Research Article

Some Results on the Signless Laplacian Spectra of Unicyclic Graphs

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We determine the second to fourth largest (resp. the second smallest) signless Laplacian spectral radii and the second to fourth largest signless Laplacian spreads together with the corresponding graphs in the class of unicyclic graphs with n vertices. Moreover, we prove that one class of unicyclic graphs are determined by their signless Laplacian spectra.

1. Introduction

Throughout the paper, $G = (V, E)$ is an undirected simple graph with n vertices and m edges. If G is connected with $m = n + c - 1$, then G is called a c -cyclic graph. Especially, if $c = 0$ or 1 , then G is called a tree or a unicyclic graph, respectively. Let $\mathbb{U}_n$ be the class of unicyclic graphs with n vertices. The neighbor set of a vertex v is denoted by $N(v)$. We write $d(v)$ for the degree of vertex v . In particular, let $\Delta(G)$ and $\delta(G)$ be the maximum degree and minimum degree of G , respectively. Let $A(G)$ be the adjacency matrix and $D(G)$ be the diagonal matrix whose (i, i) -entry is $d(v_i)$, of G , respectively. The signless Laplacian matrix of G is $Q(G) = D(G) + A(G)$. Clearly, $Q(G)$ is positive semidefinite [1] and its eigenvalues can be arranged as

$$\mu_1(G) \geq \mu_2(G) \geq \cdots \geq \mu_n(G) \geq 0. \quad (1.1)$$

Let $\mu(G)$ be the signless Laplacian spectral radius of G , namely, $\mu(G) = \mu_1(G)$. The signless Laplacian spread of G is defined as $SQ(G) = \mu_1(G) - \mu_n(G)$ [1, 2]. Let $\Phi(G, x)$ be the signless Laplacian characteristic polynomial of G , that is, $\Phi(G, x) = \det(xI - Q(G))$.

Recently, the research on the spectrum of $Q(G)$ receive much attention. Some properties of signless Laplacian spectra of graphs and some possibilities for developing the spectral theory of graphs based on $Q(G)$ are discussed in [3–5]. The largest signless Laplacian spectral radius and the largest signless Laplacian spread among the class of unicyclic graphs with n vertices were determined in [6] and [1], respectively. The smallest signless Laplacian spectral radius among the class of unicyclic graphs with n vertices was determined in [7]. In this paper, we will determine the second to fourth largest and the second smallest signless Laplacian spectral radii together with the corresponding graphs in the class of unicyclic graphs with n vertices. Moreover, we also indentify the second to fourth largest signless Laplacian spreads together with the corresponding graphs in the class of unicyclic graphs with n vertices. In the end of this paper, we will prove that a class of unicyclic graphs are determined by their signless Laplacian spectra.

2. The Signless Laplacian Spectral Radii of Unicyclic Graphs

As usually, let $K_{1,n-1}$, P_n , and C_n be the star, path, and cycle with n vertices, respectively. In the following, let S_n^3 ($n \geq 4$) be the unicyclic graph obtained by adding one edge to two pendant vertices of $K_{1,n-1}$, and let F_n , H_n , S_n^4 be the unicyclic graphs with n vertices as shown in Figure 1.

In [6], the largest signless Laplacian spectral radius in the class of unicyclic graphs was determined, and it was proved as follows.

Theorem 2.1 (see [6]). *If $U \in \mathbb{U}_n$, and $n \geq 4$, then $\mu(U) \leq \mu(S_n^3)$, where the equality holds if and only if $U \cong S_n^3$.*

Theorem 2.2. *Suppose $U \in \mathbb{U}_n$, and $n \geq 8$. (1) If $U \not\cong S_n^3$, then $\mu(U) \leq \mu(F_n)$, where the equality holds if and only if $U \cong F_n$, and $\mu(F_n)$ equals the maximum root of the equation $x^5 - (n+5)x^4 + (6n+3)x^3 - (9n-1)x^2 + (3n+8)x - 4 = 0$. (2) If $U \not\cong S_n^3$ and $U \not\cong F_n$, then $\mu(U) \leq \mu(H_n)$, where the equality holds if and only if $U \cong H_n$, and $\mu(H_n)$ equals the maximum root of the equation $x^5 - (n+5)x^4 + (6n+4)x^3 - (10n-2)x^2 + (3n+12)x - 4 = 0$. (3) If $U \not\cong S_n^3$, $U \not\cong F_n$ and $U \not\cong H_n$, then $\mu(U) \leq \mu(S_n^4)$, where the equality holds if and only if $U \cong S_n^4$, and $\mu(S_n^4)$ equals the maximum root of the equation $x^3 - (n+3)x^2 + (4n-2)x - 2n = 0$.*

In order to prove Theorem 2.2, the following lemmas are needed.

Lemma 2.3 (see [8]). $\mu(G) \leq \max\{d(v) + m(v), v \in V(G)\}$, where $m(v) = \sum_{u \sim v} d(u) / d(v)$.

Proposition 2.4. *Suppose $c \geq 1$ and G is a c -cyclic graph on n vertices with $\Delta \leq n-3$. If $n \geq 2c+5$, then $\mu(G) \leq n-1$.*

Proof. We only need to prove that $\max\{d(v) + m(v) : v \in V\} \leq n-1$ by Lemma 2.3. Suppose $d(u) + m(u) = \max\{d(v) + m(v) : v \in V\}$. We consider the next three cases.

Case 1 ($d(u) = 1$). Suppose $v \in N(u)$. Then, $d(u) + m(u) = 1 + d(v) \leq 1 + \Delta \leq n-2 < n-1$.

Case 2 ($d(u) = 2$). Suppose that $v, w \in N(u)$. Then,

$$d(u) + m(u) = 2 + \frac{d(v) + d(w)}{2} \leq 2 + \frac{2\Delta}{2} = \Delta + 2 \leq n-1. \quad (2.1)$$

Figure 1: The unicyclic graphs F_n , H_n , and S_n^4 .

Case 3 ($3 \leq d(u) \leq n-3$). Note that G has $n+c-1$ edges and $3 \leq d(u) \leq n-3$. Then,

$$d(u) + m(u) \leq d(u) + \frac{2(n+c-1) - d(u) - 2}{d(u)} = d(u) - 1 + \frac{2n+2c-4}{d(u)}. \quad (2.2)$$

Next we will prove that $d(u) - 1 + ((2n+2c-4)/d(u)) \leq n-1$, equivalently, $d(u)(n-d(u)) \geq 2n+2c-4$. Let $f(x) = (n-x)x$, where $3 \leq x \leq n-3$. Since $f'(x) = n-2x$ and $3 \leq x \leq n-3$, we have $f(x) \geq \min\{f(3), f(n-3)\} = 3(n-3) \geq 2n+2c-4$.

By combining the above arguments, the result follows. $\square$

Corollary 2.5. Suppose $U \in \mathbb{U}_n$. If $n \geq 7$ and $\Delta \leq n-3$, then $\mu(U) \leq n-1$.

Lemma 2.6 (see [6]). If G is a connected graph of order $n \geq 4$, then $\mu(G) \geq \Delta+1$, where the equality holds if and only if $G \cong K_{1,n-1}$.

Suppose B is a square matrix, let $a_{ii}(B)$ be the entry appearing in the i th row and the i th column of B . The next result gives a new method to calculate the signless Laplacian characteristic polynomial of an n -vertex graph via the aid of computer.

Lemma 2.7 (see [9]). Let G be a graph on $n-k$ ($1 \leq k \leq n-2$) vertices with $V(G) = \{v_n, v_{n-1}, \dots, v_{k+1}\}$. If G' is obtained from G by attaching k new pendant vertices, say $v_1, \dots, v_k$, to v_{k+1} , then

$$\Phi(Q(G'), x) = (x-1)^k \cdot \det(xI_{n-k} - Q(G) - B_{n-k}), \quad (2.3)$$

where $a_{11}(Q(G))$ is corresponding to the vertex v_{k+1} , and $B_{n-k} = \text{diag}\{k + (k/(x-1)), 0, \dots, 0\}$.

Example 2.8. Let F_n be the unicyclic graph as shown in Figure 1. By Lemma 2.7, we have

$$\Phi(F_n, x) = (x-1)^{n-4} \det(B), \quad \text{where } B = \begin{pmatrix} x - (n-2) - \frac{n-4}{x-1} & -1 & -1 & 0 \\ -1 & x-2 & -1 & 0 \\ -1 & -1 & x-3 & -1 \\ 0 & 0 & -1 & x-1 \end{pmatrix}. \quad (2.4)$$

By using “Matlab”, it easily follows that

$$\Phi(F_n, x) = (x-1)^{n-5} \left(x^5 - (n+5)x^4 + (6n+3)x^3 - (9n-1)x^2 + (3n+8)x - 4 \right). \quad (2.5)$$

With the similar method, by Lemma 2.7 we have

$$\Phi(H_n, x) = (x-1)^{n-5} \left(x^5 - (n+5)x^4 + (6n+4)x^3 - (10n-2)x^2 + (3n+12)x - 4 \right), \quad (2.6)$$

$$\Phi(S_n^4, x) = x(x-1)^{n-5}(x-2) \left(x^3 - (n+3)x^2 + (4n-2)x - 2n \right). \quad (2.7)$$

Proof of Theorem 2.2. Note that S_n^3 is the unique unicyclic graph with $\Delta = n-1$, and F_n, H_n, S_n^4 are all the unicyclic graphs with $\Delta = n-2$. Now suppose $U \in \mathbb{U}_n \setminus \{S_n^3, F_n, H_n, S_n^4\}$. By Lemma 2.6 and Corollary 2.5, we have $\mu(S_n^4) > n-1 \geq \mu(U)$ because $\Delta(U) \leq n-3$.

To finish the proof of Theorem 2.2, we only need to show that $\mu(S_n^4) < \mu(H_n) < \mu(F_n)$ by Theorem 2.1. By Lemma 2.6, it follows that $\mu(F_n) > n-1, \mu(H_n) > n-1$, and $\mu(S_n^4) > n-1$. When $x \geq n-1$ and $n \geq 8$, by (2.5), (2.6) and (2.7), it follows that

$$\begin{aligned} \Phi(H_n, x) - \Phi(F_n, x) &= (x-1)^{n-5} x \left(x^2 - (n-1)x + 4 \right) > 0, \\ \Phi(S_n^4, x) - \Phi(H_n, x) &= (x-1)^{n-5} \left(2x^2 + (n-12)x + 4 \right) \geq (x-1)^{n-5} (x(3n-14) + 4) > 0. \end{aligned} \quad (2.8)$$

Therefore, we have $\mu(F_n) > \mu(H_n) > \mu(S_n^4)$. Thus, Theorem 2.2 follows. $\square$

In [7], the smallest signless Laplacian spectral radius among all unicyclic graphs with n vertices was determined, and that is as follows.

Theorem 2.9 (see [7]). *If $U \in \mathbb{U}_n$, then $\mu(U) \geq 4$, where the equality holds if and only if $U \cong C_n$.*

The *lollipop* graph, denoted by $W_{n,p}$, is obtained by appending a cycle C_p to a pendant vertex of a path P_{n-p} . The next result extends the order of Theorem 2.9.

Theorem 2.10. *For any n , if $U \in \mathbb{U}_n \setminus \{C_n, W_{n,n-1}\}$, then $\mu(U) > \mu(W_{n,n-1}) > \mu(C_n)$.*

To prove Theorem 2.10, we will introduce more useful lemmas and notations.

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 , that is, adding a new vertex w and edges wu, wv in $G - uv$. An *internal path*, say $v_1 v_2 \cdots v_{s+1}$ ($s \geq 1$), 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 $v_2, \dots, v_s$ are of degree 2.

Lemma 2.11 (see [3, 10]). *Let uv be an edge of a connected graph G . If uv belongs to an internal path of G , then $\mu(G) > \mu(G_{u,v})$.*

By $G \subset G'$, we mean that G is a subgraph of G' and $G \not\cong G'$.

Lemma 2.12 (see [10]). *If $G \subset G'$ and G' is a connected graph, then $\mu(G) < \mu(G')$.*

If $u \in V(G)$ and $d(u) \geq 3$, then we called u a *branching point* of G . Let U be a connected unicyclic graph and T_v be a tree such that T_v is attached to a vertex v of the unique cycle of U . The vertex v is called the *root* of T_v , and T_v is called a *root tree* of U . Throughout this paper, we assume that T_v does not include the root v . Clearly, U is obtained by attaching root trees to some vertices of the unique cycle of U .

Proof of Theorem 2.10. In the proof of this result, we assume that the unique cycle of U is C_p . Now choose $U \in \mathbb{U}_n \setminus \{C_n\}$ such that $\mu(U)$ is as small as possible. Since $U \not\cong C_n$, U has at least one branching point. We consider the next two cases.

Case 1. There are at least two branching points in C_p .

Now suppose u and v are two branching points in C_p such that there does not exist other branching point between the shortest path in C_p connected u and v . Let $u = v_1v_2 \cdots v_s = v$ ($s \geq 2$) be the shortest path in C_p connected u and v . Since u is a branching point of U , there is at least one pendant vertex, say w , in T_u . Suppose z is the unique neighbor vertex of w in U (may be $z = u$). Let $U_1 = U - wz$ and $U_2 = U_1 - w$. Then, $U_2 \subset U$, and hence $\mu(U_2) < \mu(U)$ by Lemma 2.12. Let $U_3 = U_1 - v_1v_2 + v_1w + v_2w$. By the hypothesis, $v_1v_2 \cdots v_s$ is an internal path of U_2 . By Lemma 2.11, we can conclude that $\mu(U_3) < \mu(U_2) < \mu(U)$. But U_3 is also a unicyclic graph with n vertices and $U_3 \not\cong C_n$ because v is a branching point of U_3 , it is a contradiction to the choice of U . Thus, Case 1 is impossible.

Case 2. There is unique branching point in C_p .

Subcase 1. There is at least a branching point outside C_p .

It can be proved analogously with Case 1.

Subcase 2. There does not exist any branching point outside C_p .

Suppose u is the unique branching point in C_p . By the hypothesis, u is also the unique branching point of U . Then, U is obtained by attaching $d(u) - 2$ paths to the vertex u of C_p .

If $d(u) \geq 4$, then there are at least two paths being attaching to u . It can be proved analogously with Case 1.

If $d(u) = 3$, then U is a lollipop graph, that is, $U \cong W_{n,p}$. Let $V(W_{n,p}) = \{v_1, v_2, \dots, v_n\}$ and $E(W_{n,p}) = \{v_p v_1, v_i v_{i+1}, 1 \leq i \leq n-1\}$. If $n-p \geq 2$, since $W_{n,p} - v_{n-1}v_n \subset W_{n,p}$, $\mu(W_{n,p}) > \mu(W_{n,p} - v_{n-1}v_n) = \mu(W_{n,p} - v_n)$ by Lemma 2.12. Moreover, since $W_{n,p} - v_{n-1}v_n - v_1v_p + v_p v_n + v_n v_1$ is the graph obtained from $W_{n,p} - v_n$ by subdividing the edge v_1v_p . Thus, by Lemma 2.11 it follows that

$$\mu(W_{n,p} - v_{n-1}v_n) = \mu(W_{n,p} - v_n) > \mu(W_{n,p} - v_{n-1}v_n - v_1v_p + v_p v_n + v_n v_1) = \mu(W_{n,p+1}). \quad (2.9)$$

Therefore, $\mu(W_{n,p}) > \mu(W_{n,p+1})$. Repeating the above process, we can conclude that $\mu(W_{n,p}) > \mu(W_{n,p+1}) > \cdots > \mu(W_{n,n-1})$ holds for $n-p \geq 2$.

By combining the above arguments, $U \cong W_{n,n-1}$. □

3. The Signless Laplacian Spreads of Unicyclic Graphs

In [1], the largest signless Laplacian spread among all unicyclic graphs with n vertices was determined, as follows.

Theorem 3.1 (see [1]). *If $n \geq 8$ and $U \in \mathbb{U}_n \setminus \{S_n^3\}$, then $SQ(S_n^3) > SQ(U)$.*

The next result extends the order of Theorem 3.1 to the first four largest values.

Theorem 3.2. *If $n \geq 16$ and $U \in \mathbb{U}_n \setminus \{S_n^3, S_n^4, F_n, H_n\}$, then*

$$SQ(S_n^3) > SQ(S_n^4) > \max\{SQ(F_n), SQ(H_n)\} \geq \min\{SQ(F_n), SQ(H_n)\} > SQ(U). \quad (3.1)$$

Remark 3.3. With the aid of computer, we always have $SQ(F_n) < SQ(H_n)$. But it seems rather difficult to be proved.

To prove Theorem 3.2, we need to introduce more lemmas as follows.

Proposition 3.4. *Suppose U is a unicyclic graph on n vertices with $\Delta \leq n - 3$. If $n \geq 9$, then $SQ(U) \leq n - 1.1$.*

Proof. Note that $\mu_n(U) \geq 0$ and $SQ(U) = \mu_1(U) - \mu_n(U) \leq \mu_1(U)$. We only need to prove $\max\{d(v) + m(v) : v \in V\} \leq n - 1.1$ by Lemma 2.3. Suppose $d(u) + m(u) = \max\{d(v) + m(v) : v \in V\}$. We consider the next three cases.

Case 1 ($d(u) = 1$). Suppose $v \in N(u)$. Then, $d(u) + m(u) = 1 + d(v) \leq 1 + \Delta \leq n - 2 < n - 1.1$.

Case 2 ($d(u) = 2$). Suppose $N(u) = \{w, v\}$. Note that U is a unicyclic graph. Then, $|N(v) \cap N(w)| \leq 2$ and $|N(v) \cup N(w)| \leq n$. Therefore,

$$d(u) + m(u) = 2 + \frac{d(v) + d(w)}{2} \leq 2 + \frac{n+2}{2} < n - 1.1. \quad (3.2)$$

Case 3 ($3 \leq d(u) \leq n - 3$). Note that U has n edges and $3 \leq d(u) \leq n - 3$. By inequality (2.2), we have

$$d(u) + m(u) \leq d(u) - 1 + \frac{2n-2}{d(u)}. \quad (3.3)$$

Next we will prove that $d(u) - 1 + ((2n-2)/d(u)) \leq n - 1.1$, equivalently, $d(u)(n-d(u)-0.1) \geq 2n-2$. Let $g(x) = (n-x-0.1)x$, where $3 \leq x \leq n-3$. Since $g'(x) = n-0.1-2x$ and $3 \leq x \leq n-3$, we have $g(x) \geq \min\{g(3), g(n-3)\} > 2n-2$.

By combining the above arguments, the result follows. $\square$

Lemma 3.5. *If $n \geq 16$, then $n - 1.1 < SQ(F_n) < n - 1$.*

Proof. Let $f_1(x) = x^5 - (n+5)x^4 + (6n+3)x^3 - (9n-1)x^2 + (3n+8)x - 4$. Clearly,

$$f_1\left(\frac{1}{2n}\right) = -\frac{1}{32n^5}(80n^5 - 56n^4 - 32n^3 - 10n^2 + 10n - 1). \quad (3.4)$$

Next we will prove that $f_1(1/2n) < 0$ when $n \geq 16$. Let $\varphi(n) = 80n^5 - 56n^4 - 32n^3 - 10n^2 + 10n - 1$. When $n \geq 16$, since $\varphi'''(n) = 4800n^2 - 1344n - 192 > 0$, we have $\varphi''(n) = 1600n^3 - 672n^2 - 192n - 20 \geq \varphi''(16) = 6378476 > 0$, then $\varphi'(n) = 400n^4 - 224n^3 - 96n^2 - 20n + 10 \geq \varphi'(16) = 25272010 > 0$. Thus, $\varphi(n) \geq \varphi(16) = 80082591 > 0$, and hence $f_1(1/2n) < 0$.

With the similar method, we have

$$\begin{aligned} f_1(0.1) &= 0.2159n - 3.18749 > 0, & f_1(0.5) &= \frac{1}{32}(11 - 2n) < 0, \\ f_1(3) &= 9n - 52 > 0, & f_1(n-1) &= -20 + 21n - 5n^2 < 0, \\ f_1\left(n-1 + \frac{1}{2n}\right) &= \frac{1}{32n^5}(16n^8 - 320n^7 + 1232n^6 - 1728n^5 + 1192n^4 - 504n^3 + 140n^2 - 20n + 1) > 0. \end{aligned} \quad (3.5)$$

By (2.5), we can conclude that $1/2n < \mu_n(F_n) < 0.1$ and $n-1 < \mu_1(F_n) < n-1 + 1/2n$. Thus, $n-1.1 < SQ(F_n) = \mu_1(F_n) - \mu_n(F_n) < n-1$. $\square$

Lemma 3.6. *If $n \geq 16$, then $n-1.1 < SQ(H_n) < n-1$.*

Proof. Let $f_2(x) = x^5 - (n+5)x^4 + (6n+4)x^3 - (10n-2)x^2 + (3n+12)x - 4$. It is easily checked that

$$\begin{aligned} f_2\left(\frac{1}{2n}\right) &= -\frac{1}{32n^5}(80n^5 - 112n^4 - 40n^3 - 14n^2 + 10n - 1) < 0, \\ f_2(0.1) &= 0.2059n - 2.77649 > 0, & f_2(0.5) &= \frac{1}{32}(87 - 10n) < 0, \\ f_2(2.8) &> 0.2464n - 2.14 > 0, & f_2(n-1) &= -24 + 25n - 5n^2 < 0, \\ f_2\left(n-1 + \frac{1}{2n}\right) &= \frac{1}{32n^5}(16n^8 - 320n^7 + 1376n^6 - 1888n^5 + 1288n^4 \\ &\quad - 520n^3 + 144n^2 - 20n + 1) > 0. \end{aligned} \quad (3.6)$$

By (2.6), we can conclude that $1/2n < \mu_n(H_n) < 0.1$ and $n-1 < \mu_1(H_n) < n-1 + (1/2n)$. Thus, $n-1.1 < SQ(H_n) = \mu_1(H_n) - \mu_n(H_n) < n-1$. $\square$

Proof of Theorem 3.2. By Lemma 2.6 and (2.7), $SQ(S_n^4) = \mu_1(S_n^4) - \mu_n(S_n^4) = \mu_1(S_n^4) > n-1$. Note that S_n^3 is the unique unicyclic graph with $\Delta = n-1$, and F_n, H_n, S_n^4 are all the unicyclic graphs with $\Delta = n-2$. Now suppose $U \in \mathbb{U}_n \setminus \{S_n^3, F_n, H_n, S_n^4\}$. Then, $\Delta(U) \leq n-3$. By Lemmas 3.5 and 3.6, Theorem 3.1, and Proposition 3.4, we can conclude that

$$\begin{aligned} SQ(S_n^3) &> SQ(S_n^4) > n-1 > \max\{SQ(F_n), SQ(H_n)\} \\ &\geq \min\{SQ(F_n), SQ(H_n)\} > n-1.1 \geq SQ(U). \end{aligned} \quad (3.7)$$

This completes the proof of Theorem 3.2. $\square$

4. A Class of Unicyclic Graphs Determined by Their Signless Laplacian Spectra

A graph G is said to be *determined by its signless Laplacian spectrum* if there does not exist other nonisomorphic graph H such that H and G share the same signless Laplacian spectra (see [11]). Let $S^3(n, k)$ be the unicyclic graph on n vertices obtained by attaching k , and $n - k - 3$ pendant vertices to two vertices of C_3 , respectively. By the definition, $S^3(n, n - 3) = S_n^3$. The next theorem is the main result of this section.

Theorem 4.1. *For any $k \geq \lceil n/2 \rceil - 1$, if $8k(n - 3 - k) \neq 9(n - 3)$, then $S^3(n, k)$ is determined by its signless Laplacian spectrum.*

To prove Theorem 4.1, we need some more lemmas as follows.

Lemma 4.2 (see [12]). *If G is a graph on n vertices with vertex degrees $d_1 \geq d_2 \geq \dots \geq d_n$ and signless Laplacian eigenvalues $\mu_1 \geq \mu_2 \geq \dots \geq \mu_n$, then $\mu_2 \geq d_2 - 1$. Moreover, if $\mu_2 = d_2 - 1$, then $d_1 = d_2$, and the maximum and the second maximum degree vertices are adjacent.*

Lemma 4.3 (see [12]). *If G is a connected graph with n vertices, then $\mu_n(G) < \delta(G)$.*

Lemma 4.4 (see [7]). *In any graph, the multiplicity of the eigenvalue 0 of the signless Laplacian matrix of G is equal to the number of bipartite components of G .*

Let $\mathbb{U}(n, \Delta)$ be the class of unicyclic graphs on n vertices with maximum degree Δ .

Lemma 4.5 (see [13]). *For any $k \geq \lceil n/2 \rceil - 1$, if $U \in \mathbb{U}(n, k + 2)$, then $\mu(U) \leq \mu(S^3(n, k))$, where the equality holds if and only if $U \cong S^3(n, k)$.*

Lemma 4.6 (see [13]). *Let G be the graph with the largest signless Laplacian spectral radius in $\mathbb{U}(n, \Delta)$. If $\Delta \leq n - 2$, then there must exist some graph $G_1 \in \mathbb{U}(n, \Delta + 1)$ such that $\mu(G) < \mu(G_1)$.*

Proof of Theorem 4.1. By an elementary computation, we have

$$\Phi(S^3(n, k), x) = (x - 1)^{n-5} f_3(x), \quad (4.1)$$

where $f_3(x) = x^5 - (n + 5)x^4 + (kn + 5n - k^2 - 3k + 7)x^3 - (2kn + 7n - 2k^2 - 6k + 7)x^2 + (3n + 8)x - 4$. Now suppose that there exists another graph G such that G and $S^3(n, k)$ share the same signless Laplacian spectra. Next we will prove that $G \cong S^3(n, k)$. We only need to prove the following facts.

Fact 1. G is a connected unicyclic graph.

Proof of Fact 1. Assume that G has exactly t connected components, say $G_1, \dots, G_t$, where $t \geq 1$. By Lemma 4.4, G_i is not a bipartite graph for $1 \leq i \leq t$ because $S^3(n, k)$ is not a bipartite graph. Thus, G_i is a connected unicyclic graph for $1 \leq i \leq t$ because G has n edges (since $S^3(n, k)$ has n edges). Moreover, since $8k(n - 3 - k) \neq 9(n - 3)$, we have $f_3(4) \neq 0$. Thus, G_i is not a cycle for $1 \leq i \leq t$ because 4 is the eigenvalue of the signless Laplacian matrix of a cycle. By the above arguments, we can conclude that G_i is not a bipartite graph and has at least one pendant vertex. Thus, G_i has at least two signless Laplacian eigenvalues being

larger than 1 by Lemma 4.2, and the smallest signless Laplacian eigenvalue of G_i is less than 1 by Lemma 4.3. Therefore, by (4.1) we can conclude that $t \leq 1$, and hence G is connected. Clearly, G is a connected unicyclic graph because G has n edges. $\square$

Fact 2. $\Delta(G) \leq k + 2$.

Proof of Fact 2. Note that $k \geq \lceil n/2 \rceil - 1$. Then, $n < 2k + 3$. By Lemmas 2.3 and 2.6,

$$\Delta(G) + 1 \leq \mu(G) = \mu(S^3(n, k)) \leq \max \left\{ k + 2 + \frac{n+1}{k+2}, n - 1 - k + \frac{n+1}{n-k-1}, 2 + \frac{n+1}{2} \right\} < k + 4. \quad (4.2)$$

Thus, $\Delta(G) \leq k + 2$ holds. $\square$

Fact 3. $G \cong S^3(n, k)$.

Proof of Fact 3. By Fact 2, we have $\Delta(G) \leq k + 2$. If $\Delta(G) \leq k + 1 < \Delta(S^3(n, k))$, then $\mu(G) < \mu(S^3(n, k))$ by Lemmas 4.5 and 4.6, a contradiction. Thus, $\Delta(G) = k + 2$, and hence the result follows from Lemma 4.5 because $\mu(G) = \mu(S^3(n, k))$.

This completes the proof of Theorem 4.1. $\square$

$\square$

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