The least eigenvalues of unicyclic graphs

Zhibin Du *

Department of Mathematics, Tongji University,
Shanghai 200092, China

Abstract. Let G be a unicyclic graph on $n \geq 3$ vertices. Let $\mathbf{A}(G)$ be the adjacency matrix of G. The eigenvalues of $\mathbf{A}(G)$ are denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, which are called the eigenvalues of G. Let the unicyclic graphs G on n vertices be ordered by their least eigenvalues $\lambda_n(G)$ in non-decreasing order. For $n \geq 14$, the first six graphs in this order are determined.

Keywords: least eigenvalue, unicyclic graphs, characteristic polynomial, spectrum

1 Introduction

Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. Let $\mathbf{A}(G)$ be the adjacency matrix of G, and $\mathbf{I}$ be the identity matrix. The characteristic polynomial $det(x\mathbf{I}-\mathbf{A}(G))$ of $\mathbf{A}(G)$ is called the characteristic polynomial of G, and is denoted by $\phi(G,x)$. The eigenvalues of $\mathbf{A}(G)$ are denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$, which are called the eigenvalues of G. In particular, we say $\lambda_n(G)$ the least eigenvalue of G.

By Perron-Frobenius Theorem [4], for a connected graph G, corresponding to $\lambda_1(G)$, there is a unit eigenvector $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ with positive entries, known as the principal eigenvector of G, and $\lambda_1(G) \geq -\lambda_n(G)$ with equality if and only if G is bipartite. By interlacing Theorem [4], $\lambda_n(G) \leq -1$ if G has at least one edge.

The evaluation of graph spectral properties is an important topic in graph spectral theory. In the past several decades, many results on the

*Correspondence to Z. Du; e-mail: zhibindu@126.com

largest eigenvalue of graphs were determined, see, e.g., [1, 5, 8, 9, 10, 13, 14, 17]. Recently, the least eigenvalue of graphs has received more and more attentions. A lot of results on the least eigenvalue of graphs with some restriction can be found in [2, 3, 7, 11, 12, 15, 16, 18].

In this paper, we focus on the unicyclic graphs (the graphs with a unique cycle). Fan *et al.* [7] determined the unique graph with minimum least eigenvalue among the set of unicyclic graphs. Liu *et al.* [11] characterized the unique graph with minimum least eigenvalue among the set of unicyclic graphs with given number of pendant vertices (vertices with degree one). Zhai *et al.* [18] characterized the unique graph with minimum least eigenvalue among the set of unicyclic graphs with given diameter.

In this paper, we determine the first six minimum least eigenvalues among the set of n-vertex unicyclic graphs, where $n \geq 14$, and the corresponding graphs whose least eigenvalues achieve these values.

2 Preliminaries

Let P_n and S_n be respectively the path and the star on $n \geq 1$ vertices. Let C_n be the cycle on $n \geq 3$ vertices.

First we give some lemmas which will be used in our proof.

Lemma 2.1. [4] *Let u be a vertex of a graph G, $\varphi(u)$ be the set of the circuits containing u, and $V(Z)$ be the set of vertices in the circuit Z. Then*

$$\phi(G,x) = x\cdot\phi(G-u,x) - \sum_{uv\in E(G)} \phi(G-u-v,x) - 2\sum_{Z\in\varphi(u)} \phi(G-V(Z),x),$$

where $\phi(G-u-v,x) = 1$ if $G \cong P_2$, $\phi(G-V(Z),x) = 1$ if $G \cong C_n$.

In the following, we use Lemma 2.1 to calculate the characteristic polynomial $\phi(G,x)$ of a graph G by setting u to be a vertex of maximum degree in G.

Lemma 2.2. [6, 10] *Let G be a connected non-trivial graph, and H be a proper spanning subgraph of G. Then $\phi(H,x) > \phi(G,x)$ for $x \geq \lambda_1(G)$.*

Let $\mathbf{x}$ be a unit eigenvector of G corresponding to $\lambda_1(G)$ or $\lambda_n(G)$. We say x_v the element of $\mathbf{x}$ corresponding to $v \in V(G)$.

Lemma 2.3. [1, 6, 14] *Let G be a connected graph, $rs \in E(G)$ and $rt \notin E(G)$. Let G' be the graph obtained from G by deleting the edge rs and adding the edge rt. Let $\mathbf{x}$ ($\mathbf{x}'$, respectively) be the principal eigenvector of G (G', respectively). If $x_t \geq x_s$, then $\lambda_1(G') > \lambda_1(G)$ and $x'_t > x'_s$.*

Lemma 2.4. [9] *Let G be a unicyclic graph on $n \geq 10$ vertices. Then $\lambda_1(G) < \sqrt{n}$.*

By Perron-Frobenius Theorem [4], $-\lambda_n(G) \leq \lambda_1(G)$, and thus, $\lambda_n(G) > -\sqrt{n}$. Then we have $-\sqrt{n} < \lambda_n(G) \leq \lambda_3(P_3) = -\sqrt{2}$ if G is a unicyclic graph on $n \geq 10$ vertices.

Lemma 2.5. *Let G_0 be a connected graph with at least three vertices and let u and v be two distinct vertices of G_0. Let H_0 be a connected graph with $w \in V(H_0)$. Let G_u (G_v, respectively) be the graph obtained from G_0 and H_0 by identifying u (v, respectively) with w. Let $\mathbf{x}$ be a unit eigenvector of G_u corresponding to $\lambda_n(G_u)$, and $\mathbf{x}'$ be a unit eigenvector of G_v corresponding to $\lambda_n(G_v)$. Suppose that $|x_u| \leq |x_v|$.*

(*i*) [7] *Then $\lambda_n(G_u) \geq \lambda_n(G_v)$ with equality if and only if $\mathbf{x}$ is also a unit eigenvector of G_v corresponding to $\lambda_n(G_v)$, $x_u = x_v$ and $\sum x_j = 0$, where the summation takes on all the neighbors of w in H_0.*

(*ii*) *If $\lambda_n(G_u) > \lambda_n(G_v)$, then $|x'_u| < |x'_v|$.*

Proof. We need only to prove (ii). If $|x'_u| \geq |x'_v|$, then by (i), $\lambda_n(G_u) \leq \lambda_n(G_v)$, a contradiction. Then the result follows. □

3 The first six minimum least eigenvalues of unicyclic graphs

Let $T_n(a,b)$ be the n-vertex tree obtained by attaching a and b pendant vertices to the two end vertices of an edge, respectively, where $a+b=n-2$, $a,b \geq 0$. In particular, if $a=0$ or $b=0$, then $T_n(a,b) = S_n$.

Let $d_G(v)$ be the degree of v in G for $v \in V(G)$.

Let $C_m(T_1, T_2, \ldots, T_m)$ be the unicyclic graph with unique cycle $C_m = v_1v_2\ldots v_mv_1$ such that the deletion of all edges on C_m results in m vertex–disjoint trees $T_1, T_2, \ldots, T_m$ with $v_i \in V(T_i)$ for $i = 1, 2, \ldots, m$. If $T_i = S_r$, we require that the degree of v_i is $r+1$. If $T_i = T_r(a,b)$, we require that the degree of v_i is $a+3$.

For convenience, let $C_3(T) = C_3(T, S_1, S_1)$, $C_3(T_1, T_2) = C_3(T_1, T_2, S_1)$, $C_4(T) = C_4(T, S_1, S_1, S_1)$, and $C_4^1(T_1, T_2) = C_4(T_1, T_2, S_1, S_1)$.

Let $\mathbb{U}_1(n)$ be the set of n-vertex unicyclic graphs of form $C_3(S_a, S_b, S_c)$, where $a+b+c=n$, $a,b,c \geq 1$.

Lemma 3.1. *Let $G \in \mathbb{U}_1(n)$, where $n \geq 14$. If $G \ncong C_3(S_{n-2}), C_3(S_{n-3}, S_2)$, then $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$.*

Proof. Let $\mathbf{x}$ be a unit eigenvector of $C_3(S_a, S_b, S_c)$ corresponding to $\lambda_n = \lambda_n(C_3(S_a, S_b, S_c))$. Let u_i be a pendant neighbor of v_i in $C_3(S_a, S_b, S_c)$ if the degree of v_i is at least three, where $i = 1, 2, 3$. It is easily seen that $x_{u_i} = \frac{x_{v_i}}{\lambda_n}$ for $i = 1, 2, 3$.

Suppose that $x_{u_2} = 0$ and $x_{v_1} = x_{v_2}$. Then $x_{v_1} = x_{v_2} = 0$. Since $\lambda_n x_{v_2} = (b-1)x_{u_2} + x_{v_1} + x_{v_3}$, we have $x_{v_3} = 0$, and thus $x_{u_3} = 0$, i.e., $\mathbf{x} = 0$, a contradiction. Then either $x_{u_2} \neq 0$ or $x_{v_1} \neq x_{v_2}$.

First suppose that $a > b$. If $|x_{v_1}| < |x_{v_2}|$, then by Lemma 2.5 (i) and (ii),

$$\lambda_n(C_3(S_a, S_b, S_c)) > \lambda_n(C_3(S_{a-1}, S_{b+1}, S_c)) > \cdots > \lambda_n(C_3(S_b, S_a, S_c)),$$

a contradiction. If $|x_{v_1}| \geq |x_{v_2}|$, then by Lemma 2.5 (i) and note that either $x_{u_2} \neq 0$ or $x_{v_1} \neq x_{v_2}$, we have $\lambda_n(C_3(S_a, S_b, S_c)) > \lambda_n(C_3(S_{a+1}, S_{b-1}, S_c))$ for $b \geq 2$. If $a = b$, then whether $|x_{v_1}| \geq |x_{v_2}|$ or $|x_{v_1}| < |x_{v_2}|$, by Lemma 2.5 (i), $\lambda_n(C_3(S_a, S_b, S_c)) > \lambda_n(C_3(S_{a+1}, S_{b-1}, S_c))$. It follows that $\lambda_n(C_3(S_a, S_b, S_c)) > \lambda_n(C_3(S_{a+1}, S_{b-1}, S_c))$ for $b \geq 2$.

Let $G \in \mathbb{U}_1(n)$, and $G \ncong C_3(S_{n-2}), C_3(S_{n-3}, S_2)$, where $n \geq 14$. If $c = 1$, then by the arguments as above, $\lambda_n(G) \geq \lambda_n(C_3(S_{n-4}, S_3))$. If $c \geq 2$, then by the arguments as above, $\lambda_n(G) \geq \lambda_n(C_3(S_{n-4}, S_2, S_2)) > \lambda_n(C_3(S_{n-4}, S_3))$.

We are left to show that $\lambda_n(C_3(S_{n-4}, S_3)) > \lambda_n(C_4(T_{n-3}(n-6, 1)))$. By Lemma 2.1,

$$\phi(C_4(T_{n-3}(n-6,1)), x) = x^{n-6} f(x), \quad \phi(C_3(S_{n-4}, S_3), x) = x^{n-4} g(x),$$

where

$$f(x) = x^6 - nx^4 + (3n-12)x^2 - 2n + 12,$$
$$g(x) = x^4 - nx^2 - 2x + 3n - 13.$$

Obviously, $\lambda_n(C_4(T_{n-3}(n-6,1)))$ and $\lambda_n(C_3(S_{n-4}, S_3))$ are respectively the smallest roots of $f(x) = 0$ and $g(x) = 0$. It is easily checked that $f(x) = x^2 g(x) + h(x)$, where $h(x) = 2x^3 + x^2 - 2n + 12$. For $x < -1$, $h'(x) = 2x(3x+1) > 0$, and thus $h(x) < h(-1) = -2n + 11 < 0$. This implies that

$$f(r) = r^2 g(r) + h(r) = h(r) < 0$$

for $r = \lambda_n(C_3(S_{n-4}, S_3))$, i.e., $\lambda_n(C_4(T_{n-3}(n-6,1))) < \lambda_n(C_3(S_{n-4}, S_3))$, as desired. $\square$

Recall that $C_3(T_{n-2}(a, b))$ is the graph obtained by identifying a vertex of a triangle with the vertex of degree $a+1$ of $T_{n-2}(a, b)$. Let $\mathbb{U}_2(n)$ be the set of n-vertex unicyclic graphs of form $C_3(T_{n-2}(a,b))$, where $a+b=n-4$, $a \geq 0$, $b \geq 1$.

Lemma 3.2. *Let $G \in \mathbb{U}_2(n)$, where $n \geq 14$. If $G \ncong C_3(T_{n-2}(n-5,1))$, then $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$.*

Proof. Let $G \in \mathbb{U}_2(n)$ and $G \ncong C_3(T_{n-2}(n-5,1))$, where $n \geq 14$. Let $\mathbf{x}$ be a unit eigenvector of G corresponding to $\lambda_n = \lambda_n(G)$.

If $G \ncong C_3(T_{n-2}(n-6,2)), C_3(T_{n-2}(0,n-4))$, then by Lemma 2.5 (i),

$$\lambda_n(G) \geq \min\{\lambda_n(C_3(T_{n-2}(n-6,2))), \lambda_n(C_3(T_{n-2}(0,n-4)))\}.$$

By Lemma 2.1,

$$\phi(C_3(T_{n-2}(n-6,2)),x) = x^{n-6}(x+1)f(x),$$

$$\phi(C_3(T_{n-2}(0,n-4)),x) = x^{n-5}(x+1)g(x),$$

where

$$f(x) = x^5 - x^4 - (n-1)x^3 + (n-3)x^2 + (2n-8)x - 2n + 12,$$

$$g(x) = x^4 - x^3 - (n-1)x^2 + (n-3)x + 2n - 8.$$

Obviously, $\lambda_n(C_3(T_{n-2}(n-6,2)))$ and $\lambda_n(C_3(T_{n-2}(0,n-4)))$ are respectively the smallest roots of $f(x)=0$ and $g(x)=0$. It is easily checked that $x \cdot g(x) = f(x) + 2n - 12$, and thus

$$r \cdot g(r) = f(r) + 2n - 12 = 2n - 12 > 0$$

for $r = \lambda_n(C_3(T_{n-2}(n-6,2)))$, implying that $\lambda_n(C_3(T_{n-2}(0,n-4))) < \lambda_n(C_3(T_{n-2}(n-6,2)))$.

We are left to show that $\lambda_n(C_3(T_{n-2}(0,n-4))) > \lambda_n(C_4(T_{n-3}(n-6,1)))$. First we show that $\lambda_1(C_3(T_{n-2}(0,n-4))) < \lambda_1(C_4(T_{n-3}(n-6,1)))$. By Lemma 2.1, $\phi(C_4(T_{n-3}(n-6,1)),x) = x^{n-6}h(x)$, where

$$h(x) = x^6 - nx^4 + (3n-12)x^2 - 2n + 12.$$

Obviously, $\lambda_1(C_4(T_{n-3}(n-6,1)))$ and $\lambda_1(C_3(T_{n-2}(0,n-4)))$ are respectively the largest roots of $h(x)=0$ and $g(x)=0$. Note that $h(x) = x(x+1)g(x) + p(x)$, where $p(x) = 2x^3 - x^2 - (2n-8)x - 2n + 12$. It is easily checked that $p(-1) = 1 > 0$, $p(1) = -4n + 21 < 0$, $p(\sqrt{n}) = -3n + 8\sqrt{n} + 12 < 0$, and thus $p(x) < 0$ for $1 \leq x \leq \sqrt{n}$. By Lemma 2.4, $\lambda_1(C_3(T_{n-2}(0,n-4))) < \sqrt{n}$, now we have

$$h(r) = r(r+1)g(r) + p(r) = p(r) < 0$$

for $r = \lambda_1(C_3(T_{n-2}(0, n-4)))$, i.e., $\lambda_1(C_3(T_{n-2}(0, n-4))) < \lambda_1(C_4(T_{n-3}(n-6, 1)))$. Note that $C_4(T_{n-3}(n-6, 1))$ is a bipartite graph, and thus by Perron-Frobenius Theorem [4],

$$\begin{aligned} & -\lambda_n(C_3(T_{n-2}(0, n-4))) < \lambda_1(C_3(T_{n-2}(0, n-4))) \\ < \ & \lambda_1(C_4(T_{n-3}(n-6, 1))) = -\lambda_n(C_4(T_{n-3}(n-6, 1))), \end{aligned}$$

i.e., $\lambda_n(C_3(T_{n-2}(0, n-4))) > \lambda_n(C_4(T_{n-3}(n-6, 1)))$. $\square$

Let $\mathbb{U}_3(n)$ be the set of n-vertex unicyclic graphs of the form $C_4^1(S_a, S_b)$, where $a + b = n - 2$, $a \geq b \geq 1$.

Lemma 3.3. *Let $G \in \mathbb{U}_3(n)$, where $n \geq 14$. If $G \not\cong C_4(S_{n-3}), C_4^1(S_{n-4}, S_2)$, then $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6, 1)))$.*

Proof. Let $G \in \mathbb{U}_3(n)$ and $G \not\cong C_4(S_{n-3}), C_4^1(S_{n-4}, S_2)$, where $n \geq 14$. Note that G is a bipartite graph, and thus $\lambda_n(G) = -\lambda_1(G)$. We need only to show that $\lambda_1(G) < \lambda_1(C_4(T_{n-3}(n-6, 1)))$.

Since $b \geq 3$, it follows from Lemma 2.3 that $\lambda_1(G) \leq \lambda_1(C_4^1(S_{n-5}, S_3))$. We are left to show that $\lambda_1(C_4^1(S_{n-5}, S_3)) < \lambda_1(C_4(T_{n-3}(n-6, 1)))$.

By Lemma 2.1,

$$\phi(C_4^1(S_{n-5}, S_3), x) = x^{n-6}[x^6 - nx^4 + (4n - 20)x^2 - 2n + 12],$$

$$\phi(C_4(T_{n-3}(n-6, 1)), x) = x^{n-6}[x^6 - nx^4 + (3n - 12)x^2 - 2n + 12],$$

and thus,

$$\phi(C_4^1(S_{n-5}, S_3), x) - \phi(C_4(T_{n-3}(n-6, 1)), x) = x^{n-4}(n - 8) > 0$$

for $x \geq 1$, i.e., $\lambda_1(C_4^1(S_{n-5}, S_3)) < \lambda_1(C_4(T_{n-3}(n-6, 1)))$. $\square$

Lemma 3.4. *For $n \geq 14$,*

$$\begin{aligned} & \lambda_n(C_4(T_{n-3}(n-6, 1))) > \lambda_n(C_4^1(S_{n-4}, S_2)) \\ > \ & \lambda_n(C_3(S_{n-3}, S_2)) > \lambda_n(C_3(T_{n-2}(n-5, 1))). \end{aligned}$$

Proof. By Lemma 2.1,

$$\phi(C_3(T_{n-2}(n-5, 1)), x) = x^{n-6}(x^2 - 1)f_1(x),$$

$$\phi(C_3(S_{n-3}, S_2), x) = x^{n-4}f_2(x),$$

$$\phi(C_4^1(S_{n-4}, S_2), x) = x^{n-6}f_3(x),$$

where

$$f_1(x) = x^4 - (n-1)x^2 - 2x + n - 5,$$
$$f_2(x) = x^4 - nx^2 - 2x + 2n - 7,$$
$$f_3(x) = x^6 - nx^4 + (3n-13)x^2 - n + 5.$$

Obviously, $\lambda_n(C_3(T_{n-2}(n-5,1)))$, $\lambda_n(C_3(S_{n-3},S_2))$, $\lambda_n(C_4^1(S_{n-4},S_2))$ are respectively the smallest roots of $f_1(x)=0$, $f_2(x)=0$, $f_3(x)=0$.

Note that $f_1(x) = f_2(x) + x^2 - n + 2$. It is easily checked that $f_2(0) = 2n-7 > 0$, $f_2(-\sqrt{2}) = 2\sqrt{2} - 3 < 0$, $f_2(-\sqrt{n-2}) = 2\sqrt{n-2} - 3 > 0$, and thus $-\sqrt{n-2} < \lambda_n(C_3(S_{n-3},S_2)) < 0$. Now we have

$$f_1(r) = f_2(r) + r^2 - n + 2 = r^2 - n + 2 < 0$$

for $r = \lambda_n(C_3(S_{n-3},S_2))$, i.e., $\lambda_n(C_3(T_{n-2}(n-5,1))) < \lambda_n(C_3(S_{n-3},S_2))$.

By direct calculation, $\lambda_n(C_3(S_{n-3},S_2)) < \lambda_n(C_4^1(S_{n-4},S_2))$ for $14 \leq n \leq 19$. Suppose that $n \geq 20$. Note that $x^2 f_2(x) = f_3(x) + g(x)$, where $g(x) = -2x^3 - (n-6)x^2 + n - 5$. Then for $-\sqrt{n} < x \leq -\sqrt{2}$,

$$\begin{aligned} g'(x) &= -2x(3x+n-6) \\ &> -2x[3(-\sqrt{n}) + n - 6] \\ &= -2x(n - 3\sqrt{n} - 6) \\ &\geq -2x(20 - 3\sqrt{20} - 6) > 0, \end{aligned}$$

implying that $g(x) \leq g(-\sqrt{2}) = -n + 7 + 4\sqrt{2} < 0$. It follows that

$$r^2 f_2(r) = f_3(r) + g(r) = g(r) < 0$$

for $r = \lambda_n(C_4^1(S_{n-4},S_2))$, i.e., $\lambda_n(C_3(S_{n-3},S_2)) < \lambda_n(C_4^1(S_{n-4},S_2))$.

Now we show that $\lambda_n(C_4^1(S_{n-4},S_2)) < \lambda_n(C_4(T_{n-3}(n-6,1)))$. Note that the two graphs are both bipartite graphs. Then we need only to show that $\lambda_1(C_4^1(S_{n-4},S_2)) > \lambda_1(C_4(T_{n-3}(n-6,1)))$. Using Lemma 2.1 to $G = C_4^1(S_{n-4},S_2)$ by setting u to be the unique pendant neighbor of v_2,

$$\phi(C_4^1(S_{n-4},S_2),x) = x \cdot \phi(C_4(S_{n-4}),x) - \phi(T_{n-2}(n-5,1),x),$$

and to $G = C_4(T_{n-3}(n-6,1))$ by setting u to be the unique pendant vertex which is not incident with v_1,

$$\phi(C_4(T_{n-3}(n-6,1)),x) = x \cdot \phi(C_4(S_{n-4}),x) - \phi(C_4(S_{n-5}),x).$$

It is easily seen that $T_{n-2}(n-5,1)$ is a proper spanning subgraph of $C_4(S_{n-5})$, by Lemma 2.2, $\phi(T_{n-2}(n-5,1),x) > \phi(C_4(S_{n-5}),x)$ for $x \geq \lambda_1(C_4(S_{n-5}))$, and thus, $\phi(C_4^1(S_{n-4},S_2),x) < \phi(C_4(T_{n-3}(n-6,1)),x)$ for $x \geq \lambda_1(C_4(S_{n-5}))$, i.e., $\lambda_1(C_4^1(S_{n-4},S_2)) > \lambda_1(C_4(T_{n-3}(n-6,1)))$. $\square$

Lemma 3.5. [18] *Let G be an n-vertex unicyclic graph with diameter four, where $n \geq 10$. If $G \ncong C_4(T_{n-3}(n-6,1))$, then $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$.*

Lemma 3.6. [11] *Let $U_{n,p}$ be the n-vertex (unicyclic) graph obtained by attaching p paths of almost equal lengths to one vertex of a quadrangle. Then $U_{n,p}$ for $1 \leq p \leq n-4$ is the unique graph with minimum least eigenvalue among the set of unicyclic graphs with n vertices and p pendant vertices.*

The following result was shown in [7, 15]. For completeness, we give a different proof here.

Lemma 3.7. [7, 15] *For $n \geq 14$, $\lambda_n(C_4(S_{n-3})) > \lambda_n(C_3(S_{n-2}))$.*

Proof. By Lemma 2.1,

$$\phi(C_3(S_{n-2}), x) = x^{n-4} f(x), \quad \phi(C_4(S_{n-3}), x) = x^{n-4} g(x),$$

where

$$f(x) = x^4 - nx^2 - 2x + n - 3,$$
$$g(x) = x^4 - nx^2 + 2n - 8.$$

Obviously, $\lambda_n(C_3(S_{n-2}))$ and $\lambda_n(C_4(S_{n-3}))$ are respectively the smallest roots of $f(x) = 0$ and $g(x) = 0$. It is easily checked that $f(x) = g(x) - 2x - n + 5$. Note that $-2x - n + 5 < 0$ for $x > -\sqrt{n}$, and thus $f(r) = g(r) - 2r - n + 5 < 0$ for $r = \lambda_n(C_4(S_{n-3}))$, implying that $\lambda_n(C_3(S_{n-2})) < \lambda_n(C_4(S_{n-3}))$. ☐

Note that there are exactly $n-4$ pendant vertices in $C_3(T_{n-2}(n-5,1))$, and $C_4(S_{n-3}) \cong U_{n,n-4}$, by Lemma 3.6, $\lambda_n(C_3(T_{n-2}(n-5,1))) > \lambda_n(C_4(S_{n-3}))$, together with Lemma 3.7, we have

Lemma 3.8. *For $n \geq 14$, we have*

$$\lambda_n(C_3(T_{n-2}(n-5,1))) > \lambda_n(C_4(S_{n-3})) > \lambda_n(C_3(S_{n-2})).$$

Combining Lemmas 3.4 and 3.8, we have

Lemma 3.9. *For $n \geq 14$,*

$$\begin{aligned} & \lambda_n(C_4(T_{n-3}(n-6,1))) > \lambda_n(C_4^1(S_{n-4}, S_2)) \\ > \ & \lambda_n(C_3(S_{n-3}, S_2)) > \lambda_n(C_3(T_{n-2}(n-5,1))) \\ > \ & \lambda_n(C_4(S_{n-3})) > \lambda_n(C_3(S_{n-2})). \end{aligned}$$

Theorem 3.1. *The least eigenvalues of n-vertex unicyclic graphs with $n \geq 14$ may be ordered by the following inequalities, where G is an n-vertex unicyclic graph different from any other graph in the inequalities*:

$$\begin{aligned}\lambda_n(G) &> \lambda_n(C_4(T_{n-3}(n-6,1))) > \lambda_n(C_4^1(S_{n-4},S_2)) \\ &> \lambda_n(C_3(S_{n-3},S_2)) > \lambda_n(C_3(T_{n-2}(n-5,1))) \\ &> \lambda_n(C_4(S_{n-3})) > \lambda_n(C_3(S_{n-2})),\end{aligned}$$

and the least eigenvalues of the graphs $C_3(S_{n-2})$, $C_4(S_{n-3})$, $C_3(T_{n-2}(n-5,1))$, $C_3(S_{n-3},S_2)$, $C_4^1(S_{n-4},S_2)$, $C_4(T_{n-3}(n-6,1))$ are respectively the smallest roots of the equations on x as follows:

$$x^3 - x^2 - (n-1)x + n - 3 = 0,$$

$$x^4 - nx^2 + 2n - 8 = 0,$$

$$x^4 - (n-1)x^2 - 2x + n - 5 = 0,$$

$$x^4 - nx^2 - 2x + 2n - 7 = 0,$$

$$x^6 - nx^4 + (3n-13)x^2 - n + 5 = 0,$$

$$x^6 - nx^4 + (3n-12)x^2 - 2n + 12 = 0.$$

Proof. Let G be an n-vertex unicyclic graph, and let p be the number of pendant vertices of G. Obviously, $0 \leq p \leq n-3$.

If $p = 0$, i.e., $G \cong C_n$, then by interlacing Theorem [4],

$$\lambda_n(G) \geq -2 > -2.13578 \doteq \lambda_5(C_4(S_2)) \geq \lambda_n(C_4(T_{n-3}(n-6,1))),$$

and thus, $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$.

Suppose that $1 \leq p \leq n-6$. For $U_{n,p}$, we may choose a path on three vertices, say uvw, outside the quadrangle of $U_{n,p}$, where u is a pendant vertex of $U_{n,p}$, v is a vertex of degree two. Let G' be the graph obtained from $U_{n,p}$ by deleting the edge uv and adding the edge uw. By Lemma 2.3, $\lambda_1(U_{n,p}) < \lambda_1(G')$. Since both $U_{n,p}$ and G' are bipartite graphs, $\lambda_n(U_{n,p}) > \lambda_n(G')$. Note that there are $p+1$ pendant vertices in G', by Lemma 3.6, $\lambda_n(G') \geq \lambda_n(U_{n,p+1})$. Clearly, $U_{n,n-5} \cong C_4(T_{n-3}(n-6,1))$. Now it follows that

$$\lambda_n(U_{n,p}) > \lambda_n(U_{n,p+1}) > \cdots > \lambda_n(U_{n,n-5}) = \lambda_n(C_4(T_{n-3}(n-6,1))).$$

If $p = n-5$, then by Lemma 3.6, $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$ if $G \ncong C_4(T_{n-3}(n-6,1))$.

We have shown that $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$ if $G \not\cong C_4(T_{n-3}(n-6,1))$ and $0 \le p \le n-5$.

Suppose that $p = n-4, n-3$. Denote by r the cycle length of the unique cycle of G. Then $r = 3, 4$. If $G \notin \mathbb{U}_1(n) \cup \mathbb{U}_2(n) \cup \mathbb{U}_3(n)$, then the diameter of G is four, by Lemma 3.5, $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$. If $G \in \mathbb{U}_1(n) \cup \mathbb{U}_2(n) \cup \mathbb{U}_3(n)$, and $G \not\cong C_3(S_{n-2})$, $C_3(S_{n-3}, S_2)$, $C_3(T_{n-2}(n-5,1))$, $C_4(S_{n-3})$, $C_4^1(S_{n-4}, S_2)$, then by Lemmas 3.1, 3.2, 3.3, $\lambda_n(G) > \lambda_n(C_4(T_{n-3}(n-6,1)))$. Now the result follows from Lemma 3.9 easily. □

References

[1] F. Belardo, E.M. Li Marzi, S.K. Simić, Some results on the index of unicyclic graphs, Linear Algebra Appl. 416 (2006) 1048–1059.

[2] F.K. Bell, D. Cvetković, P. Rowlinson, S.K. Simić, Graphs for which the least eigenvalue is minimal I, Linear Algebra Appl. 429 (2008) 234–241.

[3] F.K. Bell, D. Cvetković, P. Rowlinson, S.K. Simić, Graphs for which the least eigenvalue is minimal II, Linear Algebra Appl. 429 (2008) 2168–2179.

[4] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs – Theory and Application*, 3rd edition, Johann Ambrosius Barth, Heidelberg, 1995.

[5] D. Cvetković, P. Rowlinson, Spectra of unicyclic graphs, Graphs Combin. 3 (1987) 7–23.

[6] D. Cvetković, P. Rowlinson, S. Simić, Eigenspaces of Graphs, Cambridge Univ. Press, Cambridge, 1997.

[7] Y. Fan, Y. Wang, Y. Gao, Minimizing the least eigenvalues of unicyclic graphs with application to spectral spread, Linear Algebra Appl. 429 (2008) 577–588.

[8] J. Guo, On the spectral radii of unicyclic graphs with fixed matching number, Discrete Math. 308 (2008) 6115–6131.

[9] Y. Hong, On the spectra of unicycle graph, J. East China Norm. Univ. Natur. Sci. Ed. 1 (1986) 31–34.

[10] Q. Li, K. Feng, On the largest eigenvalue of a graph, Acta Math. Appl. Sinica 2 (1979) 167–175.

[11] R. Liu, M. Zhai, J. Shu, The least eigenvalue of unicyclic graphs with n vertices and k pendant vertices, Linear Algebra Appl. 431 (2009) 657–665.

[12] M. Petrović, B. Borovićanin, T. Aleksić, Bicyclic graphs for which the least eigenvalue is minimum, Linear Algebra Appl. 430 (2009) 1328–1335.

[13] S. Simić, On the largest eigenvalue of unicyclic graphs, Publ. Inst. Math. (Beograd) 42 (56) (1987) 13–19.

[14] S.K. Simić, E.M. Li Marzi, F. Belardo, On the index of caterpillars, Discrete Math. 308 (2008) 324–330.

[15] G. Xu, Q. Xu, S. Wang, A sharp lower bound on the least eigenvalue of unicyclic graphs, J. Ninbo Univ. 16 (3) (2003) 225–227.

[16] M. Ye, Y. Fan, D. Liang, The least eigenvalue of graphs with given connectivity, Linear Algebra Appl. 430 (2009) 1375–1379.

[17] A. Yu, F. Tian, On the spectral radius of unicyclic graphs, MATCH Commun. Math. Comput. Chem. 51 (2004) 97–109.

[18] M. Zhai, R. Liu, J. Shu, Minimizing the least eigenvalue of unicyclic graphs with fixed diameter, Discrete Math. 310 (2010) 947–955.