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The Signless Laplacian Estrada Index of Unicyclic Graphs

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and

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Abstract

For a simple graph G, the signless Laplacian Estrada index is defined as $SLEE(G) = \sum_{i=1}^{n} e^{q_i}$, where $q_1, q_2, \ldots, q_n$ are the eigenvalues of the signless Laplacian matrix of G. In this paper, we first characterize the unicyclic graphs with the first two largest and smallest $SLEE$'s and then determine the unique unicyclic graph with maximum $SLEE$ among all unicyclic graphs on n vertices with a given diameter. All extremal graphs, which have been introduced in our results are also extremal with respect to the signless Laplacian resolvent energy.

Keywords: Signless Laplacian Estrada index, unicyclic graphs, extremal graphs, diameter, signless Laplacian resolvent energy.

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1. Introduction

In this paper, all graphs are simple, finite, and undirected. The vertex and edge sets of a graph G are $V(G)$ and $E(G)$, respectively. Usually, we suppose that G has n vertices and m edges. The adjacency matrix $A = A(G) = [a_{ij}]$ is the $n \times n$ symmetric matrix with zero diagonal entries and whose (i, j)-th entry is equal to 1 if i and j are adjacent in G and to 0 otherwise, for distinct $i, j \in V(G)$. The matrix $Q = Q(G) = D + A$ is known as the *signless Laplacian matrix* of G, where D is the diagonal matrix whose diagonal entry $(D)_{ii}$ is the degree of vertex i, $1 \leq i \leq n$. We denote the spectrum of Q by $(q_1, q_2, \ldots, q_n)$.

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For any graph G, the largest eigenvalue of $Q(G)$ is called the *signless Laplacian spectral radius*, *Q-spectral radius*, or *Q-index* of G. The problem of determining graphs, having the maximum spectral radius of the signless Laplacian matrix (among all graphs with given numbers of vertices and edges) is an important problem in the spectral graph theory (see [10, 11, 15]). More references about spectral properties of the signless Laplacian matrix can be found in [5, 7].

The answer to the question, "Which graphs are determined by their spectrum?" is still unknown. Reviewing the literature of the spectral graph theory, we notice that van Dam and Haemers proposed that using the signless Laplacian matrix Q in the study of graph properties is better than the other graph matrices [8]. Therefore, research on (the spectrum of) this matrix has attracted more attention of some authors.

Recently, Nasiri et al. [14], defined the *resolvent signless Laplacian Estrada index* of any non-complete graph G as $SLEE_r(G) = \sum_{i=1}^{n} \frac{2n-2}{2n-2-q_i}$, and studied the matrix $Q(G)$ with respect to this new invariant. Analogously, Cafure et al. [4], introduced the *signless Laplacian resolvent energy* of an arbitrary graph G by $RQ(G) = \sum_{i=1}^{n} \frac{1}{2n-1-q_i}$. Moreover, the spectrum of the matrix Q is the main part of another energy-like quantity of graphs, called the *signless Laplacian energy*, which is defined by Abreu et al. [1] in the following form:

$$SLE(G) = \sum_{i=1}^{n} \Big| q_i - \frac{2m}{n} \Big|.$$

Binthiya et al. [3] established an upper bound for $SLE(G)$ and $SLEE(G)$ in terms of n, m and vertex connectivity of G, where $SLEE(G)$ is the *signless Laplacian Estrada index* of the graph G. For the first time, Ayyaswamy et al. [2] defined $SLEE(G)$ as the sum of exponentials of the eigenvalues of $Q(G)$, i. e.,

$$SLEE(G) = \sum_{i=1}^{n} e^{q_i}.$$

They also determined lower and upper bounds for $SLEE$ in terms of the number of vertices and edges. In [9, 12], we investigated the unique graphs with maximum $SLEE$ among the set of all graphs with given number of cut edges, cut vertices, pendent vertices, (vertex) connectivity, edge connectivity, or diameter. In another work [13], we obtained that there exist exactly two graphs with maximum $SLEE$ in the class of all n-vertex tricyclic graphs, for $n \geq 5$.

In this paper, in order to continue our research on the signless Laplacian matrix, we study the unicyclic graphs having the first two largest and smallest $SLEE$'s, and find the unique unicyclic graph with maximum $SLEE$ among the class of all unicyclic graphs on n vertices with a given diameter.

2. Preliminaries

This section recalls some basic definitions, notations and results from [6, 9]; then it proves three useful propositions which will be used in our main results.

A *unicyclic graph* is a connected graph with the same number of vertices and edges. Hence, a unicyclic graph is a connected graph with a unique cycle. For a graph G, we denote by $T_k(G)$, its k-th signless Laplacian spectral moment, i.e., $T_k(G) = \sum_{i=1}^{n} q_i^k$. So we have,

$$SLEE(G) = \sum_{k\geq 0} \frac{T_k(G)}{k!}.$$

Definition 2.1. [6] A *semi-edge walk* of length k in a graph, say G, is an alternating sequence $W = v_1e_1v_2e_2\cdots v_ke_kv_{k+1}$ of vertices $v_1, v_2, \ldots, v_k, v_{k+1}$ and edges $e_1, e_2, \ldots, e_k$ such that two vertices v_i and v_{i+1} are (not necessarily distinct) end-vertices of the edge e_i, for any $i = 1, 2, \ldots, k$. If $v_1 = v_{k+1}$, then we say that W is a *closed semi-edge walk*.

Theorem 2.2. *[6] For a graph G, the signless Laplacian spectral moment $T_k(G)$ is equal to the number of closed semi-edge walks of length k in G.*

Let G and H be two graphs, and $x, y \in V(G)$, and $v, u \in V(H)$. We denote by $SW_k(G; x, y)$, the set of all semi-edge walks, each of which is of length k in G, starting at vertex x, and ending at vertex y. For convenience, we may denote $SW_k(G; x, x)$ by $SW_k(G; x)$, and set $SW_k(G) = \bigcup_{x\in V(G)} SW_k(G; x)$. Thus, Theorem 2.2 tells us that $T_k(G) = |SW_k(G)|$.

If for any $k \geq 0$, $|SW_k(G; x, y)| \leq |SW_k(H; v, u)|$, then we use the notation $(G; x, y) \preceq_s (H; v, u)$. Moreover, if $(G; x, y) \preceq_s (H; v, u)$, and there exists some k_0 such that $|SW_{k_0}(G; x, y)| < |SW_{k_0}(H; v, u)|$, then we write $(G; x, y) \prec_s (H; v, u)$.

Lemma 2.3. *[9] Let G be a graph and $v, u, w_1, w_2, \ldots, w_r \in V(G)$. Suppose that $E_v = \{e_1 = vw_1, \ldots, e_r = vw_r\}$ and $E_u = \{e'_1 = uw_1, \ldots, e'_r = uw_r\}$ are subsets of edges of the complement of G (i.e. $e_i, e'_i \notin E(G)$ for $i = 1, 2, \ldots, r$). Set $G_u = G + E_u$ and $G_v = G + E_v$. If $(G; v) \prec_s (G; u)$, and $(G; w_i, v) \preceq_s (G; w_i, u)$ for each $i = 1, 2, \ldots, r$, then $SLEE(G_v) < SLEE(G_u)$.*

To use the above lemma more conveniently, we say that G_u is obtained from G_v, by transferring some neighbors of v to the set of neighbors of u. In this situation, we call the vertices $w_1, \ldots, w_r$ as *transferred neighbors*, and the graph G as *transfer route*. Note that an important condition to use the above lemma is to be able to compare the number of semi-edge walks ending at vertices u and v. In the following, we present a helpful lemma to compare the number of semi-edge walks ending at some different vertices.

Lemma 2.4. *Let G be a graph and $P = v_0v_1\cdots v_l$ be a path in G such that $d(v_0) = 1$. Suppose that $v = v_r$ and $u = v_s$ such that $r + s \leq l$ and $d(v_i) = 2$*

for each $0 < i < \frac{r+s}{2}$. *If* $r+s < l$ *or* $d(v) < d(u)$, *then* $(G; v) \prec_s (G; u)$ *and* $(G; w, v) \preceq_s (G; w, u)$ *for any* $w \in V(G) \setminus \{v_0, v_1, \ldots, v_a\}$, *where* $a = \lfloor \frac{r+s}{2} \rfloor$.

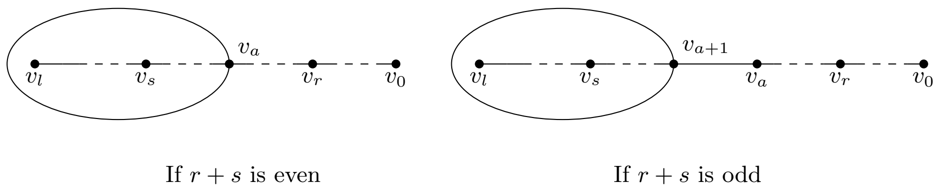

Figure 1: An illustration of the graph G in Lemma 2.4.

Proof. For each semi-edge walk W in P which does not contain the vertices v_j and the edges $e_j = v_{j-1}v_j$ for any $j > r+s$, suppose that $\overline{W}$ is a semi-edge walk in P obtained uniquely from W by replacing vertices v_t with $v_{t'}$ and the corresponding edges, where $t' = r+s-t$.

Let $W \in SW_k(G; v)$, and $r+s$ be even. In this case, v_a is the vertex which has the same distance from v and u in P. If W contains v_a more than once, then it can be decomposed uniquely to $W_1W_2W_3$, such that $W_2 \in SW_k(G; v_a)$ is as long as possible, and W_1 and W_3 are two semi-edge walks in P. Suppose that $f_k^{(1)}(W_1W_2W_3) = \overline{W_1}W_2\overline{W_3}$, and if W does not contain v_a more than once, then $f_k^{(1)}(W) = \overline{W}$. Obviously, the map $f_k^{(1)} : SW_k(G; v) \to SW_k(G; u)$ is an injection.

Let $r+s$ be odd. If W contains $e_{a+1} = v_av_{a+1}$ more than once, then it can be decomposed uniquely to $W_1e_{a+1}W_2e_{a+1}W_3$, such that W_2 is as long as possible, and W_1 and W_3 are two semi-edge walks in P. In this case set:

$$f_k^{(2)}(W_1W_2W_3) = \overline{W_1}e_{a+1}W_2e_{a+1}\overline{W_3}.$$

Also, if W does not contain $e_{a+1} = v_av_{a+1}$ more than once, then set $f_k^{(2)}(W) = \overline{W}$. The map $f_k^{(2)} : SW_k(G; v) \to SW_k(G; u)$ is also an injection.

Thus $|SW_k(G; v)| \leq |SW_k(G; u)|$ for any $k \geq 0$. Note that if $d(v) < d(u)$ then

$$T_1(G; v) = d(v) < d(u) = T_1(G; u).$$

Also, if $r+s < l$, then none of the maps $f_k^{(i)}$, for $i = 1, 2$, is covering the semi-edge walk:

$$W = v_se_{s+1}v_{s+1} \cdots v_{l-1}e_lv_le_lv_{l-1} \cdots v_{s+1}e_{s+1}v_s.$$

Therefore, $|SW_{k_0}(G; v)| < |SW_{k_0}(G; u)|$, for some $k_0 \geq 1$. Hence $(G; v) \prec_s (G; u)$.

By a similar method, we can prove that $(G; w, v) \preceq_s (G; w, u)$ for any vertex $w \in V(G) \setminus \{v_0, v_1, \ldots, v_a\}$, which completes the proof. □

A special case of the previous lemma for $r = 0$ and $s = 1$, is proved in [9, Lemma 2.5].

Corollary 2.5. *Let G be a graph containing a cycle, say $C_l = v_0v_1 \cdots v_{l-1}v_0$, such that $l > 3$. Suppose that H is the graph obtained from G by transferring neighbors $N'(v)$ of v to the set of neighbors of u, where $v = v_0$, $u = v_1$, and $N'(v) = N(v) \setminus \{u\}$. If u and v do not have a common neighbor in G, then $SLEE(G) < SLEE(H)$.*

Proof. Let G' be the transfer route graph and $P = v_0v_1 \cdots v_{l-1}$. Applying Lemma 2.4 for $r = 0$ and $s = 1$, implies that $(G'; v) \prec_s (G'; u)$ and $(G'; w, v) \preceq_s (G'; w, u)$ for any $w \in N'(v) \subseteq V(G) \setminus \{v\}$. Now, the result follows from Lemma 2.3. $\square$

Note that the result of Corollary 2.5 holds for any $v = v_i$ and $u = v_{i+1}$, because we can rewrite the cycle C_l in the form $C_l = v_iv_{i+1} \cdots v_lv_0v_1 \cdots v_{i-1}v_i$ for any $i = 0, \ldots, l$.

Lemma 2.6. *Let G be an arbitrary graph and $v, u \in V(G)$. If $d_G(v) < d_G(u)$ and $N^{np}(v) \subseteq N^{np}(u) \cup \{u\}$, where $N^{np}(x)$ is the set of all non-pendent neighbors of the vertex x, then $(G; v) \prec_s (G; u)$.*

Proof. For each $w \in N^{np}(v) \setminus \{u\}$, we correspond a vertex, say $\overline{w} = w \in N^{np}(u)$. This correspondence can be extended over $N(v) \setminus \{u\}$, because $d_G(v) < d_G(u)$. Moreover, we can assume that v corresponds to u (i.e. $\overline{v} = u$ and $\overline{u} = v$). Suppose that $k > 0$ and $W \in SW_k(G; v)$. We can decompose W into $W_1W_2W_3$, where W_1 and W_3 are as long as possible and made up of just the vertices in $\{v\} \cup N^{np}(v) \setminus \{u\}$ and the edges in $\{vw : w \in N(v) \setminus \{u\}\}$. Note that W_2 and W_3 are empty when W consists of just the above vertices and edges. Let $\overline{W_j}$ be obtained from W_j for $j = 1, 3$, by replacing each vertex x with $\overline{x}$ and each edge $e = x\,y$ with $\overline{e} = \overline{x}\,\overline{y}$. The map $f_k : SW_k(G; v) \to SW_k(G; u)$ defined by the rule $f_k(W_1W_2W_3) = \overline{W_1}W_2\overline{W_3}$ is an injection. Therefore, we have $(G; v) \prec_s (G; u)$, because $d_G(v) < d_G(u)$. $\square$

3. Maximum *SLEE* of Unicyclic Graphs

In the present section, we find the unique graphs with first and second maximum $SLEE$ among all unicyclic graphs on n vertices.

Let $q \geq 3$, and $n_i \geq 0$, where $i = 1, 2, \ldots, q$. Denoting by $C_qS(n_1, n_2, \ldots, n_q)$, the graph obtained from a cycle $C_q = v_1v_2 \cdots v_qv_1$, by attaching n_i pendent vertices to v_i for each $i = 1, 2, \ldots, q$. Also, we denote the graph $C_3S(n-3, 0, 0)$ by $G^{(1)}$, and $C_3S(n-4, 1, 0)$ by $G^{(2)}$ (see Figure 2).

Lemma 3.1. *Let G be a unicyclic graph with the unique cycle $C_q = v_1v_2 \cdots v_qv_1$. There exist $n_1, \ldots, n_q \geq 0$, such that $SLEE(G) \leq SLEE\big(C_qS(n_1, n_2, \ldots, n_q)\big)$, with equality if and only if $G \cong C_qS(n_1, n_2, \ldots, n_q)$.*

Proof. If $G \ncong C_qS(n_1, \ldots, n_q)$, then there exists a tree T on at least 3 vertices with only one vertex in C_q, say $u = v_i$, such that T is not a star with the center vertex u. Suppose that v is a non-pendant neighbor of the vertex u in T. Let

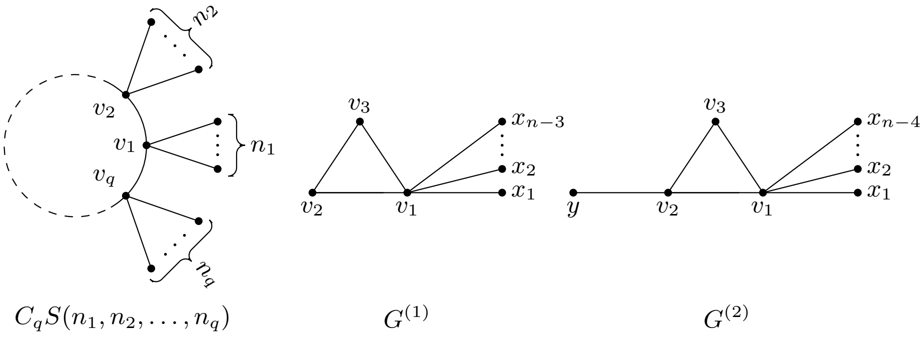

Figure 2: A demonstration of graphs $C_qS(n_1, n_2, \ldots, n_q)$, $G^{(1)}$, and $G^{(2)}$.

$N'(v) = N(v) \setminus \{u\}$, G_1 be the graph obtained from G by transferring neighbors $N'(v)$ of v to the set of neighbors of u, and G'_1 be the transfer route. By Lemma 2.4, $(G'_1; v) \prec_s (G'_1; u)$ and $(G'_1; w, v) \preceq_s (G'_1; w, u)$ for any $w \in V(G) \setminus \{v\}$. Now, by Lemma 2.3, $SLEE(G) < SLEE(G_1)$. If $G_1 \ncong C_qS(n_1, \ldots, n_q)$, then by repeating the above process, we may get a graph G_k with $SLEE(G) < SLEE(G_k)$ where $G_k \cong C_qS(n_1, \ldots, n_q)$ for some $n_1, \ldots, n_q \geq 0$. □

Lemma 3.2. *If $q \geq 3$ and $n_1, \ldots, n_q \geq 0$, then there exist $n'_1, n'_2, n'_3 \geq 0$ such that,*

$$SLEE\big(C_qS(n_1, n_2, \ldots, n_q)\big) \leq SLEE\big(C_3S(n'_1, n'_2, n'_3)\big)$$

with equality if and only if $q = 3$.

Proof. Obviously, if $q = 3$, then the equality holds true. Therefore, let $q > 3$, and $C_q = v_1v_2 \cdots v_qv_1$ be the unique cycle of $C_qS(n_1, \ldots, n_q)$. Since v_1 and v_2 do not have any common neighbors, by Corollary 2.5,

$$SLEE\big(C_qS(n_1, n_2, \ldots, n_q)\big) < SLEE\big(C_{q-1}S(n_1 + n_2 + 1, n_3, \ldots, n_q)\big).$$

By repeating this process, after $q - 3$ times, we have,

$$SLEE\big(C_qS(n_1, n_2, \ldots, n_q)\big) < SLEE\big(C_3S(q - 3 + \textstyle\sum_{i=1}^{q-2} n_i, n_{q-1}, n_q)\big).$$

□

In the following theorem, we prove that $G^{(1)}$ has the first maximum $SLEE$, and $G^{(2)}$ has the second maximum $SLEE$ among all unicyclic graphs on n vertices.

Theorem 3.3. *Let G be a unicyclic graph on n vertices. If $G \ncong G^{(1)}$, then,*

$$SLEE(G) \leq SLEE(G^{(2)}) < SLEE(G^{(1)})$$

with equality in the left part if and only if $G \cong G^{(2)}$.

Proof. Let $G \cong G^{(2)}$ (as shown in Figure 2). The graph $G^{(1)}$ is obtained from $G^{(2)}$ by transferring the pendent neighbor y of v_2 to the set of neighbors of v_1. Let H be the transfer route graph. It is easy to show that $(H; v_2) \prec_s (H; v_1)$. Therefore, Lemma 2.3 implies that $SLEE(G^{(2)}) < SLEE(G^{(1)})$.

Let $C_q = v_1 v_2 \cdots v_q v_1$ be the unique cycle of G, and $G \not\cong G^{(2)}$. We prove the theorem in three cases as follows:

Case 1. $q = 3$ and two of vertices in C_3, say v_2 and v_3, have degree 2.

In this case by removing vertices v_2 and v_3 of G, we get a tree T which is not a star with center vertex v_1. By reapplying Lemmas 2.3 and 2.4, similarly in proof of Lemma 3.1, we may get a graph G_1 from G, made up of a cycle C_3, and $n-5$ pendent vertices attached to v_1 and a pendent path $P_3 = v_1 u_1 x$ (see Figure 3), such that $SLEE(G) < SLEE(G_1)$.

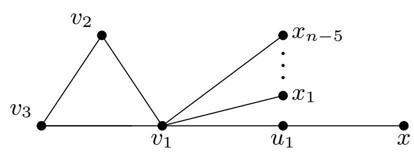

Figure 3: The graph G_1 in Case 1 of the proof.

Obviously, $G^{(2)}$ can be obtained from G_1 by transferring the neighbor x of u_1 to the set of neighbors of v_2. Let H be the transfer route graph. By Lemma 2.4, $(H; u_1) \prec_s (H; v_2)$. Therefore, Lemma 2.3 implies that $SLEE(G_1) < SLEE(G^{(2)})$.

Case 2. $q = 3$ and two of vertices in C_3, say v_1 and v_2 have degrees more than 2.

In this case, by Lemma 3.1, there exist integers $n_1, n_2, n_3 \geq 0$ such that $SLEE(G) \leq SLEE\big(C_3 S(n_1, n_2, n_3)\big)$, with equality if and only if G is isomorphic to $C_3 S(n_1, n_2, n_3)$. Without loss of generality, we may assume that $n_1 \geq n_2 \geq n_3$. If $n_3 \neq 0$, then obviously, $C_3 S(n_1 + n_3, n_2, 0)$ is obtained from $C_3 S(n_1, n_2, n_3)$ by transferring n_3 pendent neighbors of v_3 to the set of neighbors of v_1. If H is the transfer route graph, then Lemma 2.6 implies that $(H; v_3) \prec_s (H; v_1)$. Therefore, by Lemma 2.3,

$$SLEE\big(C_3 S(n_1, n_2, n_3)\big) < SLEE\big(C_3 S(n_1 + n_3, n_2, 0)\big).$$

Now, if $n_2 > 1$, then by reapplying Lemmas 2.3 and 2.6 (i. e. by transferring $n_2 - 1$ pendent neighbors of v_2 to the set of neighbors of v_1) we have,

$$SLEE\big(C_3 S(n_1 + n_3, n_2, 0)\big) < SLEE(G^{(2)}).$$

Case 3. $q > 3$.

By Lemma 3.1, there exist integers $n_1, n_2, \ldots, n_q \geq 0$, such that,

$$SLEE(G) \leq SLEE\big(C_q S(n_1, \ldots, n_q)\big),$$

with equality if and only if $G \cong C_qS(n_1,\dots,n_q)$. If $q > 4$, then by $q-4$ times reusing Corollary 2.5, as used in the proof of Lemma 3.2, we may get four integers $n'_1 \geq \cdots \geq n'_4 \geq 0$, such that $SLEE\big(C_qS(n_1,\dots,n_q)\big) < SLEE\big(C_4S(n'_1,\dots,n'_4)\big)$. Suppose that $C_4 = v_1v_2v_3v_4v_1$ and $n'_1 \neq 0$. Since v_2 and v_3 do not have any common neighbors, by Corollary 2.5, we conclude that,

$$SLEE(G) \leq SLEE\big(C_3S(n'_1, n'_2 + n'_3 + 1, n'_4)\big).$$

Now, the result follows by Case 2. □

4. Minimum *SLEE* of Unicyclic Graphs

The goal of this section is to specify unique graphs with first and second minimum $SLEE$ among all n-vertex unicyclic graphs.

Let $q \geq 3$, and $n_i \geq 0$, where $i = 1, 2, \dots, q$. Denoting by $C_qP(n_1, n_2, \dots, n_q)$, the graph obtained from a cycle $C_q = v_1v_2\cdots v_qv_1$, by attaching a pendent path on $n_i + 1$ vertices to v_i for each $i = 1, 2, \dots, q$. For convenience, we denote the graph $C_{n-1}P(1, 0, \dots, 0)$ by $G_{(2)}$ (see Figure 4).

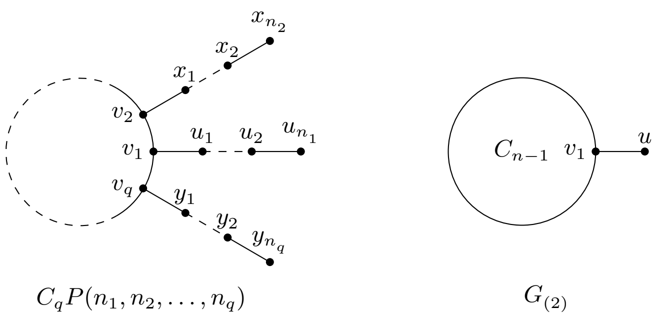

Figure 4: An illustration of the graphs $C_qP(n_1, n_2, \dots, n_q)$ and $G_{(2)}$.

Lemma 4.1. *Let G be a unicyclic graph with the unique cycle $C_q = v_1v_2\cdots v_qv_1$. There exist $n_1,\dots,n_q \geq 0$, such that $SLEE(C_qP(n_1, n_2, \dots, n_q)) \leq SLEE(G)$, with equality if and only if $G \cong C_qP(n_1, n_2, \dots, n_q)$.*

Proof. Let $G \ncong C_qP(n_1,\dots,n_q)$. Thus, G has a subgraph T containing exactly one vertex, say v_i, in C_q, and T is a tree but not a path. Let $P_{r+1} = u_0u_1\cdots u_r$ be the longest path in T with one end at v_i (i.e. $u_r = v_i$). Obviously, u_0 is a pendent vertex. Since T is not a path, there is a minimum index j, where $1 \leq j \leq r$, such that $d_T(u_j) > 2$. Let G_1 be the graph obtained from G by transferring all of vertices in $N_T(u_j) \setminus V(P_{r+1})$ from the set of neighbors of u_j to the set of neighbors of u_0. Let G'_1 be the transfer route graph. Now, by

Lemma 2.4, we have $(G'_1; u_0) \prec_s (G'_1; u_j)$ whose applying to Lemma 2.3 gives us $SLEE(G_1) < SLEE(G)$.

It is obvious that in the graph G_1, the tree which is attached to the vertex v_i has a path longer than P_{r+1}, with an end vertex v_i. Thus, by repeating this operation, we get a graph G_k such that the tree attached to v_i is a path on n_i vertices, and $SLEE(G_k) < SLEE(G)$. Now, the result follows by doing this process on every tree which has just one common vertex with C_q, and is not a path. □

Lemma 4.2. *Let $H = C_q P(n_1, n_2, \ldots, n_q)$, where $q < n$. Then,*

$$SLEE(C_q) < SLEE(G_{(2)}) \leq SLEE(H)$$

with equality on the right part if and only if $H \cong G_{(2)}$ (i.e. $q = n - 1$).

Proof. It is easy to show that $SLEE(C_q) < SLEE(G_{(2)})$. Also, if $q < n-1$, then there exists at least one index i with $n_i > 0$. Without loss of generality, we can assume that $i = 1$, and $P = v_1 u_1 u_2 \cdots u_{n_1}$ is the pendent path at v_1. Obviously $G_1 = C_{q+n_1-1} P(1, n_2, \ldots, n_q, 0, 0, \ldots, 0)$ is obtained from H by transferring the neighbor v_q of v_1 to the set of neighbors of u_{n_1-1}. By Lemmas 2.3 and 2.4, we have $SLEE(G_1) < SLEE(H)$. Now, by repeating a similar process on every pendent path of length > 0, we conclude that $SLEE(G_{(2)}) < SLEE(H)$. □

The following theorem is an immediate consequence of the previous lemmas and shows that the unique unicyclic n-vertex graph with first (respectively, second) minimum $SLEE$ is C_q (respectively, $G_{(2)}$).

Theorem 4.3. *Let G be a unicyclic graph on n vertices with the unique cycle C_q. If $q < n$, then,*

$$SLEE(C_q) < SLEE(G_{(2)}) \leq SLEE(G)$$

with equality on the right part if and only if $G \cong G_{(2)}$ (i.e. $q = n - 1$).

5. Unicyclic Graph with Maximum *SLEE* with Given Diameter

This last section determines the unique graph which has maximum $SLEE$ among the set of all unicyclic graphs with given diameter d. A *diametral path* is a shortest path between two vertices whose distance is equal to the diameter of the graph. It is well-known that C_3 is the unique unicyclic graph with diameter $d = 1$. Therefore, we consider $d \geq 2$ throughout this section.

Lemma 5.1. *Let G be a unicyclic graph with given diameter d, and $P = v_0 v_1 \cdots v_d$ be a diametral path in G. If G has maximum SLEE, then $xv_i \notin E(G)$ for any $x \in \overline{V(G)} = V(G) \setminus V(P)$ and $v_i \in V(P) \setminus \{v_a, v_{a+1}\}$, where the vertex v_a is almost in the middle of the path P (i.e. either $a = \lfloor \frac{d}{2} \rfloor$ or $a = \lfloor \frac{d}{2} \rfloor - 1$).*

Hereafter, for convenience, for any subset $X \subseteq V(G)$, set $\overline{X} = X \setminus V(P)$, and $\hat{d} = \lfloor \frac{d}{2} \rfloor$.

Proof. Suppose that i is the minimum index with $xv_i \in E(G)$ for some $x \in \overline{V(G)}$. Since G is unicyclic, there exists an index $j \in \{i+1, i+2\}$ such that v_i and v_j do not have any common neighbors belonging to $\overline{V(G)}$. If $i < \hat{d} - 1$, then by Lemmas 2.4 and 2.3 and transferring some neighbors of v_i to the set of neighbors of v_j, we may get a unicyclic graph with diameter d, which has larger $SLEE$ than G, a contradiction. Thus $\overline{N(v_i)} = \emptyset$ for each $i < \hat{d} - 1$. Similarly, we have $\overline{N(v_i)} = \emptyset$ for each $i > \hat{d} + 1$.

If d is odd, then $\overline{N(v_{\hat{d}-1})} = \emptyset$, because otherwise, in the same way as above, by transferring some neighbors of $v_{\hat{d}-1}$ to the set of neighbors of either $v_{\hat{d}}$ or $v_{\hat{d}+1}$, we obtain a unicyclic graph with diameter d, which has larger $SLEE$ than G, also a contradiction.

If d is even, then $\overline{N(v_{\hat{d}-1})} = \emptyset$ or $\overline{N(v_{\hat{d}+1})} = \emptyset$. Otherwise, we can obtain a unicyclic graph with diameter d, which has larger $SLEE$ than G, by transferring neighbors $\overline{N(v_{\hat{d}-1})}$ of $v_{\hat{d}-1}$ to the set of neighbors of either $v_{\hat{d}}$ or $v_{\hat{d}+1}$; which is again a contradiction. □

Remark. With the above notations, bear in mind if d is even and $\overline{N(v_{\hat{d}+1})} = \emptyset$, then by changing the labels of vertices of P, such that v_i gets the label u_{d-i} for each $i = 0, \ldots, d$, we have $xu_i \notin E(G)$ for any $x \in \overline{V(G)}$ and $u_i \in V(P) \setminus \{u_{\hat{d}}, u_{\hat{d}+1}\}$. Thus, we can always suppose that $a = \hat{d}$ in the previous lemma.

Let $1 \leq d \leq n-2$. We denote by G^d the graph obtained from a path on $d+1$ vertices, say $P = v_0 v_1 \cdots v_d$, by attaching $n-d-2$ pendent vertices to $v_{\hat{d}}$, and a vertex $u \in \overline{V(G)}$ to the vertices $v_{\hat{d}}$ and $v_{\hat{d}+1}$ (see Figure 5).

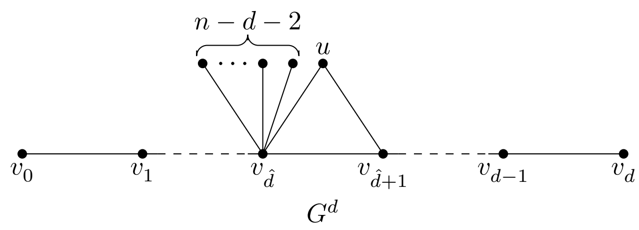

Figure 5: The unicyclic graph which has maximum $SLEE$ with given diameter d.

In the following theorem, we prove that G^d is the unique unicyclic graph which has maximum $SLEE$ among the set of all unicyclic graphs with given diameter d.

Theorem 5.2. *If G is a unicyclic graph with diameter d which has maximum $SLEE$, then $G \cong G^d$.*

Proof. By Lemma 5.1 and the previous remark, we know that the graph G has a diametral path, say $P = v_0 v_1 \cdots v_d$, such that $xv_i \notin E(G)$ for each $x \in \overline{V(G)}$ and $v_i \in V(P_{d+1}) \setminus \{v_{\hat{d}}, v_{\hat{d}+1}\}$. By Corollary 2.5, the unique cycle of G is of length 3, say $C_3 = u_1 u_2 u_3 u_1$.

By a similar method used in the proof of Lemma 3.1, we conclude that any vertex $x \in \overline{V(G)} \setminus V(C_3)$ is a pendent vertex, and C_3 has at least one common vertex with P.

We claim that $V(C_3) \cap V(P) = \{v_{\hat{d}}, v_{\hat{d}+1}\}$. In order to prove it, let C_3 have exactly one common vertex with P_{d+1}, say $u_1 = v_j$ where $j \in \{\hat{d}, \hat{d}+1\}$. If $d = 2$, then we may change our choice of P, such that C_3 and the new diametral path have exactly two vertices in common. If $d > 2$, then suppose that G_1 is the graph obtained from G by transferring neighbors $N(u_2) \setminus \{u_1\}$ of u_2 to the set of neighbors of $v_{j'}$, also H is the transfer route graph, where $\{j, j'\} = \{\hat{d}, \hat{d}+1\}$. By Lemma 2.4, $(H; u_2) \prec_s (H; v_{j'})$. Therefore, Lemma 2.3 implies that $SLEE(G) < SLEE(G_1)$, which is a contradiction. This proves our claim.

Set $u = u_3$. If $d(u) > 2$, then by transferring pendent neighbors of u to the set of neighbors of $v_{\hat{d}}$, we get a unicyclic graph with diameter d which has larger $SLEE$ than G, a contradiction. Therefore, $d(u) = 2$.

Now, if $d(v_{\hat{d}+1}) = 3$, then there is nothing to prove. Therefore, let $d(v_{\hat{d}+1}) > 3$. If d is even and $d(v_{\hat{d}}) = 3$, then by changing the labels of vertices of P, as in the previous remark, we have nothing to prove, again. So, let either d be odd or $d(v_{\hat{d}}) > 3$. Obviously, G^d can be obtained from G by transferring some neighbors of $v_{\hat{d}+1}$ to the set of neighbors of $v_{\hat{d}}$. Suppose that H is the transfer route graph. With these assumptions and using the method of the proof of Lemma 2.6, and also a correspondence between each vertex v_i and $v_{2\hat{d}+1-i}$, where $2\hat{d} + 1 - d \leq i \leq d$, we can show that $(H; v_{\hat{d}+1}) \prec_s (H; v_{\hat{d}})$. Thus, by Lemma 2.3 we have,

$$SLEE(G) < SLEE(G^d),$$

which is a contradiction. Therefore, $G \cong G^d$. □

6. Concluding Remarks

In this paper, we have determined the unicyclic graphs with the first two largest and smallest $SLEE$'s. We have also specified the unique graph with maximum $SLEE$ among all unicyclic graphs on n vertices with a given diameter. Indeed, the main idea of this paper (also [9, 12, 13]), is to use the notion of the *signless Laplacian spectral moments* of graphs to compare their $SLEE$'s.

Since the *signless Laplacian resolvent energy* of any graph, say G, is equal to $\sum_{k \geq 0} \frac{T_k(G)}{(2n-1)^{k+1}}$, it would be of interest to study this *energy-like invariant* by considering the signless Laplacian spectral moments. However, it is easy to check that the expected results for the signless Laplacian resolvent energy of graphs will be very similar to our main results. More precisely, one can check that all extremal graphs, which have been introduced in our results (including extremal graphs in [9, 12, 13]), are also extremal with respect to the signless Laplacian resolvent energy.

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