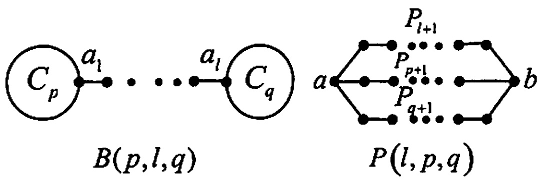

Fig. 1

vertices u and v $(u \neq v)$, the distance between u and v is the number of edges in a shortest path joining u and v. The diameter of a graph is the maximun distance between any two vertices of G. For a real number x, we use $\lfloor x \rfloor$ to represent the largest integer not greater than x and $\lceil x \rceil$ to represent the smallest integer not less than x.

An internal path of a graph G is a sequence of vertices $v_1, v_2, \cdots, v_m$ with $m \geq 2$ such that:
(1) The vertices in the sequences are distinct (except possibly $v_1 = v_m$);
(2) v_i is adjacent to $v_{i+1}, (i = 1, 2, \cdots, m-1)$;
(3) The vertex degrees $d(v_i)$ satisfy $d(v_1) \geq 3$, $d(v_2) = \cdots = d(v_{m-1}) = 2$ (unless $m = 2$) and $d(v_m) \geq 3$.

2 Preliminaries

In this section, we give the following lemmas which will be used to prove our main results.

Lemma 2.1 ([1]). Let G be a connected graph, and u, v be two vertices of G. Suppose that $v_1, v_2, \ldots, v_s \in N(v) \backslash N(u)$ $(1 \leq s \leq d(v))$ and $x = (x_1, x_2, \ldots, x_n)$ 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 vv_i and adding the edges $uv_i (1 \leq i \leq s)$. If $x_u \geq x_v$, then $q(G) < q(G^*)$.

Lemma 2.2([13]). Let u be a vertex of a connected graph G and $d(u) \geq 2$. Let $G_{k,l}(k, l \geq 0)$ be the graph obtained from G by attaching two pendant paths of lengths k and l at u, respectively. If $k \geq l \geq 1$ then

$$q(G_{k,l}) > q(G_{k+1,l-1}).$$

Lemma 2.3([4]). Suppose e be an edge of a graph G, and let $E_G(e)$ denote the set of all edges (containing no e) adjacent to e in G and $J_G(e)$ the set of all distinct line graph cycles containing e in G. Then the characteristic polynomial of G satisfies that

$$\Phi(G,x) = \frac{x-2}{x}\Phi(G-e,x) - \Sigma_{\bar{e}\in E(e)}\frac{\Phi(G-e-\bar{e},x)}{x^2}$$

$$-2\Sigma_{z\in J_G(e)}\frac{\Phi(G\setminus v(z),x)}{x^{|E(Z)|}}$$

Let G be a connected graph, and $uv \in E(G)$. The graph G_{uv} is obtained from G by subdividing the edge uv, i.e., adding a new vertex w and edges wu, wv in $G - uv$.

Lemma 2.4([17]). Let G_{uv} be the graph obtained from a connected graph G by subdividing its edge uv. Then the following holds:
(i) if uv belongs to an internal path then $q_1(G_{uv}) < q_1(G)$;
(ii) if $G \not\cong C_n$ for some $n \geq 3$, and if uv is not on the internal path then $q_1(G_{uv}) > q_1(G)$. Otherwise, if $G \cong C_n$ then $q_1(G_{uv}) = q_1(G) = 4$.

Lemma 2.5([18]). Let u be a vertex of a graph G, let $C(u)$ be the collection of all cycles containing u. Then the signless laplacian characteristic polynomial $\Psi(G)$ satisfies

$$\Psi(G,x) = (x-d(u))\Psi(G-u,x) - \sum_{v\in N(u)}\Psi(G-u-v,x)$$

$$-2\sum_{Z\in C(u)}\Psi(G\setminus V(Z),x)$$

where the first summation extends over those vertices v adjacent to u, and the second summation extends over all $Z \in C(u)$.

Lemma 2.6([18]). Let $e = uv$ be an edge of G, and let $C(e)$ be the set of all cycles containing e. Then the signless Laplacian characteristic polynomial of G satisfies

$$\Psi(G) = \Psi(G-e) - \Psi(Q_u(G-e)) - \Psi(Q_v(G-e)) - 2\sum_{Z}\Psi(Q_Z(G)),$$

where the summation extends over all $Z \in C(e)$.

Lemma 2.7([21]). Let G be a connected graph and let $e = uv$ be a non-pendant edge of G with $N(u)\bigcap N(v) = \emptyset$. 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 $q_1(G) < q_1(G^*)$.

Lemma 2.8. 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 $q_1(G_1) < q_1(G_2)$ or $q_1(G_1) < q_1(G_3)$.

Let $Q_v(G)$ denote the principal submatrix of $Q(G)$ obtained by deleting the row and column corresponding to the vertex v. Let $G = G_1u : vG_2$ be the graph obtained from two disjoint graphs G_1 and G_2 by joining a vertex u of graph G_1 to a vertex v of the graph G_2 by an edge. We call G a connected sum of G_1 at u and G_2 at v.

Lemma 2.9([22]). Let G_1 and G_2 be two graphs.
(1) Let $G = G_1u : vG_2$ be a connected sum of G_1 at u and G_2 at v, then

$$\Psi(G) = \Psi(G_1)\Psi(G_2) - \Psi(G_1)\Psi(Q_v(G_2)) - \Psi(G_2)\Psi(Q_u(G_1)).$$

(2) Let G be a connected graph with n vertices which consists of a subgraph H (with at least two vertices) and $n - |H|$ distinct pendant edges (not in H) attaching to a vertex v in H. Then

$$\Psi(G) = (x-1)^{n-|H|}\Psi(H) - (n-|H|)x(x-1)^{n-|H|-1}\Psi(Q_v(H)).$$

Lemma 2.10. Let G and H be two graphs.
(i)([23]) If $\Phi(H;x) > \Phi(G;x)$ for $x \geq q_1(H)$, then $q_1(G) > q_1(H)$;
(ii)([19]) If H is a proper subgraph of G and G is a connected graph, then $q_1(G) > q_1(H)$;
(iii)([4]) If H is a proper subgraph of G and G is a connected graph, then $\Psi(H;x) > \Psi(G;x)$, for $x \geq q_1(G)$.

Lemma 2.11([19]). Let H_0 be the graph as shown in Fig. 0. Suppose

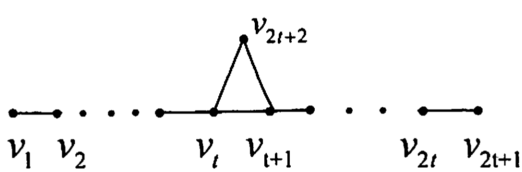

Fig. 0 H_0

that $t \geq 2$, then

$$\Psi(Q_{v_{t+1}}(H_0);x) - \Psi(Q_{v_t}(H_0);x) = x(x-2).$$

Let B_n be the matrix of order n obtained from $Q(P_{n+1})$ by deleting the row and column corresponding to some end vertex of P_{n+1}, and H_n be the matrix of order n obtained from $Q(P_{n+2})$ by deleting the rows and columns corresponding to two end vertices of P_{n+2}.

By similar reasoning as that of Lemma 2.8 of [24], we have the following result.

Lemma 2.12. Set $\Psi(P_0)=0$, $\Psi(B_0)=1$, $\Psi(H_0)=1$. We have
(1) $x\Psi(B_n)=\Psi(P_{n+1})+\Psi(P_n)$;
(2) $\Psi(P_{n+1})=(x-2)\Psi(P_n)-\Psi(P_{n-1}),(n\geq 1)$;
(3) $\Psi(P_n)=x\Psi(H_{n-1}),(n\geq 1)$;
(4) $\Psi(P_m)\Psi(P_n)-\Psi(P_{m-1})\Psi(P_{n+1})=\Psi(P_{m-1})\Psi(P_{n-1})-\Psi(P_{m-2})\Psi(P_n)$, $(m\geq 2, n\geq 2, x\neq 2)$.

Proof. We first prove that (1) and (2) hold. Considering the signless Laplacian characteristic polynomial of B_n, we have

$$\Psi(B_n)=\begin{vmatrix} x-1-1 & -1 & 0 & \cdots 0 \\ 1 & x-2 & 1 & \cdots 0 \\ 0 & 1 & x-2 & \cdots 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots x-1 \end{vmatrix}$$

$$=\Psi(P_n)-\Psi(B_{n-1}).$$

Thus we have

$$\Psi(B_{n-1})=\Psi(P_n)-\Psi(B_n). \tag{2.1}$$

From Lemma 2.8, we have

$$\Psi(P_{n+1})=(x-1)\Psi(P_n)-x\Psi(B_{n-1}). \tag{2.2}$$

Substituting Eq. (2.1) into Eq. (2.6), we have

$$\Psi(P_{n+1})=(x-1)\Psi(P_n)-x\Psi(P_n)+x\Psi(B_n)$$
$$=-\Psi(P_n)+x\Psi(B_n)$$

Hence, (1) holds. Substituting (1) into Eq. (2.2), (2) holds.

Secondly, we prove that (3) holds by employing induction on n. If $n=1,2$, the result is obvious. Suppose that $n\geq 3$. From (2) and induction, we have

$$\begin{aligned}\Psi(P_n)&=(x-2)\Psi(P_{n-1})-\Psi(P_{n-2})\\&=x(x-2)\Psi(H_{n-2})-x\Psi(H_{n-3})\\&=x[(x-2)\Psi(H_{n-2})-\Psi(H_{n-3})]\\&=x\Psi(H_{n-1}).\end{aligned}$$

Thus, (3) holds.

Finally we prove that (4) holds. From (2), we have

$$\Psi(P_m)=(x-2)\Psi(P_{m-1})-\Psi(P_{m-2}) \tag{2.3}$$

$$\Psi(P_{n+1}) = (x-2)\Psi(P_n) - \Psi(P_{n-1}). \tag{2.4}$$

From Eq. (2.4), we immediately have

$$(x-2)\Psi(P_n) = \Psi(P_{n+1}) + \Psi(P_{n-1}). \tag{2.5}$$

From Eq. (2.3) and (2.5), we immediately have

$$(x-2)\Psi(P_m)\Psi(P_n) = [(x-2)\Psi(P_{m-1}) - \Psi(P_{m-2})][\Psi(P_{n+1}) + \Psi(P_{n-1})].$$

Thus, we have

$$\begin{aligned}&(x-2)[\Psi(P_m)\Psi(P_n) - \Psi(P_{m-1})\Psi(P_{n+1})\\ &= (x-2)\Psi(P_{m-1})\Psi(P_{n-1}) - \Psi(P_{m-2})[\Psi(P_{n+1}) + \Psi(P_{n-1})].\end{aligned} \tag{2.6}$$

From (2), we have

$$\Psi(P_{n+1}) + \Psi(P_{n-1}) = (x-2)\Psi(P_n).$$

Substituting the above equation into Eq. (2.6), (4) holds. This completes the proof. □

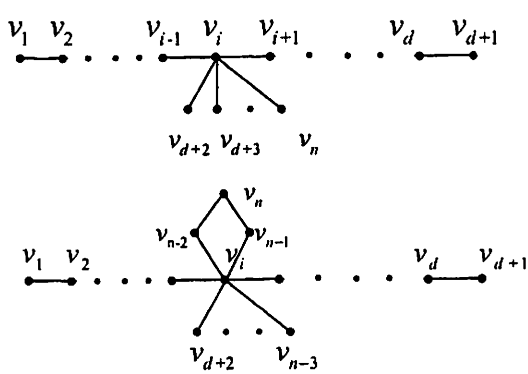

Fig.2 $P^*_{d+1}(i)$ *and* $U^*_{d+1}(i)$

We denote by $P^*_{d+1}(i)$ the graph obtained from a path $P_{d+1} : v_1v_2\cdots v_{d+1}$ and isolated vertices $v_{d+2}, \ldots, v_n$ by adding edges $v_iv_{d+2}, \ldots, v_iv_n$. Denote by $P^{\nabla\nabla}_{d+1}(i)$ 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 $P^{\triangle\nabla}_{d+1}(i)$ 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 $P^{\triangle\triangle}_{d+1}(i)$ 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 obtained

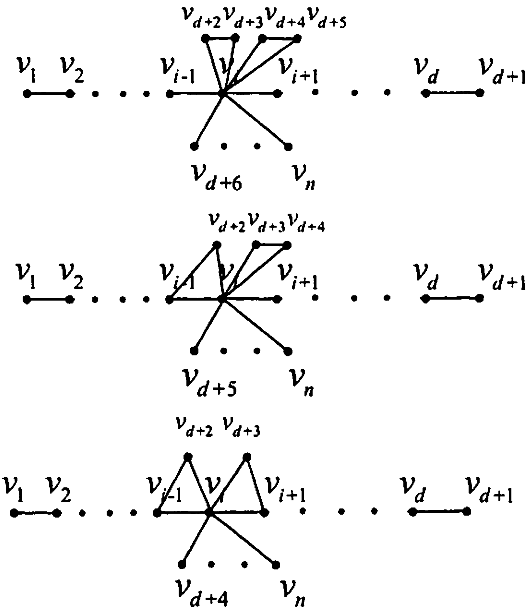

Fig. 3 $P_{d+1}^{\nabla\nabla}(i)$ $P_{d+1}^{\Delta\nabla}(i)$ $P_{d+1}^{\Delta\Delta}(i)$

from $P_{d+1}^{*}(i)$ by adding edges $v_{i-1}v_n$ and $v_{i+1}v_n$.

Lemma 2.13. Let $d \geq 3$. Then $q_1(P_{d+1}^{\Delta\Delta}(i)) \geq q_1(P_{d+1}^{\Delta\nabla}(i)) \geq q_1(P_{d+1}^{\nabla\nabla}(i))$ with the first equality if and only if $i = d$ and the second equality if and only if $i = 2$.

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

For $2 \leq i < d$, applying Lemma 2.6 to edge $v_{i+1}v_{d+3}$ of $P_{d+1}^{\Delta\Delta}(i)$ and edge $v_{d+3}v_{d+4}$ of $P_{d+1}^{\Delta\nabla}(i)$ respectively, we have

$$\Psi(P_{d+1}^{\Delta\Delta}(i)) = \Psi(P_{d+1}^{\Delta}(i)) - \Psi(Q_{v_{d+3}}(P_{d+1}^{\Delta}(i))) - \Psi(Q_{v_{i+1}}(P_{d+1}^{\Delta}(i))) -2\sum_{Z} \Psi(Q_Z(P_{d+1}^{\Delta\Delta}(i))),$$

where the summation extends over all $Z \in C(v_{i+1}v_{d+3})$.

$$\Psi(P_{d+1}^{\Delta\nabla}(i)) = \Psi(P_{d+1}^{\Delta}(i)) - \Psi(Q_{v_{d+3}}(P_{d+1}^{\Delta}(i))) - \Psi(Q_{v_{d+4}}(P_{d+1}^{\Delta}(i))) -2\sum_{Z} \Psi(Q_Z(P_{d+1}^{\Delta\nabla}(i))),$$

where the summation extends over all $Z \in C(v_{d+3}v_{d+4})$ and $P_{d+1}^{\triangle\triangle}(i) - v_{i+1} - v_{d+3}$ is a proper spanning subgraph of $P_{d+1}^{\triangle\nabla}(i) - v_{d+3} - v_{d+4}$, and $K_1 \cup P_{d-i}$ is a proper spanning subgraph of P_{d-i+1}. By Lemmas 2.10 and 2.11, we have

$$\Psi(P_{d+1}^{\triangle\nabla}(i)) - \Psi(P_{d+1}^{\triangle\triangle}(i)) > 0.$$

So, $q_1(P_{d+1}^{\triangle\triangle}(i)) \geq q_1(P_{d+1}^{\triangle\nabla}(i))$.

By similar reasoning as above, we have $q_1(P_{d+1}^{\triangle\nabla}(i)) \geq q_1(P_{d+1}^{\nabla\nabla}(i))$.

This completes the proof. □

Lemma 2.14. Let $G_1(i), G_2(i)$ and $P_{d+1}^{\theta}(i)$, shown in Fig. 4, belong to $\mathscr{B}_{n,d}$. Then

$$q_1(G_1(i)) < q_1(G_2(i)) \leq q_1(P_{d+1}^{\theta}(i)),$$

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

Proof. Applying Lemma 2.6 to edge $v_{n-2}v_{n-1}$ of $G_1(i)$ and edge v_iv_n of

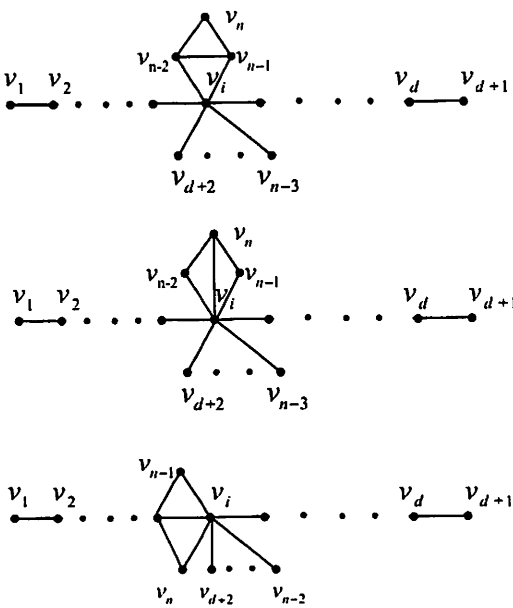

Fig. 4 $G_1(i)$ $G_2(i)$ and $P_{d+1}^{\theta}(i)$

$G_2(i)$ respectively, we have

$$\Psi(G_1(i)) = \Psi(G_1(i) - v_{n-2}v_{n-1}) - \Psi(Q_{v_{n-2}}(U_{d+1}^*(i))) - \Psi(Q_{v_{n-1}}(U_{d+1}^*(i))) - 2\sum_Z \Psi(Q_Z(G_1(i)))$$

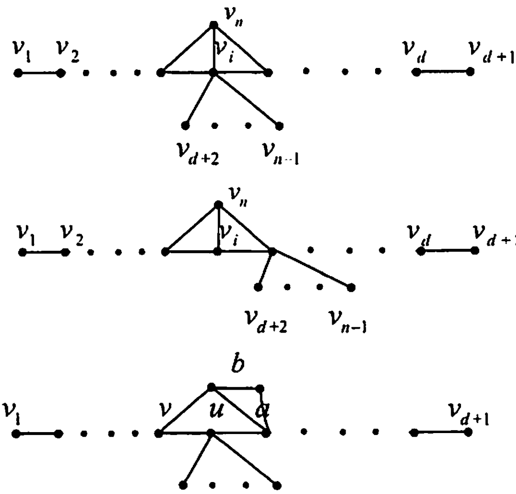

Fig. 4 $P^{+}_{d+1}(i)$ $G_3(i)$ *and* G^{+}

where the summation extends over all $Z \in C(v_{n-2}v_{n-1})$.

$$\Psi(G_2(i)) = \Psi(G_2(i) - v_iv_n) - \Psi(Q_{v_i}(U^*_{d+1}(i))) - \Psi(Q_{v_n}(U^*_{d+1}(i)))$$

$$-2\sum_Z \Psi(Q_Z(G_2(i)))$$

where the summation extends over all $Z \in C(v_iv_n)$ and $G_1(i) - v_{n-2}v_{n-1} = G_2(i) - v_iv_n$ and $G_1(i) - v_{n-2} - v_{n-1} - v_i = G_2(i) - v_i - v_n - v_{n-2}$. Note that $G_2(i) - v_i - v_n$, $G_2(i) - v_i - v_n - v_{n-2}$ are proper spanning subgraphs of $G_1(i) - v_{n-2} - v_{n-1}$, $G_1(i) - v_{n-2} - v_{n-1} - v_i$ respectively. By Lemmas 2.10 and 2.11, it is easy to see that $\Psi(G_1(i)) > \Psi(G_2(i))$. Then $q_1(G_1(i)) < q_2(G_2(i))$.

Clearly, $G_2(2) = P^{\theta}_{d+1}(2)$. For $3 \le i \le d$, applying Lemma 2.6 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

$$\Psi(G_2(i)) = \Psi(G_2(i) - v_{n-2}v_n) - \Psi(Q_{v_{n-2}}(G_2(i) - v_{n-2}v_n))$$

$$-\Psi(Q_{v_n}(G_2(i) - v_{n-2}v_n)) - 2\sum_Z \Psi(Q_Z(G_2(i)))$$

where the summation extends over all $Z \in C(v_{n-2}v_n)$.

$$\Psi(P^{\theta}_{d+1}(i)) = \Psi(P^{\theta}_{d+1}(i) - v_{i-1}v_n) - \Psi(Q_{v_{i-1}}(P^{\theta}_{d+1}(i) - v_{i-1}v_n)$$

$$-\Psi(Q_{v_n}(P^{\theta}_{d+1}(i) - v_{i-1}v_n) - 2\sum_{Z}\Psi(Q_Z(G_2(i)))$$

where the summation extends over all $Z \in C(v_{i-1}v_n)$. Applying Lemma 2.6 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 reasoning as above, we have

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

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 Lemmas 2.10 and 2.11, it is easy to see that $\Psi(G_2(i)) > \Psi(P^{\theta}_{d+1}(i))$. So, $q_1(G_2(i)) \le q_1(P^{\theta}_{d+1}(i))$.

This completes the proof. □

Lemma 2.15. If $n \ge d+4$ and $d \ge 4$ is even, then $q_1(P^{\theta}_{d+1}(\frac{d+4}{2})) < q_1(P^{\theta}_{d+1}(\frac{d+2}{2}))$.

Proof. Let $\gamma = \frac{d-2}{2}$. Then $P^{\theta}_{d+1}(\frac{d+4}{2}) \triangleq G(\gamma+1,\gamma)$, $P^{\theta}_{d+1}(\frac{d+2}{2}) \triangleq G(\gamma,\gamma+1)$. Using Lemma 2.5, we have

$$\begin{aligned}
&\Phi(P^{\theta}_{d+1}(\frac{d+4}{2})) - \Phi(P^{\theta}_{d+1}(\frac{d+2}{2}))\\
&= \Phi(G(\gamma+1,\gamma)) - \Phi(G(\gamma,\gamma+1))\\
&= (x-d(u))\Phi(G(\gamma,\gamma)) - \Phi(G(\gamma-1,\gamma)) - (x-d(u))\Phi(G(\gamma,\gamma)) + \Phi(G(\gamma,\gamma-1))\\
&= \Phi(G(\gamma,\gamma-1)) - \Phi(G(\gamma-1,\gamma))\\
&= \cdots\\
&= \Phi(G(1,0)) - \Phi(G(0,1))\\
&= (x-d(u))\Phi(G(0,0)) - \Phi(K_{1,n-d-1}) - (x-d(u))\Phi(G(0,0))\\
&\qquad + (x-d(u))^{n-d-3}\Phi(K_{1,2}) > 0
\end{aligned}$$

for $\forall x \ge q_1(P^{\theta}_{d+1}(\frac{d+4}{2}))$. So, we have $q_1(P^{\theta}_{d+1}(\frac{d+4}{2})) < q_1(P^{\theta}_{d+1}(\frac{d+2}{2}))$.

This completes the proof. □

In the similar way to the Lemma 2.14, we can prove the following Lemmas 2.16 and 2.17.

Lemma 2.16. If $n \ge d+3$ and $2 \le i-2 \le d-i+1$, then $q_1(P^{\theta}_{d+1}(i)) < q_1(P^{+}_{d+1}(i))$.

Lemma 2.17. If $d \ge 3$ and $n \ge d+3$, then $q_1(G_3(i)) < q_1(P^{+}_{d+1}(i))$.

Lemma 2.18. If $i-2 \ge d-i+2$, then $q_1(P^{+}_{d+1}(i)) < q_1(P^{+}_{d+1}(i-1))$.

Proof. Let $\alpha = i-2$ and $\beta = d-i$. Denote $P^{+}_{d+1}(i)$ by $G(\alpha,\beta)$. Similarly, denote $P^{+}_{d+1}(i-1)$ by $G(\alpha-1,\beta+1)$. Using Lemma 2.5, we have

$$\Phi(P^{+}_{d+1}(i)) - \Phi(P^{+}_{d+1}(i-1))$$

$= \Phi(G(\alpha,\beta)) - \Phi(G(\alpha-1,\beta+1))$
$= (x-d(u))\Phi(G(\alpha-1,\beta)) - \Phi(G(\alpha-2,\beta))$
$\quad -(x-d(u))\Phi(G(\alpha-1,\beta)) + \Phi(G(\alpha-1,\beta-1))$
$= \Phi(G(\alpha-1,\beta-1)) - \Phi(G(\alpha-2,\beta))$
$= \cdots$
$= \Phi(G(\alpha-\beta,0)) - \Phi(G(\alpha-\beta-1,1))$
$= (x-d(u))^{n-d-2}(x-d(u)+1)^2\Phi(P_{\alpha-\beta-2}) > 0$

for $\forall x \geq q_1(P^+_{d+1}(i))$. So, we have $q_1(P^+_{d+1}(i)) < q_1(P^+_{d+1}(i-1))$.

This completes the proof. □

3 Main results

Theorem 3.1 Let $n \geq d+4$ and $G \in \mathscr{B}_{n,d}$. If $d \geq 4$, then

$$q_1(G) \leq q_1(P^+_{d+1}(\lfloor\frac{d+2}{2}\rfloor)),$$

with equality if and only if $G = P^+_{d+1}(\lfloor\frac{d+2}{2}\rfloor)$; if $d = 3$, then $q_1(G) \leq q_1(P^\theta_4(3))$ with equality if and only if $G = P^\theta_4(3)$.

Proof. Choose $G \in \mathscr{B}_{n,d}$ and $X = (x_1, x_2, \ldots, x_n)^T$ the Perron vector of $Q(G)$, where x_i corresponds to the vertex $v_i (i = 1, 2, \ldots, n)$. We first prove some claims. □

Claim 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 of Claim 1. Otherwise, let $P_{k+1} : v_i v_{i+1} \cdots v_{i+k}$ is an internal path of G with length $k \geq 2$ and P_{k+1} does not lie 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, we have 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 shorter 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 $G^* = G' + \{v v_{i+1}\} \in \mathscr{B}_{n,d}$. By Lemmas 2.4 and 2.10, in both cases we have $q_1(G^*) > q_1(G)$, a contradiction.

Let P_{d+1} be a shortest path between two vertices of G with length d. Since $\mathscr{B}_{n,d} = \mathscr{B}^\infty_{n,d} \bigcup \mathscr{B}^\theta_{n,d}$, 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 $\infty-$graph in G. We first prove that $|V(P_{d+1}) \bigcap V(C_p)| \geq 1$ or $|V(P_{d+1}) \bigcap V(C_q)| \geq 1$. Assume, on the contrary, that $|V(P_{d+1}) \bigcap V(C_p)| = 0$ and $|V(P_{d+1}) \bigcap V(C_q)| = 0$. Let $P_k : u_1 u_2 \cdots u_k$ be a shortest path such that $u_1 \in V(P_{d+1})$ and $u_k \in$

$V(C_p)\bigcup V(C_q)$. Then $k \geq 2$. Applying Lemma 2.7 to the edge u_1u_2, we get a graph $G^* \in \mathscr{B}_{n,d}^{\infty}$ with $q_1(G^*) > q_1(G)$, a contradiction. So, we have $|V(P_{d+1})\bigcap V(C_p)| \geq 1$ or $|V(P_{d+1})\bigcap V(C_q)| \geq 1$.

Let $V' = V(P_{d+1})\bigcup V(B(p,l,q))$ and $G' = G[V']$ be the induced subgraph of G. Then G is G' with some trees attached. Applying Lemma 2.7 to the non-pendant edges, we can similarly prove that all these attached trees are stars with centers in V'. It is easy to see that G is G' with some pendant edges attached. Applying Lemma 2.8, we can further prove that all these pendant edges are attached at the same vertex of G'.

From Claim 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 $l \geq 2$, we may assume $a_1a_2 \notin E(P_{d+1})$. Applying Lemma 2.7 to a_1a_2, we get a graph $G^* \in \mathscr{B}_{n,d}^{\infty}$ with $q_1(G^*) > q_1(G)$, a contradiction. If $l = 1$ and $a_1 \notin V(P_{d+1})$, applying Lemma 2.8 to a_1 and v_i we get a graph $G^* \in \mathscr{B}_{n,d}^{\infty}$ with $q_1(G^*) > q_1(G)$, a contradiction. So, the path $a_1 \cdots a_l$ lies on P_{d+1}. We distinguish the following four cases.

Subcase 1.1. $|V(P_{d+1})\bigcap V(C_p) = V(P_{d+1})\bigcap V(C_q)| = 1$. Applying Lemma 2.8, we have $G = P_{d+1}^{\nabla\nabla}(i)$. This contradicts Lemma 2.13.

Subcase 1.2. $|V(P_{d+1})\bigcap V(C_p)| = 2$ and $|V(P_{d+1})\bigcap V(C_q)| = 1$. We may assume that $v_{i-1}v_i \in E(C_p)$ and $v_j \in V(C_q)$. By Lemma 2.8 all the pendant edges, not flying on P_{d+1}, of G must be attached at v_j. So we may further assume that $i \leq j$. By Claim 1, we have $j \leq i+1$. If $j = i+1$, applying Lemma 2.1 to v_i and v_{i+1}, by similar reasoning as the proof of Lemma 2.7, we can get a graph $G^* \in \mathscr{B}_{n,d}^{\infty}$ with $q_1(G^*) > q_1(G)$, a contradiction. Thus $i = j$, and so $G = P_{d+1}^{\Delta\nabla}(i)$. This contradicts Lemma 2.13, when $2 \leq i < d$. For $i = d$, we have $G = P_{d+1}^{\Delta\nabla}(d) = G = P_{d+1}^{\Delta\Delta}(d)$. Applying Lemma 2.1 to v_{d-1} and v_{d+1} of $P_{d+1}^{\Delta\Delta}(d)$, we have either $q_1(P_{d+1}^{\Delta\Delta}(d)) < q_1(P_{d+1}^{\theta})(2))$ or $q_1(P_{d+1}^{\Delta\Delta}(d)) < q_1(P_{d+1}^{\theta})(d))$, a contradiction.

Subcase 1.3. $|V(P_{d+1})\bigcap V(C_p)| = 1$ and $|V(P_{d+1})\bigcap V(C_q)| = 2$. By similar reasoning as Case 2, a contradiction.

Subcase 1.4. $|V(P_{d+1})\bigcap V(C_p)| = |V(P_{d+1})\bigcap V(C_q)| = 2$. We may assume that $v_{i-1}v_i \in E(C_p)$ and $v_jv_{j+1} \in V(C_q)$ and $j \geq i$. By Claim 1, we get either $j \leq i+1$ or $j = i+2, d(v_{i+1}) > 2$. If $j = i+1$ or $j = i+2, d(v_{i+1}) > 2$, applying Lemma 2.1 to vertices v_i and v_{i+1} we can get a graph $G^* \in \mathscr{B}_{n,d}^{\infty}$ with $q_1(G^*) > q_1(G)$, a contradiction. Thus $j = i$. Applying Lemma 2.1 to vertices v_{i-1} and v_{i+1} we can get a graph $G^* \in \mathscr{B}_{n,d}^{\theta}$ with $q_1(G^*) > q_1(G)$, a contradiction.

Case 2. Let $G \in \mathscr{B}_{n,d}^{\theta}$ and $P(l,p,q)$ be the θ–graph in G. By similar reasoning as Case 1, we can prove that $|V(P_{d+1})\bigcap V(P(l,p,q))| \geq 1$. Let $V' = V(P_{d+1})\bigcup V(P(l,p,q))$ 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 $P(l,p,q)$, it is easy to see that $l,p,q \geq 1$ and at most one of them is 1. Without loss of generality, we may assume that $l \leq p \leq q$. We claim that $l = 1$ and $p = q = 2$. If $l \geq 2$, by Claim 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 2.7 to aw in G (a is as given in Fig. 1), we get a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ with $q_1(G^*) > q_1(G)$, a contradiction. Thus, $l = 1$. Similarly, by Claim 1 we can show that $p \leq q \leq 3$ and that if $q = 3$ then $p = 2$. If $q = 3$, denote P_{q+1} : $auvb$ where a and b are as given in Fig. 1. By Claim 1, we have $d(u) > 2$ and $d(v) > 2$. If neither au nor vb lies on P_{d+1}, applying Lemma 2.7 to vb, we get a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ with $q_1(G^*) > q_1(G)$, a contradiction. So we may assume that au lies on P_{d+1}. If neither uv nor ab lies on P_{d+1}, applying Lemma 2.7 to vb, a contradiction. Otherwise, G must be the graph G^+ shown in Fig. 9. Applying Lemma 2.1 to u and v, we obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ with $q_1(G^*) > q_1(G)$, a contradiction. So, $l = 1, p = q = 2$.

Subcase 2.1. $|V(P_{d+1}) \bigcap V(P(l,p,q))| = 1$. Applying Lemma 2.8, we can prove that $G = G_1(i)$ or $G_2(i)$. By Lemma 2.14, we have $G = G_2(2) = P^{\theta}_{d+1}(2)$. Since $d \geq 3$, by Lemma 2.2 we have $q_1(G_2(2)) = q_(P^{\theta}_{d+1}(3))$, a contradiction.

Subcase 2.2. $|V(P_{d+1}) \bigcap V(P(l,p,q))| = 2$. 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 2.1 (and Lemma 2.2, if necessary) to u and b we get a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ with $q_1(G^*) > q_1(G)$, a contradiction. If P_{l+1} lies on P_{d+1}, by Claim 1, Lemmas 2.1 and 2.7 we can proved that all 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 $d \geq 5$, by Lemmas 2.2, 2.15 and 2.16, we have

$$q_(P^{\theta}_{d+1}(i)) \leq q_(P^{\theta}_{d+1}(\lfloor\frac{d+3}{2}\rfloor)) \leq q_(P^{\theta}_{d+1}(\lfloor\frac{d+3}{2}\rfloor)),$$

a contradiction. For $d = 4$, applying Lemmas 2.2 and 2.6, we have $q_1(P^{\theta}_5(2)) < q_1(P^{\theta}_5(3)) < q_1(P^{+}_5(3))$, and by Lemma 2.16 we have $q_1(P^{\theta}_5(4)) < q_1(P^{\theta}_5(3)) < q_1(P^{+}_5(3))$. That is to say that $q_1(P^{\theta}_5(i)) < q_1(P^{+}_5(3))$, a contradiction. For $d = 3$, by Lemma 2.6 we have $q_1(P^{\theta}_4(2)) < q_1(P^{\theta}_4(3))$. Hence $G = P^{\theta}_4(3)$.

Subcase 2.3. $|V(P_{d+1}) \bigcap V(P(l,p,q))| = 3$. Then G must be $G_0(i)$ with $n-d-2$ pendant edges attached at v_j, where $2 \leq i,j \leq d$. By Claim 1 we may assume that $i \leq j \leq i+2$. If $j = i+2$, applying Lemma 2.1 to v_j and v_{i-1}, we can obtain a graph $G^* \in \mathscr{B}^{\theta}_{n,d}$ with $q_1(G^*) > q_1(G)$, a contradiction. So G must be $P^{+}_{d+1}(i)$ or $G_3(i)$ for some i. Applying Lemma 2.17, we have $G = P_{d+1}^{+}(i)$. Applying Lemma 2.18, we have $G = P_{d+1}^{+}(\lfloor\frac{d+2}{2}\rfloor)$. For $d = 3$, applying Lemma 2.6, we have $q_1(P_4^{+}(2)) < q_1(P_4^{\theta}(3))$, a contradiction. Combining Cases 1 and 2, we have $G = P_{d+1}^{+}(\lfloor\frac{d+2}{2}\rfloor)$ for $d \geq 4$ and $G = P_4^{\theta}(3)$ for $d = 3$.

This completes the proof. □

By Lemma 2.2, we have $q_1(P_{d+1}^{+}(\lfloor\frac{d+2}{2}\rfloor)) < q_1(P_d^{+}(\lfloor\frac{d+1}{2}\rfloor))$ for $d \geq 5$. 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 2.6, by direct calculation we can show when $n \geq 9$

$$q_1(P_3^{+}(2)) > q_1(P_3^{\nabla\nabla}(2)) > q_1(P_4^{\theta}(3)) > q_1(P_5^{+}(3)).$$

Combining these inequalities and Theorem 3.1, we have the following two corollaries.

Corollary 3.1. Let $d \geq 4$, and G be a bicyclic graph on n vertices with diameter not less than d. Then

$$q_1(G) \leq q_1(P_{d+1}^{+}(\lfloor\frac{d+2}{2}\rfloor)),$$

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

Corollary 3.1. Let $n \geq 9$. Then first three graphs among all bicyclic graphs on n vertices, ordered according to their signless Laplacian spectral radius in decreasing order, are $P_3^{+}(2)$, $P_3^{\nabla\nabla}(2)$ and $P_4^{\theta}(3)$.

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