Journal of Inequalities and Applications
a SpringerOpen Journal

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Ordering non-bipartite unicyclic graphs with pendant vertices by the least Q-eigenvalue

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Abstract

A unicyclic graph is a connected graph whose number of edges is equal to the number of vertices. Fan *et al.* (Discrete Math. 313:903-909, 2013) and Liu *et al.* (Electron. J. Linear Algebra 26:333-344, 2013) determined, independently, the unique unicyclic graph whose least Q-eigenvalue attains the minimum among all non-bipartite unicyclic graphs of order n with k pendant vertices. In this paper, we extend their results and determine the first three non-bipartite unicyclic graphs of order n with k pendant vertices ordering by least Q-eigenvalue.

MSC: 05C50

Keywords: signless Laplacian; least eigenvalue; unicyclic graph; pendant vertex

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E = E(G)$, where n is called the order of G. Let $A(G)$ be the adjacency matrix of a graph G and let $D(G) = \mathrm{diag}(d_G(v_1), d_G(v_2), \ldots, d_G(v_n))$ be the diagonal matrix of degrees of G, where $d_G(v)$ or simply $d(v)$ denotes the degree of a vertex v in G. The matrix $Q(G) = D(G) + A(G)$ is called the signless Laplacian matrix (or Q-matrix) of G. Since $Q(G)$ is symmetric and positive semidefinite, it follows that its eigenvalues are real and non-negative. We simply call the eigenvalues of $Q(G)$ as the signless Laplacian eigenvalues or Q-eigenvalues of G. As usual, we shall index the eigenvalues of $Q(G)$ in nonincreasing order and denote them as $q_1(G) \geq q_2(G) \geq \cdots \geq q_n(G) \geq 0$. Denote by $\kappa(G)$ the least Q-eigenvalue of G.

For a connected graph G, Desai and Rao [3] showed that $\kappa(G) = 0$ if and only if G is bipartite, and suggested that $\kappa(G)$ can be used as a measure of non-bipartiteness of G. *For a connected non-bipartite graph G, how small can $\kappa(G)$ be?* Cardoso *et al.* [4] proposed this problem and proved that the minimum value of $\kappa(G)$ of a connected non-bipartite graph G of order n is attained solely in the unicyclic graph that arises from a cycle of order 3 by attaching a path at one of its end vertices. Wang and Fan [5] investigated how the least Q-eigenvalue of a graph changes when a bipartite branch attached at one vertex is relocated to another vertex and proved a perturbation theorem on the least Q-eigenvalue. As an application, they minimized the least Q-eigenvalue among the class of connected graphs with fixed order which contains a given non-bipartite graph as an induced subgraph. Recently, the problem of finding all graphs with the minimal least Q-eigenvalue among a given class of graphs has been studied extensively. For related results, one may refer to [1, 2, 5–12].

A c-cyclic graph G is a connected graph with n vertices and $n + c - 1$ edges. Specially, if $c = 0$, 1, or 2, then G is a tree, a unicyclic graph, or a bicyclic graph, respectively. Very recently, Fan *et al.* [1] and Liu *et al.* [2] determined, independently, the unique unicyclic graph whose least Q-eigenvalue attains the minimum among all non-bipartite unicyclic graphs of order n with k pendant vertices. In this paper, we extend their results and determine the first three non-bipartite unicyclic graphs of order n with k pendant vertices ordering by least Q-eigenvalue.

The rest of the paper is organized as follows. In Section 2, we recall some basic notions and lemmas used further, and prove two new lemmas. In Section 3, we order non-bipartite unicyclic graphs of order n with k pendant vertices. In Section 4, a conjecture is proposed.

2 Preliminaries

Denote by C_n the cycle of order n. Let $G - uv$ denote the graph obtained from G by deleting the edge $uv \in E(G)$. Similarly, $G + uv$ is the graph obtained from G by adding an edge $uv \notin E(G)$, where $u, v \in V(G)$. We write $d_G(u, v)$ or simply $d(u, v)$ for the distance in G between vertices u and v. The diameter of a connected graph G is the maximum distance between pairs of vertices in $V(G)$. For $v \in V(G)$, $N_G(v)$ or simply $N(v)$ denotes the neighborhood of v in 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.

Let $x = (x_1, x_2, \dots, x_n)^T$ be a column vector in $\mathbb{R}^n$. Then x can be considered as a function defined on $V(G)$, that is, each vertex v_i is given by the value $x(v_i) = x_i$. Then the quadratic form

$$x^T Q(G)x = \sum_{uv \in E(G)} \bigl(x(u) + x(v)\bigr)^2.$$

Let $|x(v)|$ denote the absolute value of $x(v)$. If x is an eigenvector corresponding to a Q-eigenvalue of G, then it defines on $V(G)$ naturally, *i.e.* $x(v)$ is the entry of x corresponding to v. For an arbitrary unit vector $x \in \mathbb{R}^n$, one can find in [5, 13]

$$\kappa(G) \le x^T Q(G)x, \tag{1}$$

where equality holds if and only if x is an eigenvector corresponding to $\kappa(G)$.

Let G_1 and G_2 be two vertex-disjoint graphs, and let $v_1 \in V(G_1)$, $v_2 \in V(G_2)$. $G_1(v_1) \diamond G_2(v_2)$ denotes the coalescence of G_1 and G_2, which arises from G_1, G_2 by identifying v_1 with v_2 and forming a new vertex u (see [5] for details). The graph $G_1(v_1) \diamond G_2(v_2)$ is also written as $G_1(u) \diamond G_2(u)$. If a graph G can be expressed in the form $G = G_1(u) \diamond G_2(u)$, where G_1 and G_2 are both connected and nontrivial, then G_i is called a branch of G with root u for $i = 1, 2$. Let x be a vector defined on $V(G)$. A branch H of G is called a zero branch with respect to x if $x(v) = 0$ for all $v \in V(H)$; otherwise it is called a nonzero branch with respect to x.

Lemma 2.1 ([5]) *Let G be a connected graph which contains a bipartite branch B with root v. Let x be an eigenvector of G corresponding to $\kappa(G)$.*

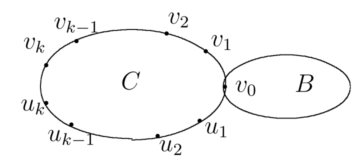

Figure 1 $C(v_0) \diamond B(v_0)$.

(i) *If* $x(v) = 0$, *then* B *is a zero branch of* G *with respect to* x.
(ii) *If* $x(v) \neq 0$, *then* $x(p) \neq 0$ *for every vertex* $p \in V(B)$.

Lemma 2.2 ([5]) *Let* G *be a connected non-bipartite graph of order* n, *and let* x *be an eigenvector of* G *corresponding to* $\kappa(G)$. *Let* T *be a tree, which is a nonzero branch of* G *with respect to* x *and with root* v. *Then* $|x(q)| < |x(p)|$ *whenever* p, q *are vertices of* T *such that* q *lies on the unique path from* v *to* p.

Lemma 2.3 ([10]) *Let* $G = C(v_0) \diamond B(v_0)$ *be a graph of order* n, *where* $C = v_0v_1v_2 \cdots v_k \times u_ku_{k-1} \cdots u_1v_0$ *is a cycle of length* $2k + 1$, *and* B *is a bipartite graph of order* $n - 2k > 1$ (*see Figure* 1). *Let* $x = (x(v_0), x(v_1), x(v_2), \dots, x(v_k), x(u_1), x(u_2), \dots, x(u_k), \dots)^T$ *be an eigenvector corresponding to* $\kappa(G)$. *Then*
(i) $|x(v_0)| = \max\{|x(w)| \mid w \in V(C)\} > 0$;
(ii) $x(v_i) = x(u_i)$ *for* $i = 1, 2, \dots, k$.

Lemma 2.4 ([10]) *Let* $G = G_1(v_2) \diamond T(u)$ *and* $G^* = G_1(v_1) \diamond T(u)$, *where* G_1 *is a non-bipartite connected graph containing two distinct vertices* v_1, v_2, *and* T *is a nontrivial tree. If there exists an eigenvector* $x = (x(v_1), x(v_2), \dots, x(v_k), \dots)^T$ *of* G *corresponding to* $\kappa(G)$ *such that* $|x(v_1)| > |x(v_2)|$ *or* $|x(v_1)| = |x(v_2)| > 0$, *then* $\kappa(G^*) < \kappa(G)$.

Lemma 2.5 ([14]) *Let* G *be a graph with* n *vertices and* m *edges. Then*

$$\kappa(G) \leq \frac{4m - 4\,\mathrm{MaxCut}(G)}{n},$$

where $\mathrm{MaxCut}(G)$ *denotes, as usual, the size of the largest bipartite subgraph of* G.

For a c-cyclic graph G, we have $\mathrm{MaxCut}(G) \geq n - 1$. This implies the following lemma.

Lemma 2.6 *Let* G *be a* c*-cyclic graph. Then* $\kappa(G) \leq \frac{4c}{n}$.

Lemma 2.7 ([15]) *Let* G *be a non-bipartite connected graph of order* n *with diameter* D. *Then* $\kappa(G) \geq \frac{1}{n(D+1)}$.

$U_n^k(g)$, shown in Figure 2, denotes the unicyclic graph of order n with odd girth g and k pendant vertices, where $g + l + k = n$. $C_3^1(n-k-1)$, $C_3^2(n-k-1)$, and $C_3^1(n-k-2)$ are the unicyclic graphs of order n with k pendant vertices, shown in Figures 2 and 3, respectively.

Lemma 2.8 *Let* $3 \leq k \leq (n-4)/\sqrt{6}$. *Then* $\kappa(C_3^2(n-k-1)) < \kappa(C_3^1(n-k-2))$.

Proof Let $\kappa = \kappa(C_3^1(n-k-2))$, and $x = (x_1, x_2, \dots, x_n)^T$ be a unit eigenvector corresponding to κ. Then $\kappa = \sum_{v_iv_j \in E(C_3^1(n-k-2))} (x_i + x_j)^2$ and $0 < \kappa < 1$ (by Lemma 2.6). From the eigenvalue

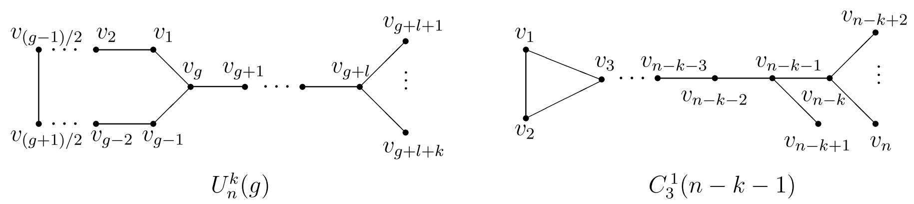

Figure 2 $U_n^k(g)$ **and** $C_3^1(n-k-1)$**.**

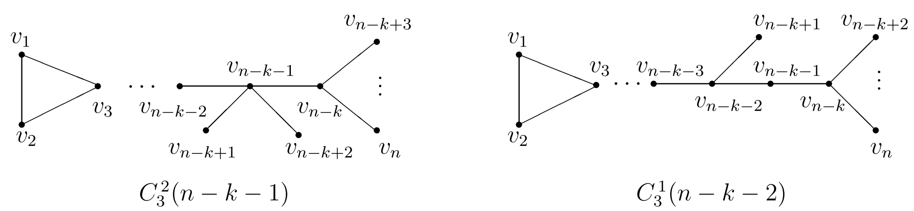

Figure 3 $C_3^2(n-k-1)$ **and** $C_3^1(n-k-2)$**.**

equation $Q(C_3^1(n-k-2))x = \kappa x$, we have $x_{n-k+2} = \cdots = x_n$,

$$\begin{aligned}
x_{n-k} &= (\kappa - 1)x_n,\\
x_{n-k-1} &= \bigl(\kappa^2 - (k+1)\kappa + 1\bigr)x_n,\\
x_{n-k-2} &= \bigl(\kappa^3 - (k+3)\kappa^2 + (2k+2)\kappa - 1\bigr)x_n,\\
x_{n-k+1} &= \frac{1}{\kappa - 1}\bigl(\kappa^3 - (k+3)\kappa^2 + (2k+2)\kappa - 1\bigr)x_n,
\end{aligned}$$

and $x_n \neq 0$.

Let $y = (y_1, y_2, \ldots, y_n)^T \in \mathbb{R}^n$, which is defined on $V(C_3^2(n-k-1))$, satisfy $y_{n-k+1} = -(x_{n-k-1} + x_{n-k-2} + x_{n-k+1})$, $y_{n-k+2} = -(x_{n-k-1} + x_{n-k+2} + x_{n-k})$, and $y_i = x_i$ for $i = 1, 2, \ldots, n-k$, $n-k+3, \ldots, n$. Then

$$\sum_{v_iv_j \in E(C_3^2(n-k-1))} (y_i + y_j)^2 = \sum_{v_iv_j \in E(C_3^1(n-k-2))} (x_i + x_j)^2 = \kappa$$

and

$$\begin{aligned}
\|y\|^2 - \|x\|^2 &= \sum_{i=1}^n y_i^2 - \sum_{i=1}^n x_i^2\\
&= \kappa\bigl(\kappa^5 - (2k+2)\kappa^4 + \bigl(k^2 + 2k - 1\bigr)\kappa^3 + (4k+6)\kappa^2\\
&\quad - \bigl(2k^2 + 6k + 3\bigr)\kappa + 2\bigr)x_n^2.
\end{aligned}$$

Let $f(t) = t^5 - (2k+2)t^4 + (k^2+2k-1)t^3 + (4k+6)t^2 - (2k^2+6k+3)t + 2$. It is not difficult to verify that $f(t) > 0$ for $0 \leq t \leq 1/(k^2+3k+2)$.

Let $z = (z_1, z_2, \ldots, z_n)^T \in \mathbb{R}^n$, which is defined on $V(C_3^1(n-k-2))$, satisfy $z_1 = z_2 = 0$, $z_{n-k+1} = (-1)^{n-k+1}(n-k-3)$,

$$z_{n-k-i} = (-1)^{n-k-i}(n-k-i-2) \quad \text{for } 0 \le i \le n-k-3,$$
$$z_{n-k+i} = (-1)^{n-k+1}(n-k-1) \quad \text{for } i = 2,3,\ldots,k.$$

Then, by (1) and $3 \le k \le (n-4)/\sqrt{6}$, we have

$$\begin{aligned}
\kappa = \kappa\bigl(C_3^1(n-k-2)\bigr) &\le \frac{z^T Q(G) z}{z^T z} \\
&= \frac{n-1}{1^2 + 2^2 + \cdots + (n-k-2)^2 + (n-k-3)^2 + (k-1)(n-k-1)^2} \\
&= \frac{6(n-1)}{2n^3 - 9n^2 - (6k^2 - 6k + 11)n + 4k^3 + 3k^2 + 17k + 42} < \frac{1}{k^2 + 3k + 2}.
\end{aligned}$$

Therefore $f(\kappa) > 0$, and so

$$\|y\|^2 - \|x\|^2 = \kappa f(\kappa) x_n^2 > 0.$$

Combining the above arguments, we have

$$\begin{aligned}
\kappa\bigl(C_3^2(n-k-1)\bigr) &\le \|y\|^{-2} \sum_{v_i v_j \in E(C_3^2(n-k-1))} (y_i + y_j)^2 < \|x\|^{-2} \sum_{v_i v_j \in E(C_3^1(n-k-2))} (x_i + x_j)^2 \\
&= \kappa.
\end{aligned}$$

□

Lemma 2.9 *Let $n \ge 120$, $k > \frac{-3+\sqrt{21}}{2} n$. Then $\kappa(C_3^1(n-k-2)) < \kappa(C_3^2(n-k-1))$.*

Proof Let $\kappa = \kappa(C_3^2(n-k-1))$, and $x = (x_1, x_2, \ldots, x_n)^T$ be a unit eigenvector corresponding to κ. Then $\kappa = \sum_{v_i v_j \in E(C_3^2(n-k-1))} (x_i + x_j)^2$ and $0 < \kappa < 1$. From the eigenvalue equation $Q(C_3^2(n-k-1))x = \kappa x$, we have $x_{n-k+3} = \cdots = x_n$,

$$\begin{aligned}
x_{n-k} &= (\kappa - 1)x_n, \\
x_{n-k-1} &= \bigl(\kappa^2 - k\kappa + 1\bigr)x_n, \\
x_{n-k+1} = x_{n-k+2} &= \frac{1}{\kappa - 1}\bigl(\kappa^2 - k\kappa + 1\bigr)x_n, \\
x_{n-k-2} &= \frac{1}{\kappa - 1}\bigl(\kappa^4 - (k+5)\kappa^3 + (5k+2)\kappa^2 - (2k+3)\kappa + 1\bigr)x_n,
\end{aligned}$$

and $x_n \neq 0$.

Let $y = (y_1, y_2, \ldots, y_n)^T \in \mathbb{R}^n$, which is defined on $V(C_3^1(n-k-2))$, satisfy that $y_{n-k+1} = -(x_{n-k-1} + x_{n-k-2} + x_{n-k+1})$, $y_{n-k+2} = -(x_{n-k-1} + x_{n-k+2} + x_{n-k})$, and $y_i = x_i$ for $i = 1,2,\ldots,n-k$, $n-k+3, n-k+4, \ldots, n$. Then

$$\sum_{v_i v_j \in E(C_3^1(n-k-2))} (y_i + y_j)^2 = \sum_{v_i v_j \in E(C_3^2(n-k-1))} (x_i + x_j)^2 = \kappa$$

and

$$\begin{aligned}\|y\|^2 - \|x\|^2 &= \sum_{i=1}^{n} y_i^2 - \sum_{i=1}^{n} x_i^2 \\ &= \frac{\kappa}{\kappa - 1}\bigl(\kappa^6 - (2k+7)\kappa^5 + \bigl(k^2 + 14k + 14\bigr)\kappa^4 - \bigl(7k^2 + 28k + 4\bigr)\kappa^3 \\ &\quad + \bigl(14k^2 + 6k + 15\bigr)\kappa^2 - \bigl(2k^2 + 14k + 1\bigr)\kappa^2 + 6\bigr)x_n^2.\end{aligned}$$

Let

$$\begin{aligned}f(t) = {} & t^6 - (2k+7)t^5 + \bigl(k^2 + 14k + 14\bigr)t^4 - \bigl(7k^2 + 28k + 4\bigr)t^3 + \bigl(14k^2 + 6k + 15\bigr)t^2 \\ & - \bigl(2k^2 + 14k + 1\bigr)t + 6.\end{aligned}$$

Then $f(0) = 6$. From $n \geq 120$ and $k > \frac{-3+\sqrt{21}}{2}n$, we have $k > \frac{-3+\sqrt{21}}{2}n > 94$, and

$$\begin{aligned}k^{12}f\bigl(1/k^2\bigr) &= 4k^{12} - 14k^{11} + 13k^{10} + 6k^9 + 8k^8 - 28k^7 - 3k^6 + 14k^5 \\ &\quad + 14k^4 - 2k^3 - 7k^2 + 1 > 0, \\ k^{12}f\bigl(3/k^2\bigr) &= -42k^{11} + 123k^{10} + 54k^9 - 54k^8 - 756k^7 - 27k^6 \\ &\quad + 1134k^5 + 1134k^4 - 486k^3 - 1701k^2 + 729 < 0, \\ f'(t) &= 6t^5 - (10k+35)t^4 + \bigl(4k^2 + 56k + 56\bigr)t^3 - \bigl(21k^2 + 84k + 12\bigr)t^2 \\ &\quad + \bigl(28k^2 + 12k + 30\bigr)t - \bigl(2k^2 + 14k + 1\bigr) < 0,\end{aligned}$$

for $0 \leq t \leq 1/30$. So $f(t)$ is strictly decreasing with respect to t in $[0, 1/30]$. Recalling that $k > \frac{-3+\sqrt{21}}{2}n$, by Lemmas 2.6 and 2.7, we find that

$$\frac{3}{k^2} < \frac{1}{n(n-k)} \leq \kappa = \kappa\bigl(C_3^2(n-k-1)\bigr) \leq \frac{4}{n} \leq \frac{1}{30}.$$

This implies that $f(\kappa) < 0$ and

$$\|y\|^2 - \|x\|^2 = \frac{\kappa}{\kappa - 1} f(\kappa) x_n^2 > 0.$$

It follows that

$$\begin{aligned}\kappa\bigl(C_3^1(n-k-2)\bigr) &\leq \|y\|^{-2} \sum_{v_iv_j \in E(C_3^1(n-k-2))} (y_i + y_j)^2 < \|x\|^{-2} \sum_{v_iv_j \in E(C_3^2(n-k-1))} (x_i + x_j)^2 \\ &= \kappa.\end{aligned}$$

□

3 Main results

Let $\mathcal{U}_n^k$ be the set of non-bipartite unicyclic graphs of order n with k pendant vertices. From [1, 2], we know that $U_n^k(3)$ is the unique graph whose least Q-eigenvalue attains the minimum among all graphs in $\mathcal{U}_n^k$. In this section, we will determine the first three graphs in $\mathcal{U}_n^k$ ordered according to their least Q-eigenvalues.

For $k = 1$, from [1], we know that $\kappa(U_n^1(3)) < \kappa(U_n^1(5)) < \kappa(U_n^1(7)) < \cdots$.

Theorem 3.1 *Let $2 \leq k \leq n-4$. Among all graphs in $\mathcal{U}_n^k \backslash \{U_n^k(3)\}$, $C_3^1(n-k-1)$ is the unique graph whose least Q-eigenvalue attains the minimum.*

Proof Let G be a graph in $\mathcal{U}_n^k \backslash \{U_n^k(3)\}$ whose least Q-eigenvalue attains the minimum, and $C_g = v_1v_2\cdots v_gv_1$ be the unique cycle of G. Then g is odd, and G can be obtained by attaching rooted trees $T_1,\ldots,T_g$ to the vertices $v_1,\ldots,v_g$ of C_g, 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 a trivial tree. Let $x = (x_1,x_2,\ldots,x_n)^T$ be a unit eigenvector corresponding to $\kappa(G)$.

First, we show that G is the cycle $C_g = v_1v_2\cdots v_gv_1$ with only one nontrivial tree attached. Otherwise, we assume that there are more than one nontrivial trees attached at two different vertices of the cycle C_g. Let v_t be a vertex of the cycle C_g such that $|x_t| \geq |x_i|$ for $i = 1,2,\ldots,g$. By Lemma 2.1, $x_t \neq 0$. Let v_l be another vertex of the cycle C_g such that $|V(T_l)| > 1$, and let

$$G_1 = G - \sum_{v\in N_{T_l}(v_l)} v_lv + \sum_{v\in N_{T_l}(v_l)} v_tv.$$

From $k \leq n-4$, we have $G_1 \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$. By Lemma 2.4, we have $\kappa(G_1) < \kappa(G)$, a contradiction. Therefore G is the cycle $C = v_1v_2\cdots v_gv_1$ with only one nontrivial tree attached. Without loss of generality, we may assume the nontrivial tree is T_g.

Second, we show that $g = 3$. Otherwise, we assume that $g \geq 5$. By Lemma 2.3, we have $x_{(g-3)/2} = x_{(g+3)/2}$. Let

$$G' = G - v_{(g-1)/2}v_{(g-3)/2} + v_{(g-1)/2}v_{(g+3)/2}.$$

Clearly, $G' \in \mathcal{U}_n^{k+1}$, and from (1) we have

$$\kappa\bigl(G'\bigr) \leq x^TQ\bigl(G'\bigr)x = x^TQ(G)x = \kappa(G).$$

Let v_t be a pendant vertex of G, and $y = (y_1,y_2,\ldots,y_n)^T$ be a unit eigenvector corresponding to $\kappa(G')$. By Lemma 2.2, we have $|y_t| > |y_g| > 0$. Let $G'' = G' - v_1v_g + v_1v_t$. It is easy to see that $G'' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$. By Lemma 2.4, we have $\kappa(G'') < \kappa(G')$. Then we have $\kappa(G'') < \kappa(G)$, a contradiction. Therefore $g = 3$.

Third, we show that G has two pendant neighbors exactly. Otherwise, suppose that G has $r \geq 3$ pendant neighbors. Let v_a be a pendant neighbor of G such that $d(v_3,v_a)$ is as large as possible, v_s and v_t be two other pendant neighbors of G. Applying Lemma 2.4 to v_s and v_t, we may obtain a graph $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$ or $G' \in \mathcal{U}_n^{k+1}$ such that $\kappa(G') < \kappa(G)$. If $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$, we have a contradiction. If $G' \in \mathcal{U}_n^{k+1}$, without loss of generality, we may assume that v_s is a pendant vertex of G'. Let u and w be two pendant vertices adjacent to v_t of G', and $G'' = G' - v_tw + uw$. Clearly, $G'' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$ and $\kappa(G'') < \kappa(G')$. Then we have $\kappa(G'') < \kappa(G)$, a contradiction. Therefore G has two pendant neighbors exactly. Let v_a be a pendant neighbor of G such that $d(v_3,v_a)$ is as large as possible, and v_b be another pendant neighbor of G.

Fourth, we show that v_b is in path $v_3 - v_a$. Otherwise, suppose that v_b is not in path $v_3 - v_a$. Employing Lemma 2.4 to vertices v_a and v_b, we may obtain a graph $G' \in \mathcal{U}_n^{k+1}$ such that $\kappa(G') < \kappa(G)$. Without loss of generality, we may assume that v_b is a pendant vertex of G'. Let u and w be two pendant vertices adjacent to v_a of G', and $G'' = G' - v_aw + uw$. Clearly, $G'' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$ and $\kappa(G'') < \kappa(G')$. Then we have $\kappa(G'') < \kappa(G)$, a contradiction. Therefore v_b is in path $v_3 - v_a$.

Fifth, we show that v_a and v_b are adjacent. Otherwise, suppose that v_a and v_b are not adjacent. Let $v_c \in N(v_b)$ be in path $v_b - v_a$, then, by Lemma 2.4, we have $|x_c| > |x_b|$. Let v_t be the pendant vertex adjacent to v_b and $G' = G - v_bv_t + v_cv_t$. Clearly, $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$ and by Lemma 2.4 we have $\kappa(G') < \kappa(G)$, a contradiction. Therefore v_a and v_b are adjacent.

Sixth, we show that $d(v_b) = 3$. Otherwise, suppose that $d(v_b) > 3$. Let v_t be the pendant vertex adjacent to v_b and $G' = G - v_bv_t + v_av_t$. Clearly, $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3)\}$. By Lemma 2.4, we have $|x_a| > |x_b|$, and by Lemma 2.4, we have $\kappa(G') < \kappa(G)$, a contradiction. Therefore $d(v_b) = 3$.

From the above arguments, we have $G = C_3^1(n-k-1)$. □

For $k = n-3$, $\mathcal{U}_n^{n-3} = \{\Delta_{r,s,t} \mid r \geq s \geq t \geq 0, r+s+t = n-3\}$, where $\Delta_{r,s,t}$ is the graph obtained from the cycle C_3 by attaching r, s, t pendent edges to the vertices v_1, v_2, and v_3 of the cycle C_3, respectively. By a similar reasoning to that of Theorem 3.1, we can prove the following theorem.

Theorem 3.2 *Let* $n \geq 8$, *and* $G \in \mathcal{U}_n^{n-3} \backslash \{\Delta_{n-3,0,0}, \Delta_{n-4,1,0}, \Delta_{n-5,2,0}\}$. *Then*

$$\kappa(\Delta_{n-3,0,0}) < \kappa(\Delta_{n-4,1,0}) < \kappa(\Delta_{n-5,2,0}) < \kappa(G).$$

Next, we will determine the graph in $\mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$ whose least Q-eigenvalue attains the minimum.

Theorem 3.3 *Let* $2 \leq k \leq n-5$. *Among all graphs in* $\mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$, $C_3^1(n-k-2)$ *or* $C_3^2(n-k-1)$ *is the graph whose least Q-eigenvalue attains the minimum.*

Proof Let G be a graph in $\mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$ whose least Q-eigenvalue attains the minimum, and let $x = (x_1, x_2, \dots, x_n)^T$ be a unit eigenvector corresponding to $\kappa(G)$. By a similar reasoning to that of Theorem 3.1, we can prove that G is the cycle $C = v_1v_2v_3v_1$ with only one nontrivial tree T_3 attached at v_3, and G has two pendant neighbors exactly. Let v_a be a pendant neighbor of G such that $d(v_3, v_a)$ is as large as possible, and v_b be another pendant neighbor of G. By a similar reasoning to that of Theorem 3.1, we can prove that v_b is in path $v_3 - v_a$.

Now we show that $d(v_b, v_a) \leq 2$. Otherwise, suppose that $d(v_b, v_a) \geq 3$. Let v_t be the pendant vertex adjacent to v_b and $v_c \in N(v_b)$ be in path $v_b - v_a$. Then, by Lemma 2.4, we have $|x_c| > |x_b|$. Let $G' = G - v_bv_t + v_cv_t$. Clearly, $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$ and $\kappa(G') < \kappa(G)$, a contradiction. Therefore $d(v_b, v_a) \leq 2$.

If $d(v_b, v_a) = 2$, then we declare $d(v_b) = 3$. Otherwise, suppose that $d(v_b) \geq 4$. Let v_t be the pendant vertex adjacent to v_b and let $G' = G - v_bv_t + v_av_t$. Clearly, $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$ and $\kappa(G') < \kappa(G)$, a contradiction. Therefore $d(v_b) = 3$ and $G = C_3^1(n-k-2)$.

If $d(v_b, v_a) = 1$, then we declare $d(v_b) = 4$. Otherwise, suppose that $d(v_b) \geq 5$. Let v_t be the pendant vertex adjacent to v_b and let $G' = G - v_bv_t + v_av_t$. Clearly, $G' \in \mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$ and $\kappa(G') < \kappa(G)$, a contradiction. Therefore $d(v_b) = 4$ and $G = C_3^2(n-k-1)$.

From the above arguments, we have $G = C_3^1(n-k-1)$ or $C_3^2(n-k-1)$. □

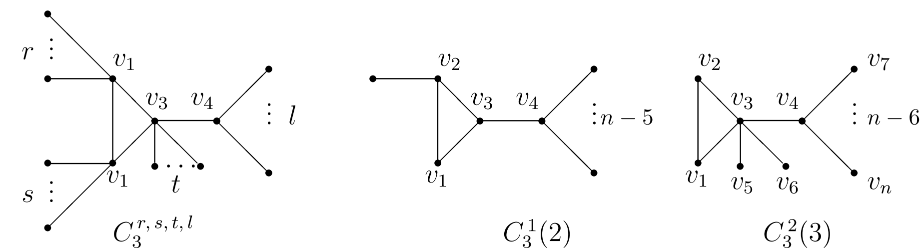

Figure 4 $C_3^{r,s,t,l}$, $C_3^1(2)$, and $C_3^2(3)$.

For $k = n-4$, $\mathcal{U}_n^{n-4} = \{C_3^{r,s,t,l} \mid l \geq 1, r \geq 0, s \geq 0, t \geq 0, r+s+t+l = n-4\}$, where $C_3^{r,s,t,l}$, shown in Figure 4, denotes the unicyclic graph of order n with $n-4$ pendant vertices. $C_3^1(2)$ and $C_3^2(3)$, shown in Figure 4, are the unicyclic graphs of order n with $n-4$ pendant vertices.

Theorem 3.4 *Let $n \geq 7$. Among all graphs in $\mathcal{U}_n^{n-4} \backslash \{U_n^{n-4}(3), C_3^1(3)\}$, $C_3^1(2)$ is the unique graph whose least Q-eigenvalue attains the minimum.*

Proof By a similar reasoning to that of Theorem 3.3, we can prove that $C_3^2(3)$ or $C_3^1(2)$ is the graph whose least Q-eigenvalue attains the minimum among all graphs in $\mathcal{U}_n^{n-4} \backslash \{U_n^{n-4}(3), C_3^1(3)\}$. Let $\kappa = \kappa(C_3^2(3))$ and let $x = (x_1, x_2, \ldots, x_n)^T$ be an eigenvector corresponding to κ. From the eigenvalue equations, we have $x_1 = x_2$, $x_5 = x_6$, $x_7 = \cdots = x_n$,

$$(\kappa - 2)x_1 = x_1 + x_3,$$

$$(\kappa - 5)x_3 = 2x_1 + x_4 + 2x_5,$$

$$(\kappa - n + 5)x_4 = x_3 + (n-6)x_7,$$

$$(\kappa - 1)x_5 = x_3,$$

$$(\kappa - 1)x_7 = x_4.$$

Since x is an eigenvector, it follows that $\kappa = \kappa(C_3^2(3))$ is the least root of the equation

$$f(x) \triangleq \begin{vmatrix} x-3 & -1 & 0 & 0 & 0 \\ -2 & x-5 & -1 & -2 & 0 \\ 0 & -1 & x-n+5 & 0 & -n+6 \\ 0 & -1 & 0 & x-1 & 0 \\ 0 & 0 & -1 & 0 & x-1 \end{vmatrix} = 0.$$

By an easy computation, we can obtain

$$f(x) = x^5 - (n+5)x^4 + (9n-17)x^3 - (19n-65)x^2 + (7n-16)x - 4.$$

Similarly, from the eigenvalue equation, we can prove that $\kappa(C_3^1(2))$ is the least root of

$$g(x) \triangleq x^6 - (n+6)x^5 + (9n-2)x^4 - (25n-48)x^3 + (25n-58)x^2 - (7n-8)x + 4 = 0.$$

By Lemma 2.6, we have $0 < \kappa(C_3^2(3)), \kappa(C_3^1(2)) \le 4/n$. Note that for $n \ge 12$,

$$(x-1)f(x) - g(x) = x\big((n-10)x^3 - (3n-34)x^2 + (n-23)x + 4\big) > 0$$

for $0 < x \le 4/n$. It follows that $g(\kappa(C_3^2(3))) < 0$. This implies that $\kappa(C_3^1(2)) < \kappa(C_3^2(3))$.

For $7 \le n \le 11$, by computation, we can verify that $\kappa(C_3^1(2)) < \kappa(C_3^2(3))$.

From the above arguments, we have $\kappa(C_3^1(2)) < \kappa(C_3^2(3))$ for $n \ge 7$. □

Combining Theorem 3.3 and Lemma 2.8, we have the following theorem.

Theorem 3.5 *Let $3 \le k \le (n-4)/\sqrt{6}$. Among all graphs in $\mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$, $C_3^2(n-k-1)$ is the unique graph whose least Q-eigenvalue attains the minimum.*

Combining Theorem 3.3 and Lemma 2.9, we have the following theorem.

Theorem 3.6 *Let $n \ge 120$, $k > \frac{-3+\sqrt{21}}{2}n$. Among all graphs in $\mathcal{U}_n^k \backslash \{U_n^k(3), C_3^1(n-k-1)\}$, $C_3^1(n-k-2)$ is the unique graph whose least Q-eigenvalue attains the minimum.*

4 Discussion

According to Lemmas 2.8 and 2.9, we propose the following conjecture.

Conjecture 4.1 There exists a real number α with $0 < \alpha < 1$ such that, for any $\varepsilon > 0$, there exists a sufficiently large N such that

$$\kappa\big(C_3^2(n-k-1)\big) < \kappa\big(C_3^1(n-k-2)\big)$$

for all $n \ge N$ and all $3 \le k \le (\alpha - \varepsilon)n$, and

$$\kappa\big(C_3^2(n-k-1)\big) > \kappa\big(C_3^1(n-k-2)\big)$$

for all $n \ge N$ and all $(\alpha + \varepsilon)n \le k \le n-5$.

If Conjecture 4.1 is true, then, by Lemmas 2.8 and 2.9, $\sqrt{6}/6 \le \alpha \le (\sqrt{21}-3)/2$, where α is the same as in Conjecture 4.1.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

All authors completed the paper together. All authors read and approved the final manuscript.

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Acknowledgements

The first author is very grateful to Professor Yong-Gao Chen for his help. This work is supported by the National Natural Science Foundation of China (Nos. 11171290, 11271315) and the Natural Science Foundation of Jiangsu Province (BK20151295).

Received: 1 October 2015 Accepted: 28 April 2016 Published online: 10 May 2016

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