On the least signless Laplacian eigenvalue of non-bipartite unicyclic graphs with both given order and diameter*

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Abstract

Let A be the $(0,1)$-adjacency matrix of a simple graph G and D be the diagonal matrix $\mathrm{diag}(d_1, d_2, \ldots, d_n)$, where d_i is the degree of the vertex v_i. $Q(G) = D + A$ is called the signless Laplacian of G. In this paper, we characterize the extremal graph in which the least signless Laplacian eigenvalue attains the minimum among all the non-bipartite unicyclic graphs with both given order and diameter.

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1 Introduction

All graphs considered here are connected, undirected and simple (i.e., loops and multiple edges are not allowed). Let $G = G[V(G), E(G)]$ be a graph with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, where $|V(G)| = n$ is the order and $|E(G)| = m$ is the size of G. For a graph G, the adjacency matrix of G is defined to be a matrix $A(G) = [a_{ij}]$, where $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. The degree matrix of

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G is denoted by $D(G) = diag(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$, where $d_G(v)$ or simply $d(v)$ denotes the degree of a vertex v in the graph G. The matrix $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix (or Q-matrix) of G. Note that $Q(G)$ is nonnegative, symmetric and positive semidefinite, so its eigenvalues are real and nonnegative. We simply call the eigenvalues of $Q(G)$ as the signless Laplacian eigenvalues or Q-eigenvalues of G and the eigenvalues can be arranged as:

$$q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0.$$

The signless Laplacian eigenvalues of a graph have recently attracted more and more researchers' attention, see [2-5] for the survey on this topic. One reason for this is that the signless Laplacian spectrum seems to be more informative than other commonly used graph matrices [2]. While there are many results about the largest eigenvalue of the signless Laplacian, the properties of its least eigenvalue are less well studied. A fundamental fact is that $q_n(G) = 0$ if and only if G is bipartite. This was firstly proven in 1994, in a notable early paper of Desai and Rao [7], who even suggested the use of $q_n(G)$ as a measure of non-bipartiteness of G. In a recent work, Lima et al. [6] survey the known results and presents some new ones about the least signless Laplacian eigenvalues of graphs. Cardoso et al. [1] prove that the minimum value of the least eigenvalue of the signless Laplacian of a connected non-bipartite graph with a prescribed number of vertices is attained solely in the unicyclic graph obtained from a triangle by attaching a path at one of its endvertices. Wang and Fan [11] investigate how the least eigenvalue of the signless Laplacian of a graph changes by relocating a bipartite branch from one vertex to another vertex, and minimize the least eigenvalue of the signless Laplacian among the class of connected graphs with fixed order which contains a given non-bipartite graph as an induced subgraph. For more results about $q_n(G)$, the reader is referred to [8-10].

A connected graph G with order n is called a unicyclic graph if $|E(G)| = n$. The diameter of a connected graph G is the maximum distance between pairs of vertices in $V(G)$. The girth of a graph G is the length of the shortest cycle in G. In this paper, we proceed to investigate the least signless Laplacian eigenvalues of non-bipartite unicyclic graphs. We characterize the extremal graph in which the least signless Laplacian eigenvalue attains the minimum among all the non-bipartite unicyclic graphs with both given order and diameter. Furthermore, we also characterize the extremal graph whose least signless Laplacian eigenvalue attains the minimum among all the non-bipartite unicyclic graphs with given order, girth and diameter.

2 Preliminary

Denote by C_n and P_n the cycle and the path, respectively, each on n vertices. Let $G-u$, $G-uv$ denote the graph that arises from G by deleting the vertex $u \in V(G)$ and the graph that arises from G by deleting 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 $u, v \in V(G)$. A pendant vertex of G is a vertex of degree 1. A pendant neighbor of G is a vertex adjacent to a pendant vertex. For $v \in V(G)$, $N_G(v)$ or simply $N(v)$ denotes the set of all neighbors of the vertex v in G. If the length of a path P is equal to the diameter, then the path P is called a diameter-path. We write $d_G(u,v)$ or simply $d(u,v)$ for the distance in G between vertices u and v, and $sgn(a)$ for the sign of the real number a.

Let $X = (x_1, x_2, \ldots, x_n)^T \in R^n$. Then X can be considered as a function defined on $V(G)$, that is, each vertex v_i is mapped to $x_i = x(v_i)$. If X is an eigenvector associated to a $Q-$eigenvalue, then it defines on G naturally, i.e. $x(v)$ is the entry of X corresponding to v. One can find in [6] that

$$X^TQ(G)X = \sum_{uv \in E(G)} [x(u) + x(v)]^2.$$

In addition, for an arbitrary unit vector $X \in R^n$,

$$q_n(G) \leq X^TQ(G)X,$$

with equality if and only if X is an eigenvector corresponding to $q_n(G)$.

Let G_1 and G_2 be two vertex-disjoint graphs, and let $v_1 \in V(G_1)$, $v_2 \in V(G_2)$. The coalescence of G_1 and G_2, denoted by $G_1(v_1) \diamond G_2(v_2)$, is obtained from G_1, G_2 by identifying v_1 with v_2 and forming a new vertex u (see [11] for detail). The graph $G_1(v_1) \diamond G_2(v_2)$ is also written as $G_1(u) \diamond G_2(u)$. If a connected graph G can be expressed in the form $G = G_1(u) \diamond G_2(u)$, where G_1 and G_2 are both nontrivial and connected, then G_1 is called a branch of G with root u. Clearly G_2 is also a branch of G in the above definition. Let X be a vector defined on $V(G)$. A branch H of G is called a zero branch with respect to X if $x(p) = 0$ for all $p \in V(H)$; otherwise it is called a nonzero branch with respect to X.

Lemma 2.1 ([11]) *Let G be a connected graph which contains a bipartite branch H with root u. Let X be an eigenvector of G corresponding to $q_n(G)$.*

(i) *If $x(u) = 0$, then H is a zero branch of G with respect to X.*

(ii) *If $x(u) \neq 0$, then $x(p) \neq 0$ for every vertex $p \in V(H)$. Furthermore, for every vertex $p \in V(H)$, $x(p)x(u)$ is either positive or negative, depending on whether p is or is not in the same part of the bipartite graph H as u; consequently, $x(p)x(q) < 0$ for each edge $pq \in E(H)$.*

Lemma 2.2 ([11]) *Let $G = G_1(v_2) \diamond G_2(u)$ and $G^* = G_1(v_1) \diamond G_2(u)$ be two graphs of order n, where G_1 is a connected graph containing two distinct vertices v_1, v_2, and G_2 is a connected bipartite graph containing a vertex u. If there exists an eigenvector $X =(x(v_1), x(v_2), \ldots, x(v_k), \ldots, x(u), \ldots)^T$ of G corresponding to $q_n(G)$ such that $|x(v_1)| \geq |x(v_2)|$, then $q_n(G^*) \leq q_n(G)$, with equality only if $|x(v_1)| = |x(v_2)|$ and $d_{G_2}(u)x(u) = -\sum_{v \in N_{G_2}(u)} x(v)$.*

Lemma 2.3 ([11]) *Let $G = G_1(v_2) \diamond S(u)$ and $G^* = G_1(v_1) \diamond S(u)$, where G_1 is a connected non-bipartite graph containing two distinct vertices v_1, v_2, and S is a nontrivial star with the center u. If there exists an eigenvector $X = (x(v_1), x(v_2), \ldots, x(v_k), \ldots, x(u), \ldots)^T$ of G corresponding to $q_n(G)$ such that $|x(v_1)| > |x(v_2)|$ or $|x(v_1)| = |x(v_2)| > 0$, then $q_n(G^*) < q_n(G)$.*

Lemma 2.4 ([11]) *Let G be a connected non-bipartite graph of order n, and let X be an eigenvector of G corresponding to $q_n(G)$. Let T be a tree, which is a nonzero branch of G with respect to X and with root u. Then $|x(q)| < |x(p)|$ whenever p, q are vertices of T such that q lies on the unique path from u to p.*

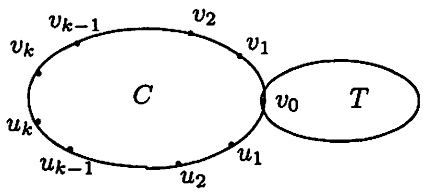

Fig. 2.1. G

Lemma 2.5 *Let G be a unicyclic graph with n vertices, $C = v_0v_1v_2\ldots v_k u_ku_{k-1}\ldots u_1v_0$ be the unique cycle in G. Suppose that $d_G(v_i) = 2$ and $d_G(u_i) = 2$ for $i = 1, \ldots, k$ (see Fig. 2.1). Then there exists an eigenvector $X = (x(v_0), x(v_1), x(v_2), \ldots, x(v_k), x(u_1), x(u_2), \ldots, x(u_k), \ldots)^T$ corresponding to $q_n(G)$, which satisfies the following:*

(i) $|x(v_0)| = \max\{|x(w)|\,|w \in V(C)\} > 0$;
(ii) $x(v_i) = x(u_i)$ *for* $i = 1, 2, \ldots, k$;
(iii) $x(v_i)x(v_{i-1}) \leq 0$ *and* $x(u_i)x(u_{i-1}) \leq 0$ *for* $i = 1, 2, \ldots, k$.

Proof. Suppose $Y = (y(v_0), y(v_1), \ldots, y(v_k), y(u_1), \ldots, y(u_k), \ldots)^T$ is an eigenvector corresponding to $q_n(G)$. If $|V(T)| = 1$, without loss of generality, we may assume that $|y(v_0)| = \max\{|y(w)|\,|w \in V(C)\}$. If $|V(T)| > 1$, we claim that

$$|y(v_0)| = \max\{|y(w)|\,|w \in V(C)\}.$$

Otherwise, without loss of generality, we suppose $|y(v_i)| > |y(v_0)|$ for some $1 \le i \le k$. Let

$$G' = G - \sum_{w \in N_T(v_0)} v_0 w + \sum_{w \in N_T(v_0)} v_i w.$$

By Lemma 2.2, $q_n(G') < q_n(G)$, which is a contradiction because $G' \cong G$. Furthermore, we claim $y(v_0) \neq 0$. Otherwise, by Lemma 2.1, T is a zero branch with respect to X. Then $X = 0$, which is a contradiction because X is an eigenvector.

If for $1 \le i \le k$, $y(v_i) = 0$, $y(u_i) = 0$, Lemma 2.5 holds obviously. Suppose that there exists $y(v_i) \neq 0$ or $y(u_i) \neq 0$ for some $1 \le i \le k$.

Let $Y' = (y'(v_0), y'(v_1), \ldots, y'(v_k), y'(u_1), \ldots, y'(u_k), \ldots)^T \in R^n$ satisfying that

$$y'(w) = \begin{cases} y(v_0), & w = v_0; \\ y(u_i), & w = v_i \ for \ i = 1,\ 2,\ \ldots,\ k; \\ y(v_i), & w = u_i \ for \ i = 1,\ 2,\ \ldots,\ k; \\ y(w), & others. \end{cases}$$

Then

$$q_n(G) \le \frac{Y'^T Q(G) Y'}{Y'^T Y'} = \frac{Y^T Q(G) Y}{Y^T Y} = q_n(G).$$

Hence Y' is also an eigenvector of G corresponding to $q_n(G)$. Let $Z = Y + Y'$. Since $z(v_0) = 2y(v_0) \neq 0$, it follows that $Z \neq 0$ and Z is also an eigenvector of G corresponding to $q_n(G)$ which satisfies both (i) and (ii).

Let $X = (x(v_0), x(v_1), \ldots, x(v_k), x(u_1), \ldots, x(u_k), \ldots)^T$ satisfying that

$$x(w) = (-1)^{d_G(v_0, w)} |z(w)| \ \ for \ \ w \in V(G).$$

Then

$$q_n(G) \le \frac{X^T Q(G) X}{X^T X} \le \frac{Z^T Q(G) Z}{Z^T Z} = q_n(G).$$

As a result, X is also an eigenvector of G corresponding to $q_n(G)$ which satisfies (i), (ii) and (iii). □

Lemma 2.6 *Let $3 \le k < n$ be odd, and let G be a unicyclic graph obtained from the cycle $C = v_1 v_2 \ldots v_k v_1$ by attaching rooted trees $T_1, \ldots, T_k$ to the vertices $v_1, \ldots, v_k$, respectively, where T_i contains the root vertex v_i and $|V(T_i)| = 1$ means $V(T_i) = \{v_i\}$. Let*

$$G' = G - \sum_{i=2}^{k} \sum_{w \in N_{T_i}(v_i)} v_i w + \sum_{i=2}^{k} \sum_{w \in N_{T_i}(v_i)} v_1 w.$$

Then $d(G') \le d(G)$.

Proof. Let $d(G') = d'$, $P = v_{i_1} v_{i_2} \dots v_{i_{d'}} v_{i_{d'+1}}$ be a diameter-path of G'. It is not difficult to see that at least one of v_{i_1} and $v_{i_{d'+1}}$ is a pendent vertex. Now we distinguish two cases to show that $d(G') \le d(G)$.

Case 1. Both v_{i_1} and $v_{i_{d'+1}}$ are pendent vertices. If v_{i_1} and $v_{i_{d'+1}}$ are on two different rooted trees T_i and T_j, then v_1 is a vertex in the path P. Let $P_1 = v_{i_1} \dots v_1$, $P_2 = v_1 \dots v_{i_{d'+1}}$. Without loss of generality, we assume that the path P_1 is in T_i and the path P_2 is in T_j. Then $v_{i_1} \dots v_i$ is the unique path from v_{i_1} to v_i of G, and $v_j \dots v_{i_{d'+1}}$ is the unique path from $v_{i_{d'+1}}$ to v_j of G. Therefore $d_G(v_{i_1}, v_{i_{d'+1}}) > d'$, namely $d(G') < d(G)$.

If both v_{i_1} and $v_{i_{d'+1}}$ are on the same rooted tree T_i, then P is also the unique path from v_{i_1} to $v_{i_{d'+1}}$ of G. Therefore $d(G') \le d(G)$.

Case 2. One of v_{i_1} and $v_{i_{d'+1}}$ is a pendent vertex, the other is a vertex of the cycle. Without loss of generality, we assume that v_{i_1} is a vertex of the cycle and $v_{i_{d'+1}}$ is on the tree T_i, then $i_1 = \lfloor \frac{k+2}{2} \rfloor$ or $i_1 = \lceil \frac{k+2}{2} \rceil$. Let v_t is a vertex of the cycle such that $d_G(v_t, v_i) = \lfloor \frac{k}{2} \rfloor$. Then $D_G(v_t, v_{i_{d'+1}}) = d'$. Therefore $d(G') \le d(G)$. □

Let $k \ge 3$ be odd. Let $C^*_{k,l}$ be the graph of order n obtained by attaching a cycle C_k to an end vertex of a path P_{l+1} and attaching $n-k-l$ pendant edges to the other end vertex of the path P_{l+1} (see Fig. 2.2). And $l = 0$ means attaching $n-k$ pendant edges to the vertex v_k of C_k.

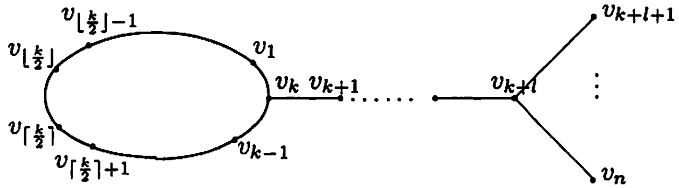

Fig. 2.2. $C^*_{k,l}$

Lemma 2.7 *Let $3 \le k \le n-2$ be odd, and let both $C^*_{k,l}$ and $C^*_{k,l+1}$ have order n. Then $q_n(C^*_{k,l+1}) < q_n(C^*_{k,l})$.*

Proof. Let $Y = (y(v_1), y(v_2), \dots, y(v_k), \dots)^T$ be an eigenvector corresponding to $q_n(C^*_{k,l})$ satisfying Lemma 2.5. By Lemmas 2.4 and 2.5, we have $0 < |y(v_{k+l})| < |y(v_{k+l+1})|$. Note that

$$C^*_{k,l+1} = C^*_{k,l} - \sum_{j=k+l+2}^{n} v_{k+l} v_j + \sum_{j=k+l+2}^{n} v_{k+l+1} v_j.$$

By Lemma 2.2, we have $q_n(C^*_{k,l+1}) < q_n(C^*_{k,l})$. □

3 Main results

Theorem 3.1 *Among all the non-bipartite unicyclic graphs with both given order n and given diameter d, we have*

(i) *if $d = 1$, then the graph is isomorphic to K_3;*

(ii) *if $d \geq 2$, then the least signless Laplacian eigenvalue of a graph attains the minimum uniquely at $C^*_{3,\,d-2}$.*

Proof. (i) It is easy to verify that if $d(G) = 1$ then $G = K_3$.

(ii) Suppose that $d \geq 2$. Let G be a non-bipartite unicyclic graph with both given order n and given diameter d, and $C = v_1 v_2 \dots v_k v_1$ (k is odd) be the unique cycle in G. A unicyclic graph is either a cycle or a cycle with trees attached. Then G can be obtained by attaching rooted trees T_1, ..., T_k to the vertices v_1, ..., v_k, respectively, where T_i contains the root vertex v_i. $|V(T_i)| = 1$ means that $V(T_i) = \{v_i\}$ and in this case T_i is called a trivial tree. Now we assume that $G \neq C^*_{3,\,d-2}$, it suffices to prove that $q_n(C^*_{3,\,d-2}) < q_n(G)$.

Case 1. $G = C^*_{k,\,l}$ and G is not an odd cycle. Then G has at least one pendent vertex. Since $G \neq C^*_{3,\,d-2}$, it follows that $k > 3$. Let $Y = (y(v_1), y(v_2), \dots, y(v_k), \dots)^T$ be an eigenvector corresponding to $q_n(G)$ satisfying Lemma 2.5. Then

$$q_n(G) = \frac{Y^T Q(G) Y}{Y^T Y},$$

and we may assume that $|y(v_k)| = \max\{|y(v_i)|\,|i = 1, 2, \dots, k\} > 0$,

$$|y(v_i)| \leq |y(v_k)| \leq |y(v_{k+l})|, \quad 1 \leq i \leq k.$$

Let

$$G^* = G - v_1 v_k - \sum_{i=1}^{\lfloor \frac{k}{2} \rfloor - 1} v_i v_{i+1} + \sum_{i=1}^{\lfloor \frac{k}{2} \rfloor - 1} v_i v_{k+l} + v_{\lfloor \frac{k}{2} \rfloor} v_{\lceil \frac{k}{2} \rceil + 1},$$

and $Z = (z(v_1), z(v_2), \dots, z(v_k), \dots)^T \in R^n$, in which $z(w)$ corresponds to the vertex w of G satisfying

$$z(w) = \begin{cases} -\mathrm{sgn}(y(v_{k+l}))(|y(v_{k+l})| + |y(v_i) + y(v_{i-1})|), & w = v_i\ ,\ i = 1,\ \dots,\ \lfloor \frac{k}{2} \rfloor - 1; \\ y(w), & \text{others}, \end{cases}$$

where $v_0 = v_k$. Then

$$Z^T Q(G^*) Z = Y^T Q(G) Y, \qquad Z^T Z \geq Y^T Y.$$

As a result, we get that

$$q_n(G^*) \leq \frac{Z^T Q(G^*) Z}{Z^T Z} \leq \frac{Y^T Q(G) Y}{Y^T Y} = q_n(G).$$

By $k > 3$, we claim that $q_n(G^*) < q_n(G)$. Otherwise, suppose $q_n(G^*) = q_n(G)$. Then Z is an eigenvector corresponding to $q_n(G^*)$ and $Z^TZ = Y^TY$. Therefore,

$$[q_n(G^*) - 1]z(v_1) = z(v_{k+l}), \ |y(v_1) + y(v_k)| = 0,$$

and so

$$-\text{sgn}(y(v_{k+l}))\,(q_n(G^*)-1)\,(|y(v_{k+l})|+|y(v_k)+y(v_1)|) = \text{sgn}(y(v_{k+l}))\,|y(v_{k+l})|.$$

It follows that

$$q_n(G^*)|y(v_{k+l})| = (1 - q_n(G^*))\,|y(v_k) + y(v_1)|) = 0.$$

Since $q_n(G^*) \neq 0$, then $y(v_{k+l}) = 0$. Noting that

$$|y(v_i)| \leq |y(v_k)| \leq |y(v_{k+l})| = 0, \quad i = 1, 2, \ldots .k,$$

by Lemma 2.1, we have $Y = 0$. This is a contradiction because Y is an eigenvector corresponding to $q_n(G)$. Therefore $q_n(G^*) < q_n(G)$.

Note that $G^* = C^*_{3,\,t}$, $t = l + \lfloor \frac{k}{2} \rfloor - 1$,

$$t + 2 = d(C^*_{3,\,t}) = d(G^*) = d(G) = d.$$

Therefore $t = d - 2$. Namely $q_n(C^*_{3,\,d-2}) < q_n(G)$.

Case 2. G is the cycle $C = v_1v_2 \ldots v_kv_1$ with only one nontrivial tree attached, and $G \neq C^*_{k,\,l}$. Without loss of generality, we assume that T_k is the nontrivial tree. Then T_k have at least two pendant neighbors. Let $X = (x(v_1), x(v_2), \ldots, x(v_k), \ldots)^T$ be an eigenvector corresponding to $q_n(G)$ satisfying Lemma 2.5. Then

$$|x(v_k)| = \max\{|x(w)| \;|w \in V(C)\} > 0,$$

and so T_k is a nonzero branch with respect to X. Namely, $|x(v_i)| > 0$ for any $v_i \in V(T_k)$. Let

$$|x(v_c)| = \max\{|x(v_i)|\,|v_i \in V(T_k), v_i \text{ is not a pendant vertex}\}.$$

Denote by P the unique path from v_k to v_c in G. By Lemma 2.4, we know that any vertex adjacent to v_c and not in P must be a pendant vertex.

Suppose that v_b is another pendant neighbor and $v_{i_1}, \ldots, v_{i_t}$ are all the pendant vertices adjacent to v_b. Then $|v_c| \geq |v_b| > 0$. Let

$$G' = G - \sum_{j=1}^{t} v_bv_{i_j} + \sum_{j=1}^{t} v_cv_{i_j}.$$

By Lemma 2.3, we have $q_n(G') < q_n(G)$. It is not difficult to see $d(G') \leq d(G)$.

If G' has at least two pendant neighbors, repeating the above procedure, we can transform G' into a non-bipartite unicyclic graph $G_1 = C^*_{k,l}$ of order n, and

$$q_n(G_1) = q_n(C^*_{k,l}) < q_n(G), \qquad d(G_1) = d(C^*_{k,l}) \leq d(G).$$

Let $d_1 = d(G_1)$. Then $d_1 \leq d$. By Case 1, we have

$$q_n(C^*_{3,d_1-2}) \leq q_n(G_1),$$

with equality if and only if $k = 3$. Furthermore, by Lemma 2.7, we have

$$q_n(C^*_{3,d-2}) \leq q_n(C^*_{3,d_1-2}) \leq q_n(G_1) < q_n(G).$$

Case 3. There are at least two nontrivial trees attaching at the cycle $C = v_1v_2\dots v_kv_1$. Let T_i and T_j be two nontrivial trees. Suppose $Y = (y(v_1), y(v_2), \dots, y(v_k), \dots)^T$ is an eigenvector corresponding to $q_n(G)$. Without loss of generality, we may assume that $|y(v_i)| \geq |y(v_j)|$. Let

$$G' = G - \sum_{w \in N_{T_j}(v_j)} v_j w + \sum_{w \in N_{T_j}(v_j)} v_i w.$$

By Lemma 2.2, we have $q_n(G') \leq q_n(G)$. If G' has more than one nontrivial trees attached at the cycle $C = v_1v_2\dots v_kv_1$, repeating the above procedure, we can transform G' into a non-bipartite unicyclic graph G_1 of order n, where G_1 is the cycle $C = v_1v_2\dots v_kv_1$ with only one nontrivial tree attached and $q_n(G_1) \leq q_n(G)$. By Lemma 2.6, we have $d(G_1) \leq d(G)$. Let $d_1 = d(G_1)$. Then $d_1 \leq d$.

If $G_1 \neq C^*_{k,l}$, by Case 2, we have

$$q_n(C^*_{3,d_1-2}) < q_n(G_1) \leq q_n(G).$$

Furthermore, by Lemma 2.7, we have

$$q_n(C^*_{3,d-2}) \leq q_n(C^*_{3,d_1-2}) < q_n(G_1) \leq q_n(G).$$

If $G_1 = C^*_{k,l}$, noting that G has more than one nontrivial trees attached at the cycle $C = v_1v_2\dots v_kv_1$, then $l = 0$. It follows that all the trees attached at the cycle $C = v_1v_2\dots v_kv_1$ are star. If $k > 3$, by Case 1, we have

$$q_n(C^*_{3,d_1-2}) < q_n(G_1) \leq q_n(G).$$

Furthermore, by Lemma 2.7, we have

$$q_n(C^*_{3,\,d-2}) \le q_n(C^*_{3,\,d_1-2}) < q_n(G_1) \le q_n(G).$$

If $k = 3$, then $G_1 = C^*_{3,\,0}$. It follows that G is C_3 with at least two vertices attached by pendant edges. Namely, $d(G) = 3$. By Lemma 2.7, we have

$$q_n(C^*_{3,\,d-2}) = q_n(C^*_{3,\,1}) < q_n(C^*_{3,\,0}) = q_n(G_1) \le q_n(G).$$

Case 4. $G = C_n$. Let $Y = (y(v_1), y(v_2), \ldots, y(v_k), \ldots)^T$ be an eigenvector corresponding to $q_n(G)$ satisfying Lemma 2.5. Then

$$q_n(G) = \frac{Y^T Q(G) Y}{Y^T Y},$$

and we may assume that $|y(v_n)| = \max\{|y(v_i)|\,|i = 1, 2, \ldots, n\} > 0$, and $y(v_i) = y(v_{n-i}),\ i = 1, 2, \ldots, \lfloor \frac{n}{2} \rfloor$. Let

$$G^* = G - v_1 v_n - \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} v_i v_{i+1} + \sum_{i=1}^{\lfloor \frac{n}{2} \rfloor - 1} v_i v_{n-i} + v_{\lfloor \frac{n}{2} \rfloor} v_{\lceil \frac{n}{2} \rceil + 1},$$

and $Z = (z(v_1), z(v_2), \ldots, z(v_n))^T \in R^n$, in which $z(w)$ corresponds to the vertex w of G satisfying

$$z(w) = \begin{cases} -y(v_i), & w = v_i\ ,\ i = 1,\ \ldots,\ \lfloor \frac{k}{2} \rfloor - 1; \\ y(w), & \text{others.} \end{cases}$$

Then

$$Z^T Q(G^*) Z \le Y^T Q(G) Y, \qquad Z^T Z = Y^T Y.$$

Therefore

$$q_n(G^*) \le \frac{Z^T Q(G^*) Z}{Z^T Z} \le \frac{Y^T Q(G) Y}{Y^T Y} = q_n(G).$$

Note that G^* is a unicyclic graph with order n, girth 3 and diameter d. If $G^* \ne C^*_{3,\,d-2}$, by Case 2, we have

$$q_n(C^*_{3,\,d-2}) < q_n(G^*) \le q_n(G).$$

If $G^* = C^*_{3,\,d-2}$, then $d = 2$ and $n = 5$. Namely, $G = C_5$. Using the well known mathematics software Matlab, it is easy to compute that

$$q_5(C^*_{3,\,0}) < q_5(C_5) = q_n(G).$$

Combining Cases 1-4, if $G \ne C^*_{3,\,d-2}$, we have $q_n(C^*_{3,\,d-2}) < q_n(G)$. □

In a same way as Theorem 3.1, we can characterize the extremal graph whose least signless Laplacian eigenvalue attains the minimum among the non-bipartite unicyclic graphs with given order n, girth g and diameter d.

Theorem 3.2 *Among all the non-bipartite unicyclic graphs with order n, girth g and diameter d, we have*

(i) *if $d = 1$, then the graph is isomorphic to K_3;*

(i) *if $g = n$, then the graph is isomorphic to C_n;*

(iii) *if $d \geq 2$ and $g < n$, then the least signless Laplacian eigenvalue of a graph attains the minimum uniquely at $C^*_{g,d-\lceil \frac{g}{2} \rceil}$.*

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