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THE (SIGNLESS) LAPLACIAN SPECTRAL RADIUS OF UNICYCLIC AND BICYCLIC GRAPHS WITH n VERTICES AND k PENDANT VERTICES

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Abstract. In this paper, the effects on the signless Laplacian spectral radius of a graph are studied when some operations, such as edge moving, edge subdividing, are applied to the graph. Moreover, the largest signless Laplacian spectral radius among the all unicyclic graphs with n vertices and k pendant vertices is identified. Furthermore, we determine the graphs with the largest Laplacian spectral radii among the all unicyclic graphs and bicyclic graphs with n vertices and k pendant vertices, respectively.

Keywords: Laplacian matrix, signless Laplacian matrix, spectral radius

MSC 2010: 05C50, 05C75

1. Introduction

Throughout the paper, $G = (V, E)$ is a connected undirected simple graph with $V = \{v_1, v_2, \ldots, v_n\}$ and $E = \{e_1, e_2, \ldots, e_m\}$. Especially, if $m = n$ or $m = n + 1$, then G is called a unicyclic or bicyclic graph, respectively. The notation $N(v)$ is used to denote the neighbors of vertex v. The degree of vertex v, written by $d(v)$, is $d(v) = |N(v)|$. Specially, we use $\Delta(G)$ to indicate the maximum degree of G. If $d(v) = 1$, then v is called a pendant vertex of G. Let the adjacency matrix, degree matrix of G be $A(G) = [a_{ij}]$, $D(G) = \operatorname{diag}\{d(v_1), d(v_2), \ldots, d(v_n)\}$, respectively. The *Laplacian matrix* of G is $L(G) = D(G) - A(G)$ and the *signless Laplacian matrix* of G is $Q(G) = D(G) + A(G)$. Denote the spectral radii of $A(G)$, $L(G)$ and $Q(G)$

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by $\varrho(G)$, $\lambda(G)$, and $\mu(G)$, respectively. For the relation between $\lambda(G)$ and $\mu(G)$, it is well known that

Proposition 1.1 ([15], [14]). *$\lambda(G) \leqslant \mu(G)$, the equality holds if and only if G is bipartite.*

If G is connected, by the Perron-Frobenius Theorem of non-negative matrices, $\mu(G)$ has multiplicity one and there exists a unique positive unit eigenvector corresponding to $\mu(G)$. We refer to such an eigenvector as the *Perron vector* of $\mu(G)$.

Our terminology and notation are standard except as indicated. For terminology and notation not defined here, we refer the readers to [1], [2], [4]–[6], [10], [12], [13], [17], [18] and the references therein.

It is well known that graph spectrum has great important application in many fields. Several graph spectra, i.e., spectra of $A(G)$, $L(G)$ and $Q(G)$, have been defined in [3]. The spectra of $A(G)$, $L(G)$ are well studied (for instance see [4], [6], [8], [12], [13]), but the spectrum of $Q(G)$ seems to be less well known. It is not until recent years, some researchers found that the spectrum of $Q(G)$ has a strong connection with the structure of the graph (see [7], [10]). Thus, more and more mathematicians became interested in it and devoted themselves to the study [2], [5], [7], [10].

The problem concerning graphs with maximal or minimal spectral radius over a given class of graphs proposed in [1] has been studied extensively. In this direction, Wu et al. [17] determined the unique tree with the largest spectral radius in the class of trees with n vertices and k pendant vertices, and Guo [9] identified the graphs with the largest spectral radius in the class of unicyclic and bicyclic graphs with n vertices and k pendant vertices, respectively. Very recently, Geng et al. [6] obtained the unique tricyclic graph with the largest spectral radius in the class of tricyclic graphs with n vertices and k pendant vertices. In this paper, we shall consider the similar problem for signless Laplacian spectral radius and Laplacian spectral radius. We determine the unique graph with the largest signless Laplacian spectral radius among all unicyclic graphs with n vertices and k pendant vertices, and the graphs with the largest Laplacian spectral radii among all unicyclic graphs and bicyclic graphs with n vertices and k pendant vertices, respectively.

The paper is organized as follows. In the second section, we obtain some properties for the signless Laplacian spectral radius of a graph when some operations, such as edge moving, edge subdividing, are applied to the graph. In the third section, we determine the graphs with the largest signless Laplacian spectral radius and the largest Laplacian spectral radius among all unicyclic graphs having n vertices and k pendant vertices, respectively. In the fourth section, we identify the graph with the largest Laplacian spectral radius among all bicyclic graphs having n vertices and k pendant vertices.

2. Some properties of the signless Laplacian spectral radius

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

Let $X(G)$ be the line graph of G. It is well known that (for example, see [13], p. 23):

$$\mu(G) = 2 + \varrho(X(G)). \tag{1}$$

In the study of spectral theory, the effects on the spectrum are observed when some operations, such as edge moving, edge subdividing, are applied to the graph. For example, the following lemmas are stated for the spectral radius of the adjacency matrix.

Lemma 2.1 ([12]). *Let uv be an edge of a graph G satisfying $d(u) \geqslant 2$ and $d(v) \geqslant 2$, and suppose that two new paths $P\colon uu_1u_2\ldots u_k$ and $Q\colon vv_1v_2\ldots v_m$ of length k and m ($k \geqslant m \geqslant 1$) are attached to G, respectively, to form $M_{k,m}$, where $u_1, u_2, \ldots, u_k$ and $v_1, v_2, \ldots, v_m$ are distinct new vertices. Then, we have $\varrho(M_{k,m}) > \varrho(M_{k+1,m-1})$.*

Suppose v is a vertex of a connected graph G with at least two vertices. Let $G_{k,l}$ ($l \geqslant k \geqslant 1$) be the graph obtained from G by attaching two new paths $P\colon v(=v_0)v_1v_2\ldots v_k$ and $Q\colon v(=u_0)u_1u_2\ldots u_l$ of length k and l, respectively, at v, where $v_1, v_2, \ldots, v_k$ and $u_1, u_2, \ldots, u_l$ are distinct new vertices. Let $G_{k-1,l+1} = G_{k,l} - v_{k-1}v_k + u_lv_k$. It has been proved that

Lemma 2.2 ([12]). *Let G be a connected graph on $n \geqslant 2$ vertices. If $l \geqslant k \geqslant 1$, then*

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

By $G \subset G'$, we mean that G is a subgraph of G' and $G \ncong G'$. It is well known that (for example, see [13], p. 17–18):

Lemma 2.3. *If $G \subset G'$ and G' is a connected graph, then $\varrho(G) < \varrho(G')$.*

By Lemma 2.3, it immediately follows

Proposition 2.1. *If $G \subset G'$ and G' is a connected graph, then $\mu(G) < \mu(G')$.*

Proof. Since $G \subset G'$ and G' is a connected graph, then $X(G) \subset X(G')$ and $X(G')$ is a connected graph. This implies that $\varrho(X(G)) < \varrho(X(G'))$. Bearing in mind the equality (1), then the result follows. $\square$

Lemma 2.4 ([4]). *Suppose $M_{n\times n}$ is a symmetric, nonnegative matrix, y is an n-tuple positive vector and μ' is a positive real number. If $My \leqslant \mu' y$ and $My \neq \mu' y$, then $\varrho_1(M) < \mu'$, where $\varrho_1(M)$ is the largest eigenvalue of M.*

With the help of the above lemmas, we can obtain the similar results on $\mu(G)$ for the general connected graphs.

1. Edge moving operation

Theorem 2.1. *Let G be a connected graph on $n \geqslant 2$ vertices. If $l \geqslant k \geqslant 1$, then*

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

Proof. We consider the next two cases.

Case 1. $k = 1$. Without loss of generality, suppose $e_1 = vv_1$, $e_2 = vu_1$, $e_3 = u_1u_2$, $\ldots$, $e_{l+1} = u_{l-1}u_l$, $e_t = u_lv_1$. Then $G_{1,l}$, $G_{0,l+1}$, $X(G_{1,l})$, $X(G_{0,l+1})$ are the graphs as shown in Fig. 1. Let $G_1 = X(G_{1,l}) \setminus \{wv_{e_1} \colon w \neq v_{e_2}\}$, then $G_1 \subset X(G_{1,l})$, thus $\varrho(G_1) < \varrho(X(G_{1,l}))$ follows from Lemma 2.3.

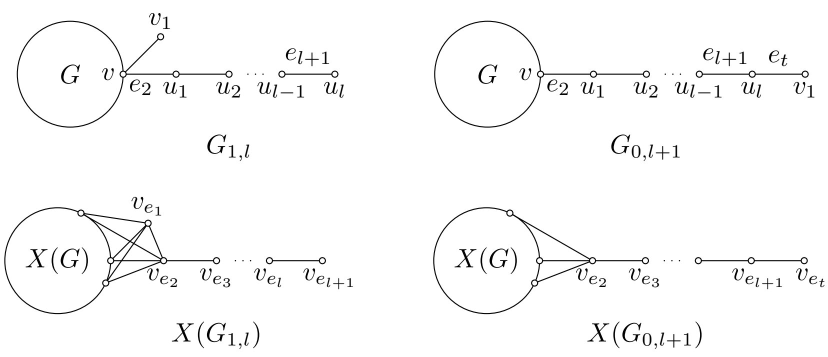

Fig. 1

Subcase 1.1. $l = 1$. It is easy to see that $G_1 \cong X(G_{0,l+1})$, this implies that $\varrho(X(G_{0,l+1})) = \varrho(G_1) < \varrho(X(G_{1,l}))$. Thus, the result follows from equality (1).

Subcase 1.2. $l \geqslant 2$. By Lemma 2.2, we have $\varrho(X(G_{0,l+1})) < \varrho(G_1) < \varrho(X(G_{1,l}))$. Thus, the result follows from equality (1).

Case 2. $k \geqslant 2$. Without loss of generality, suppose $e_1 = vv_1$, $e_2 = v_1v_2, \ldots$, $e_k = v_{k-1}v_k$ and $e_{k+1} = vu_1$, $e_{k+2} = u_1u_2, \ldots$, $e_{k+l} = u_{l-1}u_l$, $e_t = u_lv_k$. Then $G_{k,l}$, $G_{k-1,l+1}$, $X(G_{k,l})$, $X(G_{k-1,l+1})$ are the graphs as shown in Fig. 2. By Lemma 2.1, it follows that $\varrho(X(G_{k-1,l+1})) < \varrho(X(G_{k,l}))$. Bearing in mind the equality (1), the result follows.

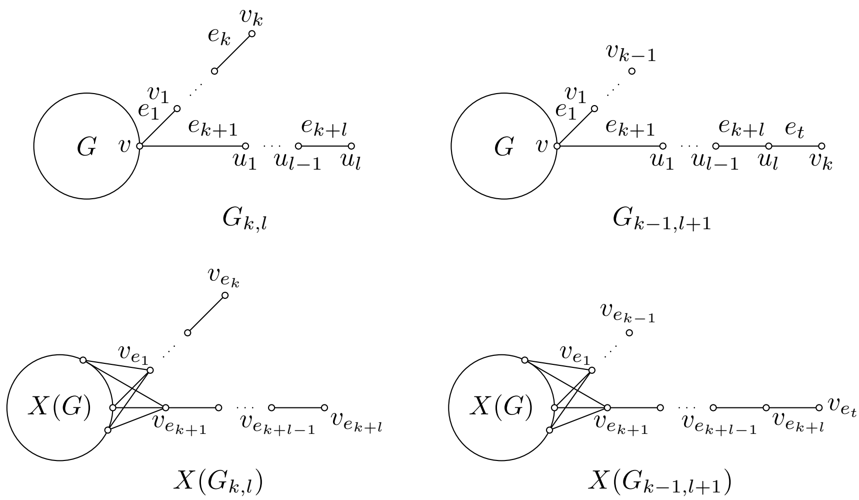

Fig. 2

By combining the above discussion, the assertion follows. □

By Proposition 1.1 and Theorem 2.1, we have

Corollary 2.1 ([8])**.** *Let G be a connected bipartite graph on $n \geqslant 2$ vertices. If $l \geqslant k \geqslant 1$, then $\lambda(G_{k,l}) > \lambda(G_{k-1,l+1})$.*

Lemma 2.5 ([18])**.** *Let $G = (V(G), E(G))$ be a connected simple graph with $uv_i \in E(G)$ and $wv_i \notin E(G)$ for $i = 1, \ldots, k$. Let $G' = (V'(G), E'(G))$ be a new graph obtained from G by deleting edges uv_i and adding edges wv_i for $i = 1, \ldots, k$. Let $x = (x_1, x_2, \ldots, x_n)^T$ be a Perron vector of $\mu(G)$. If $x_w \geqslant x_u$, then $\mu(G) < \mu(G')$.*

2. Edge subdividing operation

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 $G - uv$. An *internal path*, say $v_1v_2 \ldots v_{s+1}$ $(s \geqslant 1)$, is a path joining v_1 and v_{s+1} (which need not be distinct) such that v_1 and v_{s+1} have degree greater than 2, while all other vertices $v_2, \ldots, v_s$ are of degree 2. A *pendant path* of a graph is a path with one of its end vertices having degree one and all the internal vertices having degree two. Clearly, a pendant path of length one is a pendant edge.

Theorem 2.2. *Let uv be an edge of the connected graph G.*
(1) *If uv belongs to a pendant path of G, then $\mu(G^*_{u,v}) > \mu(G)$.*
(2) *If uv belongs to an internal path of G, then $\mu(G^*_{u,v}) < \mu(G)$.*

Proof. (1) Since $G \subset G^*_{u,v}$, then $\mu(G^*_{u,v}) > \mu(G)$ follows from Proposition 2.1.

(2) For convenience, we assume $v_1 v_2 \ldots v_a$ $(a \geqslant 2)$ is an internal path of G and $x = (x_1, x_2, \ldots, x_n)^T$ is the Perron vector of $\mu(G)$, where x_i (> 0) corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$. Without loss of generality, suppose that $x_1 \leqslant x_a$, and $x_t = \min\{x_t, x_{t+1}, \ldots, x_a\}$ such that $x_t < x_i$ for $1 \leqslant i \leqslant t-1$. We divide the proof into the next two cases.

Case 1. $t = 1$. Let $G' = G - v_1v_2 + v_1w + wv_2$, where $w \notin V(G)$. It is easy to see that $G^*_{u,v} \cong G'$. Let $y = (y_1, y_w, y_2, \ldots, y_n)^T$, where $y_w = y_1 = x_1$ and $y_i = x_i$ for $2 \leqslant i \leqslant n$. This implies that y is an $(n+1)$-tuple positive vector. Let $s = \sum\limits_{v_j \in N(v_1)} x_j - x_2$, where $N(v_1)$ is the set of neighbors of v_1 in G. Then,

$$(Q(G')y)_1 = d(v_1)x_1 + s + y_w = s + (d(v_1)+1)x_1,$$
$$(\mu(G)y)_1 = \mu(G)y_1 = \mu(G)x_1 = d(v_1)x_1 + s + x_2.$$

Since $x_1 \leqslant x_2$, then $(Q(G')y)_1 \leqslant (\mu(G)y)_1$. Moreover, we have

$$(Q(G')y)_w = 2y_w + x_1 + x_2 = 3x_1 + x_2,$$
$$(\mu(G)y)_w = \mu(G)y_w = \mu(G)x_1 = d(v_1)x_1 + s + x_2.$$

Since $d(v_1) \geqslant 3$, $s > 0$, thus $(Q(G')y)_w < (\mu(G)y)_w$.

For the other vertex v_j $(j \neq 1, w)$, we have $(Q(G')y)_j = (\mu(G)y)_j$. Combining the above discussion, we can conclude that $Q(G')y \leqslant \mu(G)y$ and $Q(G')y \neq \mu(G)y$, thus $\mu(G^*_{u,v}) = \mu(G') < \mu(G)$ follows from Lemma 2.4.

Case 2. $1 < t < a$. Let $G' = G - v_{t-1}v_t + v_{t-1}w + wv_t$, where $w \notin V(G)$. It is easy to see that $G^*(u,v) \cong G'$. Let $y = (y_1, \ldots, y_{t-1}, y_w, y_t, \ldots, y_n)^T$, where $y_w = x_t$ and $y_i = x_i$ for $1 \leqslant i \leqslant n$. This implies that y is an $(n+1)$-tuple positive vector. Then

$$(Q(G')y)_w = 2y_w + x_{t-1} + x_t = x_{t-1} + 3x_t,$$
$$(\mu(G)y)_w = \mu(G)y_w = \mu(G)x_t = 2x_t + x_{t-1} + x_{t+1}.$$

Since $x_t \leqslant x_{t+1}$, thus $(Q(G')y)_w \leqslant (\mu(G)y)_w$. Moreover, we have

$$(Q(G')y)_t = 2x_t + y_w + x_{t+1} = 3x_t + x_{t+1},$$
$$(\mu(G)y)_t = \mu(G)y_t = \mu(G)x_t = 2x_t + x_{t-1} + x_{t+1}.$$

Since $x_t < x_{t-1}$, thus $(Q(G')y)_t < (\mu(G)y)_t$.

For the other vertex v_j ($j \neq t, w$), we have $(Q(G')y)_j = (\mu(G)y)_j$. Combining the above discussion, we can conclude that $Q(G')y \leqslant \mu(G)y$ and $Q(G')y \neq \mu(G)y$, thus $\mu(G^*_{u,v}) = \mu(G') < \mu(G)$ follows from Lemma 2.4.

By combining the above arguments, we have $\mu(G^*_{u,v}) < \mu(G)$. This completes the proof. □

Corollary 2.2. *Suppose uv is an edge of the connected bipartite graph G.*

(1) *If uv belongs to a pendant path of G, then $\lambda(G^*_{u,v}) > \lambda(G)$.*

(2) *If uv belongs to an internal path of G and $G^*_{u,v}$ is also a bipartite graph, then $\lambda(G^*_{u,v}) < \lambda(G)$.*

Proof. We only prove (1), because (2) can be proved similarly. It is easy to see that $G^*_{u,v}$ is also bipartite as G is bipartite, then $\lambda(G^*_{u,v}) = \mu(G^*_{u,v}) > \mu(G) = \lambda(G)$ follows from Proposition 1.1 and Theorem 2.2. Thus (1) holds. □

3. The largest $\mu(G)$ (resp. $\lambda(G)$) in the class of unicyclic graphs with n vertices and k pendant vertices

Let G be a connected graph and let T be a tree such that T is attached to a vertex v of G. The vertex v is called the *root* of T. Throughout this paper, we assume that T does not include the root. Given u, $v \in V(G)$, the symbol $d(u,v)$ is used to denote the *distance* between u and v, i.e., the length of (number of edges in) the shortest path that connects u and v in G. Paths $P_{l_1}, \ldots, P_{l_k}$ are said to *have almost equal lengths* if $l_1, \ldots, l_k$ satisfy $|l_i - l_j| \leqslant 1$ for $1 \leqslant i \leqslant j \leqslant k$.

For integers n, k, let $\mathbb{U}_n(k)$ denote the class of connected unicyclic graphs with n vertices and k pendant vertices, and let $\mathbb{U}_n(t,k)$ be the class of connected unicyclic graphs on n vertices and k pendant vertices with the unique cycle of length t. The notation $W_n(t,k)$ denotes the unicyclic graph on n vertices obtained from a cycle, say C_t, by attaching k paths of almost equal lengths to one vertex of C_t. Obviously, $W_n(t,k) \in \mathbb{U}_n(t,k) \subseteq \mathbb{U}_n(k)$.

Lemma 3.1. *Suppose t and k are integers with $t \geqslant 3$ and $1 \leqslant k \leqslant n-t$. If $G \in \mathbb{U}_n(t,k)$, then $\mu(G) \leqslant \mu(W_n(t,k))$, with equality holding if and only if $G \cong W_n(t,k)$.*

Proof. Choose $G \in \mathbb{U}_n(t,k)$ such that the signless Laplacian spectral radius of G is as large as possible. Denote the vertex set of G by $\{v_1, \ldots, v_n\}$ and the Perron vector of $\mu(G)$ by $x = (x_1, \ldots, x_n)^T$, where x_i (> 0) corresponds to the vertex v_i ($1 \leqslant i \leqslant n$).

We first prove that G is a graph obtained by attaching some tree to only one vertex of C_t. On the contrary, assume that there exist trees T_1, T_2 attached to v_1, v_2 of C_t, respectively. Without loss of generality, suppose $x_1 \leqslant x_2$. Note that there must be some vertex $u \in V(T_1) \cap N(v_1)$ such that $u \notin N(v_2)$, let

$$G_1 = G - v_1u + v_2u,$$

then $G_1 \in \mathbb{U}_n(t,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

Thus, G is a graph obtained by attaching some tree T to one vertex, say v_1, of C_t. We now prove that each vertex v of T has degree $d(v) \leqslant 2$. On the contrary, assume there exists one vertex $v_i \in V(T)$ such that $d(v_i) \geqslant 3$ and $d(v_i, v_1)$ is as small as possible.

If $x_1 \geqslant x_i$, since $d(v_i) \geqslant 3$, then there must exist one vertex $u \in N(v_i)$ such that $d(v_1, u) > d(v_1, v_i)$. Clearly, $u \notin N(v_1)$. Let

$$G_1 = G - uv_i + uv_1,$$

then $G_1 \in \mathbb{U}_n(t,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

If $x_1 < x_i$, we consider the next two cases.

Case 1. $d(v_i, v_1) = 1$. Assume $C_t = v_1v_2v_3\ldots v_tv_1$. Clearly, $v_2 \notin N(v_i)$. Let

$$G_1 = G - v_1v_2 + v_iv_2,\ \ G_2 = G_1 - v_iv_2 - v_2v_3 + v_iv_3,\ \ G_3 = G_2 - v_2,\ \ G_4 = G_2 + v_2v_s,$$

where v_s is a pendant vertex of G.

By Lemma 2.5, $\mu(G) < \mu(G_1)$. Since $k \geqslant 1$, then $d(v_1) \geqslant 3$. Thus, $v_1v_tv_{t-1}\ldots v_3v_i$ or $v_iv_1v_tv_{t-1}\ldots v_3v_i$ is in an internal path of G_3. By Theorem 2.2, $\mu(G_1) < \mu(G_3) < \mu(G_4)$. Thus, we can conclude that $\mu(G) < \mu(G_4)$. But $G_4 \in \mathbb{U}_n(t,k)$, a contradiction to the choice of G.

Case 2. $d(v_i, v_1) \geqslant 2$. Suppose $P = v_1v_2\ldots v_lv_i$ is the unique path of length l from v_1 to v_i, then $l \geqslant 2$ by $d(v_i, v_1) \geqslant 2$. Let

$$G_1 = G - v_iv_l - v_lv_{l-1} + v_iv_{l-1},\ \ G_2 = G_1 - v_l,\ \ G_3 = G_1 + v_lv_s,$$

where v_s is a pendant vertex of G.

Clearly, $G_3 \in \mathbb{U}_n(t,k)$. By the choice of v_i, $v_1v_2\ldots v_{l-1}v_i$ is an internal path of G_2. By Theorem 2.2, we have $\mu(G) < \mu(G_2) < \mu(G_3)$, a contradiction.

Thus, G is a graph obtained by attaching k paths to the vertex v_1 of C_t. Finally, we prove that $G \cong W_n(t,k)$, i.e., the k paths have almost equal lengths. On the contrary, assume that there exist two paths, say P_{l_1} and P_{l_2}, such that $l_1 - l_2 \geqslant 2$ and $l_2 \geqslant 2$. Denote $P_{l_1} = u_1\ldots u_{l_1}$ and $P_{l_2} = w_1\ldots w_{l_2}$, where $u_1 = v_1 = w_1$. Let

$$G_1 = G - u_{l_1-1}u_{l_1} + w_{l_2}u_{l_1},$$

then $G_1 \in \mathbb{U}_n(t,k)$. By Theorem 2.1, $\mu(G) < \mu(G_1)$, a contradiction to the choice of G.

By combining the above arguments, we have $G \cong W_n(t,k)$. This completes the proof. □

Lemma 3.2. *Suppose t and k are integers with $t \geqslant 4$ and $1 \leqslant k \leqslant n-t$. Then,*

$$\mu(W_n(t,k)) < \mu(W_n(t-1,k)).$$

Proof. By the definition, $W_n(t,k)$ is the graph obtained by attaching k paths of almost equal lengths to v_1 of C_t. Assume $C_t = v_1v_2v_3\ldots v_tv_1$. Let

$$G_1 = W_n(t,k) - v_1v_2 - v_2v_3 + v_1v_3,\ \ G_2 = G_1 - v_2,\ \ G_3 = G_1 + v_2v_s,$$

where v_s is a pendant vertex of $W_n(t,k)$.

Since $k \geqslant 1$, then $d(v_1) \geqslant 3$. Thus, $v_1v_3v_4\ldots v_tv_1$ is an internal path of G_2. By Theorem 2.2, $\mu(W_n(t,k)) < \mu(G_2) < \mu(G_3)$. Moreover, note that $G_3 \in \mathbb{U}_n(t-1,k)$, thus we can conclude that $\mu(W_n(t,k)) < \mu(G_3) \leqslant \mu(W_n(t-1,k)$ by Lemma 3.1. □

For $G \in \mathbb{U}_n(k)$, it has been proved (see [9]) that $\varrho(G) \leqslant \varrho(W_n(3,k))$, with equality holding if and only if $G \cong W_n(3,k)$. The next theorem shows the similar result to $\mu(G)$ for $G \in \mathbb{U}_n(k)$

Theorem 3.1. *Suppose k is an integer with $1 \leqslant k \leqslant n-3$. If $G \in \mathbb{U}_n(k)$, then*

$$\mu(G) \leqslant \mu(W_n(3,k)),$$

and the equality holds if and only if $G \cong W_n(3,k)$.

Proof. Since $k \geqslant 1$ and $G \in \mathbb{U}_n(k)$, then there exists an integer t ($\geqslant 3$) such that $G \in \mathbb{U}_n(t,k)$. By Lemmas 3.1–3.2, it follows that $\mu(G) \leqslant \mu(W_n(t,k)) \leqslant \mu(W_n(3,k))$, with equality holding if and only if $G \cong W_n(3,k)$. This completes the proof of the assertion. □

In the following, we shall determine the unique graph with the largest Laplacian spectral radius in the class of unicyclic graphs with n vertices and k pendant vertices. By Proposition 1.1 and Lemma 3.1, it follows

Lemma 3.3. *Suppose t is a positive even number and k is an integer with $1 \leqslant k \leqslant n-t$. If $G \in \mathbb{U}_n(t,k)$, then $\lambda(G) \leqslant \lambda(W_n(t,k))$, with equality holding if and only if $G \cong W_n(t,k)$.*

Lemma 3.4. *Suppose t ($\geqslant 5$) is a positive odd number and k is an integer with $1 \leqslant k \leqslant n-t$. If $G \in \mathbb{U}_n(t,k)$, then $\lambda(G) < \lambda(W_n(t-1,k))$.*

Proof. Since t is odd, by Proposition 1.1 and Lemmas 3.1–3.2 we have $\lambda(G) < \mu(G) \leqslant \mu(W_n(t,k)) < \mu(W_n(t-1,k)) = \lambda(W_n(t-1,k))$. Thus, the result follows. □

Lemma 3.5. *Suppose t and k are integers with $t \geqslant 4$ and $1 \leqslant k \leqslant n-t$. If $G \in \mathbb{U}_n(t,k)$, then $\lambda(G) \leqslant \lambda(W_n(4,k))$, with equality holding if and only if $G \cong W_n(4,k)$.*

Proof. We divide the proof into the following two cases.

Case 1. t is even. We may assume that $t \geqslant 6$. By Proposition 1.1, Lemmas 3.2 and 3.3, we have $\lambda(G) \leqslant \lambda(W_n(t,k)) = \mu(W_n(t,k)) < \mu(W_n(t-1,k)) < \mu(W_n(t-2,k)) = \lambda(W_n(t-2,k))$. Since t is even, by repeating the above process, we can conclude that $\lambda(G) < \lambda(W_n(4,k))$ for $t \geqslant 6$.

Case 2. t is odd. Since $t \geqslant 5$, then $\lambda(G) < \lambda(W_n(t-1,k))$ follows from Lemma 3.4. Combining with Case 1, we have $\lambda(G) < \lambda(W_n(t-1,k)) \leqslant \lambda(W_n(4,k))$.

By combining the above arguments, the result follows. □

Lemma 3.6 ([8]). *Let v be a vertex of a connected graph G and suppose that $v_1,\ldots,v_s$ are pendant vertices of G which are adjacent to v. Let G^* be the graph obtained from G by adding any b $\bigl(1 \leqslant b \leqslant \frac{1}{2}s(s-1)\bigr)$ edges between $v_1,\ldots,v_s$. Then, $\lambda(G) = \lambda(G^*)$.*

The next lemma gives an upper bound for $\lambda(G)$, which does not exceed n.

Lemma 3.7 ([16]). $\lambda(G) \leqslant \max\{|N(u) \cup N(v)| \colon u,v \in V(G)\}$.

The next lemma gives a lower bound for $\lambda(G)$.

Lemma 3.8 ([14]). *If G is a graph with at least one edge, then $\lambda(G) \geqslant \Delta(G)+1$, where equality holds if and only if $\Delta(G) = n-1$.*

Theorem 3.2. *Suppose k is an integer with $1 \leqslant k \leqslant n-4$. If $G \in \mathbb{U}_n(k)$, then*

$$\lambda(G) \leqslant \lambda(W_n(4,k)),$$

where the equality holds if and only if $G \cong W_n(4,k)$.

P r o o f. Since $k \geqslant 1$ and $G \in \mathbb{U}_n(k)$, then there exists an integer t ($\geqslant 3$) such that $G \in \mathbb{U}_n(t,k)$. If $t \geqslant 4$, the result follows from Lemma 3.5. Next we shall consider the case of $t = 3$.

By the definition, $\mathbb{U}_n(3,k)$ denotes the class of connected unicyclic graphs on n vertices having k pendant vertices and a cycle $C_3 = v_1v_2v_3v_1$. Choose $G \in \mathbb{U}_n(3,k)$ such that the Laplacian spectral radius of G is as large as possible.

We first proved that G is a graph by attaching some tree to only one vertex of C_3. On the contrary, assume that there exist trees T_1, T_2 attached to v_1, v_2 of C_3, respectively. Note that $1 \leqslant k \leqslant n-4$. By Lemmas 3.7–3.8 we have

$$\lambda(G) \leqslant \max\{|N(u) \cup N(v)|\colon\ u, v \in V(G)\} \leqslant k+3 = \Delta(W_n(3,k))+1 < \lambda(W_n(3,k)).$$

But $W_n(3,k) \in \mathbb{U}_n(3,k)$, it is a contradiction to the choice of G.

Thus, G is a graph obtained by attaching some tree to one vertex, say v_1, of C_3. Let $T = G - v_2v_3$, then T is a tree. By Lemma 3.6, $\lambda(G) = \lambda(T)$. Next we shall prove that $\lambda(T) < \lambda(W_n(4,k))$.

Choose a pendant vertex, say u, of $V(T)$ such that $d(v_1,u)$ is as large as possible in T. Let $G_1 = T + uv_2$. Since $T \subset G_1$, then $\lambda(T) = \mu(T) < \mu(G_1)$ follows from Proposition 2.1.

Note that G_1 contains a cycle, say C_a, clearly $a \geqslant 4$ because $1 \leqslant k \leqslant n-4$, thus $G_1 \in \mathbb{U}_n(a,k)$. By Lemmas 3.1–3.2, $\mu(G_1) \leqslant \mu(W_n(a,k)) \leqslant \mu(W_n(4,k))$.

Combining the above arguments, we can conclude that

$$\lambda(G) = \lambda(T) = \mu(T) < \mu(G_1) \leqslant \mu(W_n(4,k)) = \lambda(W_n(4,k)).$$

This completes the proof. □

4. The largest $\lambda(G)$ in the class of bicyclic graphs with n vertices and k pendant vertices

Let G be a bicyclic graph. The *base* of G, denoted by $\hat{G}$, is the (unique) minimal connected bicyclic subgraph of G. It is easy to see that $\hat{G}$ is the unique bicyclic subgraph of G containing no pendant vertices, while G can be obtained from $\hat{G}$ by attaching trees to some vertices of $\hat{G}$.

Let C_p and C_q be two vertex-disjoint cycles. Suppose that $u \in V(C_p)$ and $v \in V(C_q)$. In [9], Guo introduced the graph $B(p,l,q)$ (Fig. 3), which is arisen from C_p and C_q by joining u and v by a path $(u=)v_1v_2\dots v_l(=v)$ of length $l-1$, where $l=1$ means identifying u and v.

Let P_{p+1}, P_{q+1} and P_{l+1} be three vertex-disjoint paths, where $p,l,q \geqslant 1$ and at most one of them is 1. Identifying the three initial vertices and terminal vertices of them, respectively, the resulting graph (Fig. 3), denoted by $P(p,l,q)$, is also reported in [9].

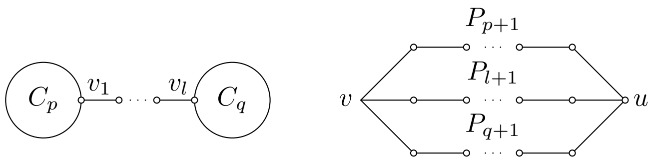

Fig. 3. The graphs $B(p,l,q)$ and $P(p,l,q)$.

For integers n, k, let $\mathbb{B}(n,k)$ be the class of connected bicyclic graphs with n vertices and k pendant vertices. Now we define the following two kinds of bicyclic graphs with n vertices and k pendant vertices:

$$\mathbb{B}_1(n,k) = \{G \in \mathbb{B}(n,k)\colon\ \hat{G} = B(p,l,q)\},$$
$$\mathbb{B}_2(n,k) = \{G \in \mathbb{B}(n,k)\colon\ \hat{G} = P(p,l,q)\}.$$

The girth of G is the length of a shortest cycle in G and its length is denoted by $g(G)$. For convenience, we introduced more notation as follows.

$$\mathcal{B}^1(n,k) = \{G \in \mathbb{B}_1(n,k)\colon\ g(G) \geqslant 4\}, \quad \mathcal{B}^2(n,k) = \{G \in \mathbb{B}_1(n,k)\colon\ g(G) = 3\},$$
$$\mathcal{B}^3(n,k) = \{G \in \mathbb{B}_2(n,k)\colon\ g(G) \geqslant 4\}, \quad \mathcal{B}^4(n,k) = \{G \in \mathbb{B}_2(n,k)\colon\ g(G) = 3\}.$$

It is easy to see that

$$\mathbb{B}(n,k) = \mathbb{B}_1(n,k) \cup \mathbb{B}_2(n,k),$$
$$\mathbb{B}_1(n,k) = \mathcal{B}^1(n,k) \cup \mathcal{B}^2(n,k),$$
$$\mathbb{B}_2(n,k) = \mathcal{B}^3(n,k) \cup \mathcal{B}^4(n,k).$$

Let W_1 be the graph on n vertices obtained from $B(4,1,4)$ by attaching k paths of almost equal lengths to the vertex of degree 4. Let W_2 and W_3 be the graphs on n vertices arisen from $P(3,1,3)$ by attaching k paths of almost equal lengths to one vertex of degree 3 and one vertex of degree 2, respectively. Let W_4 and W_5 be the graphs on n vertices obtained from $P(2,2,2)$ by attaching k paths of almost equal lengths to one vertex of degree 3 and one vertex of degree 2, respectively.

Let $m(v)$ denote the average of the degrees of the vertices adjacent to v, i.e., $m(v) = \sum_{u \in N(v)} d(u)/d(v)$.

Lemma 4.1 ([11]).

$$\lambda(G) \leqslant \max\Big\{\frac{d(u)(d(u)+m(u)) + d(v)(d(v)+m(v))}{d(u)+d(v)} \colon\ uv \in E(G)\Big\}.$$

Lemma 4.2. *If* $1 \leqslant k \leqslant n-7$, *then* $\lambda(W_i) < \lambda(W_1)$ *holds for* $2 \leqslant i \leqslant 5$.

Proof. By Lemmas 3.8 and 4.1, we have

$$\begin{aligned}\lambda(W_2) &\leqslant \max\Big\{\frac{d(u)(d(u)+m(u)) + d(v)(d(v)+m(v))}{d(u)+d(v)} \colon\ uv \in E(W_2)\Big\}\\ &= \max\Big\{\frac{k^2+9k+32}{k+6}, \frac{k^2+9k+25}{k+5}, \frac{k^2+9k+19}{k+4}\Big\}\\ &\leqslant k+5 = \Delta(W_1)+1 < \lambda(W_1).\end{aligned}$$

By Lemmas 3.7–3.8, we have

$$\lambda(W_3) \leqslant \max\{|N(u) \cup N(v)| \colon\ u, v \in V(W_3)\} = k+5 = \Delta(W_1)+1 < \lambda(W_1).$$

It can be proved similarly as $\lambda(W_3) < \lambda(W_1)$ that $\lambda(W_4) < \lambda(W_1)$ and $\lambda(W_5) < \lambda(W_1)$.

By combining the above discussion, the assertions follow. □

Lemma 4.3. *If* $1 \leqslant k \leqslant n-7$ *and* $G \in \mathcal{B}^1(n,k)$, *then* $\mu(G) \leqslant \mu(W_1)$, *with equality holding if and only if* $G \cong W_1$.

Proof. Choose $G \in \mathcal{B}^1(n,k)$ such that $\mu(G)$ is as large as possible. Denote the vertex set of G by $\{v_1, \ldots, v_n\}$ and the Perron vector of $\mu(G)$ by $x = (x_1, \ldots, x_n)^T$, where x_i (> 0) corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$.

Suppose $\hat{G} = B(p,l,q)$, and $v_1 \ldots v_l$ is the unique path from $v_1 \in V(C_p)$ to $v_l \in V(C_q)$. We claim that $l = 1$. Assume, on the contrary, that $l > 1$. Without loss of generality, suppose that $x_1 \geqslant x_l$. Clearly, there exists some vertex $u \in N(v_l) \cap V(C_q)$, and $u \notin N(v_1)$. Let

$$G_1 = G - v_l u + v_1 u,$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction. Hence, $l = 1$.

We now prove that G is the graph that arises from $B(p,1,q)$ by attaching a tree to the vertex of degree 4, say v_1, in $B(p,1,q)$. Assume that there exists a vertex v_i of $B(p,1,q)$ such that $v_i \neq v_1$ and there exists a tree T attached to v_i. By symmetry, we may assume that $v_i \in V(C_p)$.

If $x_1 \geqslant x_i$, choose $u \in N(v_i) \cap V(T)$, clearly $u \notin N(v_1)$. Let

$$G_1 = G - v_i u + v_1 u,$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

If $x_1 < x_i$, suppose $\{u, v\} = N(v_1) \cap V(C_q)$, clearly $u, v \notin N(v_i)$. Let

$$G_1 = G - v_1 u - v_1 v + v_i u + v_i v,$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

Thus, G is a graph obtained by attaching one tree, say T, to the vertex v_1 of $B(p,1,q)$. We now prove that each vertex of T has degree $d(v) \leqslant 2$. On the contrary, assume there exists one vertex $v_i \in V(T)$ such that $d(v_i) \geqslant 3$.

If $x_1 \geqslant x_i$, since $d(v_i) \geqslant 3$, then there must exist some vertex $u \in N(v_i)$ such that $d(v_1, u) > d(v_1, v_i)$. Clearly, $u \notin N(v_1)$. Let

$$G_1 = G - uv_i + v_1 u$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

If $x_1 < x_i$, suppose $\{u, v\} = N(v_1) \cap V(C_q)$, clearly $u, v \notin N(v_i)$. Let

$$G_1 = G - v_1 u - v_1 v + v_i u + v_i v,$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

Thus, G is a graph obtained by attaching k paths to the vertex v_1 of $B(p,1,q)$. Next we shall prove that $p = q = 4$. On the contrary, we assume that $p > 4$ and $C_p = v_1 v_2 \ldots v_p v_1$. Let

$$G_1 = G - v_1 v_2 - v_2 v_3 + v_1 v_3, \quad G_2 = G_1 - v_2, \quad G_3 = G_1 + v_2 v_s,$$

where v_s is a pendant vertex of G.

Note that $v_1v_3\dots v_pv_1$ is an internal path of G_2, then $\mu(G) < \mu(G_2)$ follows from Theorem 2.2. Moreover, since $G_2 \subset G_3$, by Proposition 2.1 it follows that $\mu(G_2) < \mu(G_3)$. Thus, we can conclude that $\mu(G) < \mu(G_3)$. But $G_3 \in \mathcal{B}^1(n,k)$, a contradiction. Thus, $p = 4$. By the same reason, $q = 4$.

Finally, we prove that $G \cong W_1$, i.e., the k paths have almost equal lengths. On the contrary, if there exist two paths, say P_{l_1} and P_{l_2}, such that $l_1 - l_2 \geqslant 2$ and $l_2 \geqslant 2$. Denote $P_{l_1} = u_1\dots u_{l_1}$ and $P_{l_2} = w_1\dots w_{l_2}$, where $u_1 = v_1 = w_1$. Let

$$G_1 = G - u_{l_1-1}u_{l_1} + w_{l_2}u_{l_1},$$

then $G_1 \in \mathcal{B}^1(n,k)$. By Theorem 2.1, $\mu(G) < \mu(G_1)$, a contradiction.

By combining the above arguments, we have $G \cong W_1$. This completes the proof.

□

Corollary 4.1. *If $1 \leqslant k \leqslant n-7$ and $G \in \mathcal{B}^1(n,k)$, then $\lambda(G) \leqslant \lambda(W_1)$, with equality holding if and only if $G \cong W_1$.*

Proof. By Proposition 1.1 and Lemma 4.3, we have

$$\lambda(G) \leqslant \mu(G) \leqslant \mu(W_1) = \lambda(W_1).$$

Thus, the conclusion follows from Lemma 4.3.

Lemma 4.4. *If $1 \leqslant k \leqslant n-7$ and $G \in \mathcal{B}^2(n,k)$, then $\lambda(G) < \lambda(W_1)$.*

Proof. Choose $G \in \mathcal{B}^2(n,k)$ such that $\lambda(G)$ is as large as possible. Without loss of generality, we assume that $p \geqslant q$ in the proof of this lemma. By the definition, $\hat{G} = B(p,l,3)$. Suppose that $C_q(= C_3) = v_1v_2v_3v_1$, where $d(v_1) \geqslant 3$ in $B(p,l,3)$. Two cases occur as follows.

Case 1. If there exists a vertex w ($w = v_2$ or v_3) of degree 2 in C_3 of $B(p,l,3)$ such that there exists a tree T attached to w, by Lemmas 3.7–3.8 it follows that

$$\lambda(G) \leqslant \max\{|N(u) \cup N(v)|\colon\ u,v \in V(G)\} \leqslant k+5 = \Delta(W_1)+1 < \lambda(W_1).$$

Case 2. There exists no tree attached to v_2 or/and v_3 in C_q $(= C_3)$ of $B(p,l,3)$. Let

$$G_1 = G - v_2v_3.$$

Then, $\lambda(G) = \lambda(G_1)$ follows from Lemma 3.6. Note that $G_1 \in \mathbb{U}_n(k+2)$ and $k+2 < n-4$, by Theorem 3.2 we have $\lambda(G_1) \leqslant \lambda(W_n(4,k+2))$. Choose two different pendant vertices, say u and v, of $V(W_n(4,k+2))$ such that $d(v_i,u)$ and

$d(v_i, v)$ are as large as possible in $W_n(4, k+2)$, where v_i is the unique vertex of degree greater than 4 in $W_n(4, k+2)$. Let

$$G_2 = W_n(4, k+2) + uv.$$

Since $W_n(4, k+2) \subset G_2$, by Proposition 2.1 we have $\mu(W_n(4, k+2)) < \mu(G_2)$. Note that $G_2 \in \mathcal{B}^1(n, k)$, then $\mu(G_2) \leqslant \mu(W_1)$ by Lemma 4.3.

Combining the above discussion and Proposition 1.1, we can conclude that

$$\lambda(G) = \lambda(G_1) \leqslant \lambda(W_n(4, k+2)) = \mu(W_n(4, k+2)) < \mu(G_2) \leqslant \mu(W_1) = \lambda(W_1).$$

By the above arguments, we have $\lambda(G) < \lambda(W_1)$. This completes the proof. □

Lemma 4.5. *If* $1 \leqslant k \leqslant n-7$ *and* $G \in \mathcal{B}^3(n, k)$, *then* $\mu(G) \leqslant \max\{\mu(W_2), \mu(W_3), \mu(W_4), \mu(W_5)\}$.

Proof. Choose $G \in \mathcal{B}^3(n, k)$ such that $\mu(G)$ is as large as possible. Denote the vertex set of G by $\{v_1, \ldots, v_n\}$ and the Perron vector of $\mu(G)$ by $x = (x_1, \ldots, x_n)^T$, where x_i (> 0) corresponds to the vertex v_i $(1 \leqslant i \leqslant n)$. Without loss of generality, we assume that $l = \min\{p, l, q\}$ in the proof of this lemma.

We first prove that G is the graph obtained from $P(p, l, q)$ by attaching some tree to only one vertex of $P(p, l, q)$. On the contrary, assume there exist trees T_i and T_j attached to v_i and v_j of $P(p, l, q)$, respectively. By symmetry, we may assume that $x_i \geqslant x_j$. Choose $u \in N(v_j) \cap V(T_j)$, clearly $u \notin N(v_i)$. Let

$$G_1 = G - v_j u + v_i u.$$

Then, $G_1 \in \mathcal{B}^3(n, k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

Thus, G is the graph arisen from $P(p, l, q)$ by attaching some tree, say T, to unique vertex, say v_1, of $P(p, l, q)$. We now prove that every vertex v of T has degree $d(v) \leqslant 2$. On the contrary, assume that there exists $v_j \in V(T)$ such that $d(v_j) \geqslant 3$.

If $x_j \leqslant x_1$, since $d(v_j) \geqslant 3$, then there must exist some vertex $u \in N(v_j)$ such that $d(v_1, u) > d(v_1, v_j)$. Clearly, $u \notin N(v_1)$. Let

$$G_1 = G - uv_j + uv_1,$$

then $G_1 \in \mathcal{B}^3(n, k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

If $x_j > x_1$, suppose $u \in N(v_1) \cap V(P(p, l, q))$, clearly $u \notin N(v_j)$. Let

$$G_1 = G - v_1 u + v_j u,$$

then $G_1 \in \mathcal{B}^3(n, k)$. By Lemma 2.5, $\mu(G) < \mu(G_1)$, a contradiction.

Thus, G is a graph obtained by attaching k paths to some vertex v_1 of $P(p,l,q)$. We divide the proof into the next two cases.

Case 1. $d(v_1)=3$ in $P(p,l,q)$.

Subcase 1.1. $l=1$. We shall prove that $p=q=3$. On the contrary, assume that $p\geqslant 4$. Suppose $P_{p+1}=v_1v_2\dots v_{p+1}$, then $d(v_1)\geqslant 4$ and $d(v_{p+1})=3$. Let

$$G_1=G-v_1v_2-v_2v_3+v_1v_3,\quad G_2=G_1-v_2,\quad G_3=G_1+v_2v_s,$$

where v_s is a pendant vertex of G.

Note that $v_1v_3\dots v_{p+1}$ is an internal path of G_2 and $G_2\subset G_3$, then $\mu(G)<\mu(G_2)<\mu(G_3)$ follows from Proposition 2.1 and Theorem 2.2, a contradiction to the choice of G. Thus, $p=3$. By the same reason, $q=3$. Thus, G is a graph obtained by attaching k paths to one vertex of degree 3 of $P(3,1,3)$. By Theorem 2.1, we have $G\cong W_2$.

Subcase 1.2. $l\geqslant 2$. By the same method as Subcase 1.1, we can prove that $G\cong W_4$.

Case 2. $d(v_1)=2$ in $P(p,l,q)$.

Subcase 2.1. $l=1$. By the same method as Subcase 1.1, we can prove that $G\cong W_3$.

Subcase 2.2. $l\geqslant 2$. By the same method as Subcase 1.1, we can prove that $G\cong W_5$.

By the above arguments, this completes the proof. □

Corollary 4.2. *If $1\leqslant k\leqslant n-7$ and $G\in\mathcal{B}^3(n,k)$, then $\lambda(G)<\lambda(W_1)$.*

P r o o f. By Proposition 1.1,

$$\max\{\mu(W_2),\mu(W_3),\mu(W_4),\mu(W_5)\}=\max\{\lambda(W_2),\lambda(W_3),\lambda(W_4),\lambda(W_5)\}.$$

Combining with Proposition 1.1, Lemmas 4.2 and 4.5, we have

$$\lambda(G)\leqslant\mu(G)\leqslant\max\{\lambda(W_2),\lambda(W_3),\lambda(W_4),\lambda(W_5)\}<\lambda(W_1).$$

Thus, the conclusion follows. □

Lemma 4.6. *If $1\leqslant k\leqslant n-7$ and $G\in\mathcal{B}^4(n,k)$, then $\lambda(G)<\lambda(W_1)$.*

P r o o f. If $G\in\mathcal{B}^4(n,k)$, by Lemmas 3.7–3.8 it follows that

$$\lambda(G)\leqslant\max\{|N(u)\cup N(v)\colon\ u,v\in V(G)\}\leqslant k+5=\Delta(W_1)+1<\lambda(W_1).$$

This completes the proof. □

By Corollaries 4.1–4.2, Lemmas 4.4 and 4.6, we can conclude

Theorem 4.1. *If* $1 \leqslant k \leqslant n-7$ *and* $G \in \mathbb{B}(n,k)$, *then*

$$\lambda(G) \leqslant \lambda(W_1),$$

where the equality holds if and only if $G \cong W_1$.

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