Electronic Journal of Graph Theory and Applications **6** (1) (2018), 190–200

Electronic Journal of Graph Theory and Applications

On maximum signless Laplacian Estrada index of graphs with given parameters II

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Abstract

The signless Laplacian Estrada index of a graph G 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. Following the previous work in which we have identified the unique graphs with maximum signless Laplacian Estrada index with each of the given parameters, namely, number of cut edges, pendent vertices, (vertex) connectivity, and edge connectivity, in this paper we continue our characterization for two further parameters: diameter and number of cut vertices.

Keywords: Estrada index, signless Laplacian Estrada index, extremal graph, diameter, cut vertex
Mathematics Subject Classification : 05C12, 05C35, 05C50
DOI: 10.5614/ejgta.2018.6.1.14

1. Introduction

Let $G = (V, E)$ be a simple, finite, and undirected graph with vertex set $V(G)$, the edge set $E(G)$, and $|V(G)| = n$. The adjacency matrix $\mathbf{A} = \mathbf{A}(G) = [a_{ij}]$ of G is the binary matrix, where the element a_{ij} is equal to 1 if vertices i and j are adjacent, and 0 otherwise. The matrices $\mathbf{L} = \mathbf{D} - \mathbf{A}$ and $\mathbf{Q} = \mathbf{D} + \mathbf{A}$, where $\mathbf{D} = diag(d_1, d_2, \ldots, d_n)$ is the diagonal matrix of vertex degrees, are known as the *Laplacian matrix* and *signless Laplacian matrix* of G. The spectrum of $\mathbf{Q}$ is denoted by $(q_1, q_2, \ldots, q_n)$.

Received: 3 July 2016, Revised: 11 February 2018, Accepted: 24 March 2018.

Spectral graph theory is the study of properties of a graph in relationship to the eigenvalues of matrix $\mathbf{M}$ associated with the graph. This theory is called $\mathbf{M}$-*theory* (see [5–7]). The spectral graph theory is widely used in various fields such as physics, chemistry, computer sciences, and mathematics (see [2–5, 13–16, 18]). For some special graphs, $\mathbf{Q}$-theory is equivalent to other theories. For example, for regular graphs $\mathbf{Q}$-theory is equivalent to $\mathbf{A}$-theory and $\mathbf{L}$-theory, or the matrices $\mathbf{L}$ and $\mathbf{Q}$ are similar if and only if G is a bipartite graph [8, 9, 12]. For studying various graph properties, some evidence is presented that the positive semi-definite matrix $\mathbf{Q}$ might be better suited than the other graph matrices (see [9]).

For a graph G, Ayyaswamy et al. [1] introduced the innovative notion of the *signless Laplacian Estrada index* as

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

They also established lower and upper bounds for $SLEE$ in terms of the number of vertices and edges. Previously in [10], we investigated the unique graphs with maximum $SLEE$ among the set of all graphs with given number of cut edges, pendent vertices, (vertex) connectivity and edge connectivity. Moreover, we studied the signless Laplacian Estrada index of unicyclic and tricyclic graphs in [11, 17].

In this paper, we continue our research by determining the unique graphs with maximum $SLEE$ according to two further parameters: diameter and number of cut vertices. Our main results are the following two theorems:

Theorem 1.1. *If G has maximum $SLEE$ with diameter d, $2 < d < n-1$, then $G \cong H_{d,1}$, (see Figure 1).*

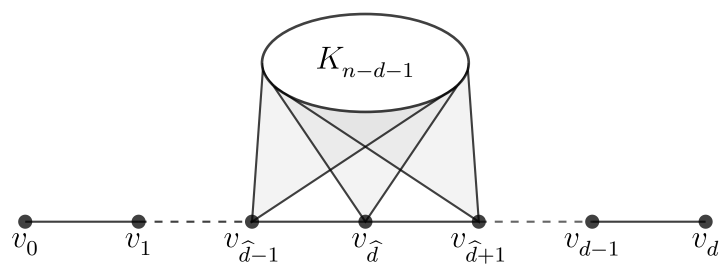

Figure 1. Graph $H_{d,1}$.

Theorem 1.2. *If G has maximum $SLEE$ on n vertices with r cut vertices, $0 \leq r \leq n-2$, then $G \cong G_n^r$, where G_n^r is the graph obtained from K_{n-r} by attaching $n-r$ pendent paths of orders $n_1, n_2, \ldots, n_{n-r}$ to its vertices; such that each vertex of K_{n-r} has exactly one pendent path and also $\mid n_i - n_j \mid \leq 1$ for $1 \leq i, j \leq n-r$. More precisely, each pendent path is of order $\lfloor \frac{r}{n-r} \rfloor$ or $\lfloor \frac{r}{n-r} \rfloor + 1$. For example, the graphs G_6^r with $r = 0, 1, 2, 3, 4$ are shown in Figure 2.*

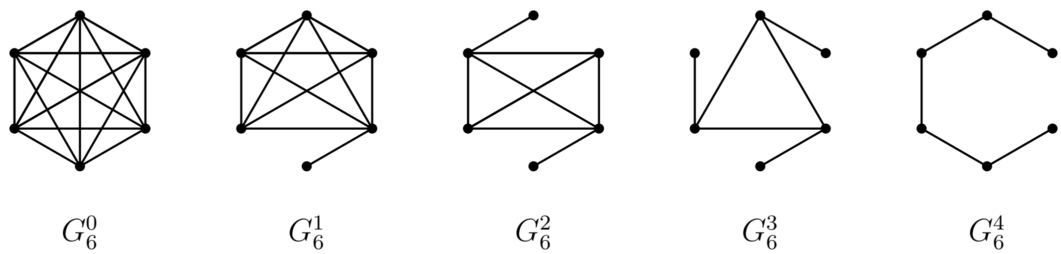

Figure 2. The graphs G_6^r with $r = 0, 1, 2, 3, 4$.

2. Preliminaries and Lemmas

In this section, initially, basic definitions, notations, and concepts used in the study are introduced and some findings proved in [8, 10] are restated as well. Then, relevant propositions required to prove the results reported in the next sections are given and proved.

Definition 2.1. [8] A *semi-edge walk* of length k in graph G is an alternating sequence $W = v_1e_1v_2e_2 \dots v_ke_kv_{k+1}$, where $v_1, v_2, \dots, v_k, v_{k+1} \in V(G)$, and $e_1, e_2, \dots, e_k \in E(G)$ such that the vertices v_i and v_{i+1} are (not necessarily distinct) end points of edge e_i, for any $i = 1, 2, \dots, k$. If $v_1 = v_{k+1}$, then we say W is a *closed semi-edge walk*.

By following [10], we denote the k-th signless Laplacian spectral moment of the graph G by $T_k(G)$, i.e., $T_k(G) = \sum_{i=1}^{n} q_i^k$.

Theorem 2.1. *[8] For a graph G, the signless Laplacian spectral moment T_k is equal to the number of closed semi-edge walks of length k.*

Note that, by Taylor expansions, we have

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

Bearing this relation in mind, one can find that for two n-vertex graphs G and H, if $T_k(G) \geq T_k(H)$ for all $k \geq 0$, then $SLEE(G) \geq SLEE(H)$. So, to compare the signless Laplacian Estrada indices of two graphs, we can compare their signless Laplacian spectral moments.

By $(G; v, u) \preceq_s (G'; v', u')$ we mean $|SW_k(G; v, u)| \leq |SW_k(G'; v', u')|$, for any $k \geq 0$. Moreover, if $(G; v, u) \preceq_s (G'; v', u')$ and there exists some k_0 such that we have $|SW_{k_0}(G; v, u)| < |SW_{k_0}(G'; v', u')|$, then we write $(G; v, u) \prec_s (G'; v', u')$. Let $SW_k(G; v) = SW_k(G; v, v)$. Similarly, we may define $(G; v) \preceq_s (G'; v')$ and $(G; v) \prec_s (G'; v')$. By the above notations, we have

$$T_k(G) = \sum_{v\in V(G)} |SW_k(G; v)|.$$

The notation $G \preceq_s G'$ means that $T_k(G) \leq T_k(G')$, for each $k \geq 0$. If $G \preceq_s G'$ and for some k_0, $T_{k_0}(G) < T_{k_0}(G')$, then we use the notation $G \prec_s G'$. Also, if $T_k(G) = T_k(G')$, for each $k \geq 0$, then we write $G =_s G'$.

Lemma 2.1. *[10] Let G be a graph. If an edge e does not belong to $E(G)$, then $G \prec_s G+e$, thus $SLEE(G) < SLEE(G+e)$.*

Lemma 2.2. *[10] 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. Let $G_u = G + E_u$ 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 $G_v \prec_s G_u$, thus $SLEE(G_v) < SLEE(G_u)$.*

For a vertex v and an edge e, let $SW_k(G; v, [e])$ be the set of all closed semi-edge walks of length k in the graph G, starting at vertex v and containing e.

Lemma 2.3. *Let G be a graph and $H = G + e$, such that $e = uv \in E(\overline{G})$. If $(G; v) \preceq_s (G; u)$, then $(H; v) \preceq_s (H; u)$. Moreover, if $(G; v) \prec_s (G; u)$, then $(H; v) \prec_s (H; u)$.*

Proof. We know that for each $z \in \{u, v\}$ and $k \geq 0$,

$$|SW_k(H; z)| = |SW_k(G; z)| + |SW_k(H; z, [e])|.$$

Since $(G; v) \preceq_s (G; u)$, $|SW_k(G; v)| \leq |SW_k(G; u)|$, for each $k \geq 0$. Thus, there is a bijection $f_k : SW_k(G; v) \to A_k \subseteq SW_k(G; u)$, for each $k \geq 0$. It is enough to show that $|SW_k(H; v, [e])| \leq |SW_k(H; u, [e])|$, for each $k \geq 0$. Let $W \in SW_k(H; v, [e])$. We can uniquely decompose W to $W = W_1 e W_2 e \ldots e W_r$, such that $W_i \in SW_{k_i}(G; x, y)$, where $x, y \in \{u, v\}$, $k_i \geq 0$ and $1 \leq i \leq r$. Note that W_i is a semi-edge walk in G and does not contain e, thus the decomposition is unique. For each W_i , exactly one of the following cases occurs:

1) $W_i \in SW_{k_i}(G; v, v)$. In this case, we set $h(W_i) = f_{k_i}(W_i)$. Thus, $h(W_i) \in A_{k_i} \subseteq SW_{k_i}(G; u, u)$.

2) $W_i \in A_{k_i} \subseteq SW_{k_i}(G; u, u)$. In this case, set $h(W_i) = f_{k_i}^{-1}(W_i) \in SW_{k_i}(G; v, v)$.

3) $W_i \in SW_{k_i}(G; u, u) \setminus A_{k_i}$, or $W_i \in SW_{k_i}(G; u, v)$, or $W_i \in SW_{k_i}(G; v, u)$. We consider $h(W_i) = W_i$ for the first case, and $h(W_i) = W_i^{-1}$ for the last two cases.

Now, it is easy to show that the map $h_k : SW_k(H; v, [e]) \to SW_k(H; u, [e])$ by the rule $h_k(W) = h_k(W_1 e W_2 e \ldots W_r) = h(W_1) e h(W_2) e \ldots e h(W_r)$ is an injection.

Note that if there exists k_0 such that $|SW_{k_0}(G; v)| < |SW_{k_0}(G; u)|$, then f_{k_0} is not surjective. Thus, h_{k_0} is not a surjection and we have

$$|SW_{k_0}(H; v, [e])| < |SW_{k_0}(G; u, [e])|$$

which implies that $(H; v) \prec_s (H; u)$. □

Lemma 2.4. *Let G be a graph and $H = G + e$, such that $e = uv \in E(\overline{G})$ and $(G; v) \preceq_s (G; u)$. If there exists a vertex $x \in V(G)$ such that $(G; x, v) \preceq_s (G; x, u)$, then $(H; x, v) \preceq_s (H; x, u)$. Moreover, if $(G; v) \prec_s (G; u)$ or $(G; x, v) \prec_s (G; x, u)$, then $(H; x, v) \prec_s (H; x, u)$.*

Proof. Since $(G; v) \preceq_s (G; u)$, there is a bijection $f_k : SW_k(G; v) \to A_k \subseteq SW_k(G; u)$, for each $k \geq 0$. Similarly, since $(G; x, v) \preceq_s (G; x, u)$, for each $k \geq 0$, there is a bijection

$$g_k : SW_k(G; x, v) \to B_k \subseteq SW_k(G; x, u).$$

It is obvious that for each $k \geq 0$,

$$|SW_k(H; x, z)| = |SW_k(G; x, z)| + |SW_k(H; x, z, [e])|$$

where $z \in \{v, u\}$. It is enough to show that for each $k \geq 0$,

$$|SW_k(H; x, v, [e])| \leq |SW_k(H; x, u, [e])|.$$

Let $W \in SW_k(H; x, v, [e])$. W can be decomposed uniquely to $W_1eW_2e \dots eW_r$, where W_i is a semi-edge walk of length k_i in G. Three cases will be considered as follows for W_1:

1) If $W_1 \in SW_{k_1}(G; x, v)$, set $h_1(W_1) = g_{k_1}(W_1) \in B_{k_1} \subseteq SW_{k_1}(G; x, u)$.
2) If $W_1 \in B_{k_1} \subseteq SW_{k_1}(G; x, u)$, set $h_1(W_1) = g_{k_1}^{-1}(W_1) \in SW_{k_1}(G; x, v)$.
3) If $W_1 \in SW_{k_1}(G; x, u) \setminus B_{k_1}$, set $h_1(W_1) = W_1$.

If $1 < i \leq r$, then three cases will be considered as follows for W_i:

1) If $W_i \in SW_{k_i}(G; v)$, then set $h_i(W_i) = f_{k_i}(W_i) \in A_{k_i}$.
2) If $W_i \in A_{k_i} \subseteq SW_{k_i}(G; u)$, then set $h_i(W_i) = f_{k_i}^{-1}(W_i) \in SW_{k_i}(G; v)$.
3) If $W_i \in SW_{k_i}(G; u) \setminus A_{k_i}$, $W_i \in SW_{k_i}(G; v, u)$ or $W_i \in SW_{k_i}(G; u, v)$, then set $h_i(W_i) = W_i$ for the first case, and $h_i(W_i) = W_i^{-1}$ for the last two cases.

One can easily see that the map $h_k : SW_k(H; x, v, [e]) \to SW_k(H; x, u, [e])$ by the rule $h_k(W) = h_k(W_1eW_2e \dots W_r) = h_1(W_1)eh_2(W_2)e \dots eh_r(W_r)$ is injective.

The second part of the lemma is clear. □

3. The proof of Theorem 1.1

For $x \in V(G)$, the *eccentricity* $e(x)$ of x is defined as $e(x) = max\{d(x, y) : y \in V(G)\}$. The *diameter* $d(G)$ is the maximum eccentricity over all vertices, whereas the *radius* $r(G)$ is the minimum eccentricity. Also, x is a *central vertex* if $e(x) = r(G)$ and a *diametrical path* is a shortest path between two vertices whose distance is equal to $d(G)$. For the sake of convenience, we denote $\lceil \frac{d}{2} \rceil$ by $\widehat{d}$, which is the smallest integer number greater than $\frac{d}{2}$. It is obvious that K_n is the unique graph with diameter 1. Also, the path on n vertices P_n is the unique graph with diameter $n - 1$. Furthermore, $K_n - e$ is the graph with the greatest signless Laplacian spectral moments, and so the maximum $SLEE$, with diameter 2, where e is an edge of K_n.

Lemma 3.1. *Let G be a graph with diameter d and $P_{d+1} = v_0v_1 \dots v_d$ be a diametrical path in G. If $d \geq 2$ and $x \in V(G) \setminus V(P_{d+1})$, then x has at most 3 neighbors in $V(P_{d+1})$.*

Proof. Suppose that x has neighbors $v_{i_1}, v_{i_2}, \ldots, v_{i_r}$ in P_{d+1}, where $r > 3$ and $i_1 < i_2 < \ldots < i_r$. Since $i_r - i_1 > 2$, the path $P' = v_0v_1 \ldots v_{i_1}xv_{i_r}v_{i_r+1} \ldots v_d$ from v_0 to v_d has a length $d - i_r + i_1 + 2 < d$, which is a contradiction. □

Let $n > 4$, $2 < d < n-1$, and $1 \leq j \leq \widehat{d}$. We denote by $\mathcal{H}_{d,j}$ the set of all graphs $H_{d,j}$; each of these members are constructed from K_{n-1-d} and $P_{d+1} = v_0v_1 \ldots v_d$ by attaching each vertex of K_{n-d-1} to exactly 3 vertices of P_{d+1}, such that for each $x \in V(K_{n-d-1})$ there exists an index i, where $\widehat{d} - j \leq i \leq \widehat{d} + j - 2$, and x is attached to v_i, v_{i+1}, and v_{i+2}. Therefore, none of vertices v_i, where $0 \leq i < \widehat{d} - j$ or $\widehat{d} + j < i \leq d$, has a neighbor in K_{n-d-1}. Note that $v_{\widehat{d}}$ is a central vertex of the path P_{d+1}. For example, all graphs $H_{4,2}$ with $n = 7$ are shown in Figure 3.

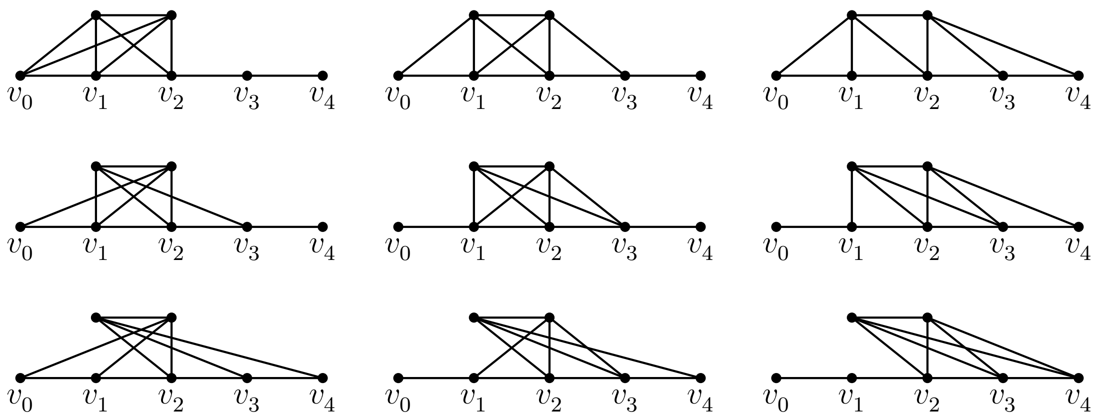

Figure 3. All graphs $H_{4,2}$ with $n = 7$.

Lemma 3.2. *Let $n > 4$, $2 < d < n-1$, and $2 \leq j \leq \widehat{d}$. If $H_j \in \mathcal{H}_{d,j}$, then either $H_j \in \mathcal{H}_{d,j-1}$, or there exists a graph, say $H_{j-1} \in \mathcal{H}_{d,j-1}$, such that $H_j \prec_s H_{j-1}$, resulting $SLEE(H_j) < SLEE(H_{j-1})$.*

Proof. Let $H_j \in \mathcal{H}_{d,j}$ and $N_K(v_i) = N(v_i) \cap V(K_{n-1-d})$, where $0 \leq i \leq d$ and $N(v_i)$ is the set of vertices that are adjacent to v_i. For a better understanding of the proof, our argument is divided into two parts; that is, first we discuss $N_K(v_{\widehat{d}-j})$ and then, proceed to $N_K(v_{\widehat{d}+j})$. Let $H_j \notin \mathcal{H}_{d,j-1}$. If $N_K(v_{\widehat{d}-j}) = \emptyset$, then we set $H'_{j-1} = H_j$. In this case, we have $H'_{j-1} =_s H_j$. Let $N_K(v_{\widehat{d}-j}) \neq \emptyset$. For convenience, suppose that $v = v_{\widehat{d}-j}$, $y = v_{\widehat{d}-j+1}$, $z = v_{\widehat{d}-j+2}$, and $u = v_{\widehat{d}-j+3}$. By the definition of $\mathcal{H}_{d,j}$, it is obvious that $N_K(v) \subseteq N_K(y) \subseteq N_K(z)$ and $N_K(v) \cap N_K(u) = \emptyset$. Let $E = \{vx : x \in N_K(v)\}$, $E' = \{ux : x \in N_K(v)\}$, $H'_j = H_j - E$, and $H'_{j-1} = H'_j + E'$. By Lemma 2.2, in order to show that $H_j \prec_s H'_{j-1}$, it is enough to prove the following statements:

1) $(H'_j; v) \prec_s (H'_j; u)$.

2) $(H'_j; x, v) \preceq_s (H'_j; x, u)$, for each $x \in N_K(v)$.

In order to prove (1), we begin with the following claim:
Claim. $(H'_j; y) \preceq_s (H'_j; z)$:

To prove the claim, let $W \in SW_k(H'_j - e; y)$, where $e = yz$ and $k \geq 0$. We can decompose W to $W = W_1W_2W_3$, where W_1 and W_3 are as long as possible and consist of just the vertices $v_0, v_1, \dots, y$ and edges in $\{v_tv_{t+1} : 0 \leq t \leq \widehat{d} - j\} \cup \{yx : x \in N_K(y)\}$; where also $W_2 \in SW_{k_2}(H'_j - e; x, w)$, such that $x, w \in N_K(y) \subseteq N_K(z)$. Suppose that W'_i is obtained from W_i, for $i = 1, 3$, by replacing each vertex v_t with v_a, each edge v_tv_{t+1} with v_av_{a-1}, and each edge yx with zx; where $x \in N_K(y)$ and $a = 2\widehat{d} - 2j - t + 3$ (in fact the distance between vertices v_t and y is equal to the distance between vertices v_a and z in P_{d+1}). It is easy to show that the map $f'_k : SW_k(H'_j - e; y) \to SW_k(H'_j - e; z)$, defined by the rule $f'_k(W_1W_2W_3) = W'_1W_2W'_3$, is injective; thus, $(H'_j - e; y) \preceq_s (H'_j - e; z)$. Now, the claim follows from Lemma 2.3.

For each $k \geq 0$, let $f_k : SW_k(H'_j; y) \to SW_k(H'_j; z)$ be an injection. If $W \in SW_k(H'_j; v)$, then W can be decomposed to $W = W_1W_2W_3$, where $W_2 \in SW_{k_2}(H'_j; y)$ is as long as possible. Let W'_i be obtained form W_i for each $i = 1, 3$; by replacing each vertex v_t with v_a and each edge v_tv_{t+1} with v_av_{a-1}, where $a = 2\widehat{d} - 2j - t + 3$. The map $g_k : SW_k(H'_j; v) \to SW_k(H'_j; u)$, defined by the rule $g_k(W_1W_2W_3) = W'_1f_{k_2}(W_2)W'_3$, is injective. Note that if $j > 2$ or d is even, then the path $v_0v_1 \dots v$ is a proper subgraph of the path $v_dv_{d-1} \dots u$. Also, if d is odd and $j = 2$, then $N_K(u) \neq \emptyset$, which implies that $deg_{H'_j}(v) = 2 < deg_{H'_j}(u)$. Therefore, $(H'_j; v) \prec_s (H'_j; u)$, which is (1).

We use a similar procedure to prove statement (2): First, we claim that:

Claim. For each $x \in N_K(v)$, $(H'_j; x, y) \preceq_s (H'_j; x, z)$.

In order to prove the claim, let $x \in N_K(v)$ and $W \in SW_k(H'_j - e; x, y)$, where $e = yz$. We can decompose W to $W = W_1W_2$, such that $W_1 \in SW_{k_1}(H'_j - e; x, w)$ is as long as possible, where $w \in N_K(y)$ and $W_2 \in SW_{k_2}(H'_j - e; w, y)$. Suppose that W'_2 is obtained from W_2 by replacing each vertex v_t with v_a, the edge wy with wz and each edge v_tv_{t+1} with v_av_{a-1}, where $a = 2\widehat{d} - 2j - t + 3$. One can easily see that the map $h'_k : SW_k(H'_j - e; x, y) \to SW_k(H'_j - e; x, z)$, defined by the rule $h'_k(W_1W_2) = W_1W'_2$, is injective. Resulting, $(H'_j - e; x, y) \preceq_s (H'_j - e; x, z)$. Now, the claim is obtained from Lemma 2.4.

Consider $h_k : SW_k(H'_j; x, y) \to SW_k(H'_j; x, z)$ is an injective map for each $k \geq 0$. Let $W \in SW_k(H'_j; x, v)$. We can decompose W to $W = W_1W_2$, where $W_1 \in SW_{k_1}(H'_j; x, y)$ and is as long as possible; where also $W_2 \in SW_{k_2}(H'_j; y, v)$. Let W'_2 be obtained from W_2 by replacing each vertex v_t with v_a and each edge v_tv_{t+1} with v_av_{a-1}, where $a = 2\widehat{d} - 2j - t + 3$. It is elementary to show that the map $l_k : SW_k(H'_j : x, v) \to SW_k(H'_j; x, u)$, defined by the rule $l_k(W_1W_2) = h_{k_1}(W_1)W'_2$, is an injection. Thus, $(H'_j; x, v) \preceq_s (H'_j; x, u)$ for each $x \in N_K(v)$, from which statement (2) follows. Now, by the above discussion and lemma 2.2, we have $H_j \preceq_s H'_{j-1}$, with equality if and only if $H'_{j-1} \cong H_j$. The first part of the argument ends here.

If $N_K(v_{\widehat{d}+j})$ is empty or d is odd and $j = 2$, then $H'_{j-1} \in \mathcal{H}_{d,j-1}$. In this case, set $H_{j-1} = H'_{j-1}$ and of course $H_{j-1} =_s H'_{j-1}$. Let $H'_{j-1} \notin \mathcal{H}_{d,j-1}$, then $N_K(v_{\widehat{d}+j})$ is not empty. By repeating the above discussion for $v = v_{\widehat{d}+j}$, $y = v_{\widehat{d}+j-1}$, $z = v_{\widehat{d}+j-2}$, and $u = v_{\widehat{d}+j-3}$, we get the graph $H_{j-1} = H'_{j-1} - E + E'$, such that $H_{j-1} \in \mathcal{H}_{d,j-1}$ and $H'_{j-1} \prec_s H_{j-1}$. Therefore,

$$H_j \preceq_s H'_{j-1} \preceq_s H_{j-1} \in \mathcal{H}_{d,j-1},$$

these equalities hold if and only if graphs are isomorphic. □

Now, we may prove the main result of this section.

Proof of Theorem 1.1. Suppose that G is a graph, having the greatest signless Laplacian spectral moments, and so the maximum $SLEE$, with diameter d. Let $P_{d+1} = v_0v_1 \dots v_d$ be a diametrical path in G, and H be the graph obtained from G by adding some edges such that:

(a) For each $x \in V(G) \setminus V(P_{d+1})$, x is a neighbor of exactly 3 vertices of P_{d+1} in H, say v_i, v_{i+1} and v_{i+2}.

(b) $H - V(P_{d+1})$ is a complete graph on $n - 1 - d$ vertices.

By Lemma 3.1, such a graph H exists. Obviously, we have $H \in \mathcal{H}_{d,j}$ for some j, where $1 \leq j \leq \widehat{d}$ and $G \preceq_s H$, with equality if and only if $G \cong H$. If $j > 1$, then by Lemma 3.2, we may get a sequence of graphs, say $H_{d,j-1}, H_{d,j-2}, \dots, H_{d,1}$, such that for each t, $H_{d,t} \in \mathcal{H}_{d,t}$ and

$$G \preceq_s H \preceq_s H_{d,j-1} \preceq_s H_{d,j-2} \preceq_s \dots \preceq_s H_{d,1},$$

these equalities hold if and only if the graphs are isomorphic. Since the diameter of $H_{d,1}$ is d and G has the greatest signless Laplacian spectral moments among the set of all graphs with diameter d, $G =_s H_{d,1}$ which implies that $G \cong H_{d,1}$, as expected. □

4. The proof of Theorem 1.2

A *cut vertex* of a graph is a vertex whose removal increases the number of components of the graph. Let G be a connected graph and x be a vertex of G. A *block* of G is defined to be a maximal subgraph without cut vertices. A *pendent path* at x in a graph G is a path in which no vertex other than x is incident with any edge of G outside the path, where $deg_G(x) \geq 3$. In particular, we consider a vertex x as a pendent path at x of length zero in G only when x is neither a pendent vertex nor a cut vertex of G. Let G and H be two vertex-disjoint connected graphs, such that $x \in V(G)$ and $y \in V(H)$. We denote the *coalescence* of G and H by $G(x) \circ H(y)$, which is obtained by identifying the vertex x of G with the vertex y of H.

Lemma 4.1. *Let H_1 and H_2 be two graphs, $P_s = y_0y_1 \dots y_{s-1}$ be a path on s vertices, $u \in V(H_2)$, and $xy \in E(H_1)$ such that $x \neq y$. Let $G = \big(H_1(y) \circ P_s(y_0)\big)(x) \circ H_2(u)$. If H_2 contains a path $Q_{s+2} = ux_1x_2 \dots x_{s+1}$, then $G \prec_s G - E_y + E_{x_1}$ – thus $SLEE(G) < SLEE(G - E_y + E_{x_1})$ – where $E_y = \big\{yw : w \in N_{H_1}(y) \setminus \{x\}\big\}$, $E_{x_1} = \big\{x_1w : w \in N_{H_1}(y) \setminus \{x\}\big\}$, and $N_{H_1}(y)$ is the set of vertices of H_1 that are neighbors of y (see Figure 4).*

Proof. Let $G' = G - E_y$. By Lemma 2.2, it is enough to show that $(G'; y) \prec_s (G'; x_1)$ and $(G'; w, y) \preceq_s (G'; w, x_1)$, for each $w \in N_{H_1}(y) \setminus \{x\}$. Let $P'_{s+1} = xy_0y_1 \dots y_{s-1}$, $A_k = SW_k(G'; y) \setminus SW_k(P'_{s+1}; y)$, and $B_k = SW_k(G'; x_1) \setminus SW_k(Q_{s+2}; x_1)$. Since P'_{s+1} is a proper subgraph of Q_{s+2}, it is easy to show that $|SW_k(p'_{s+1}; y)| \leq |SW_k(Q_{s+2}; x_1)|$ and inequality is strict for some $k = k_0 \geq s$. Let $W \in A_k$. We can decompose W to $W_1W_2W_3$, such that $W_2 \in SW_{k_2}(G'; x)$ and is as long as possible; also $W_1 \in SW_{k_1}(G'; y, x), W_3 \in SW_{k_3}(G'; x, y)$ and $k = k_1 + k_2 + k_3$. Let W'_j be obtained from W_j by replacing each y_i with x_{i+1}, where $j = 1, 3$

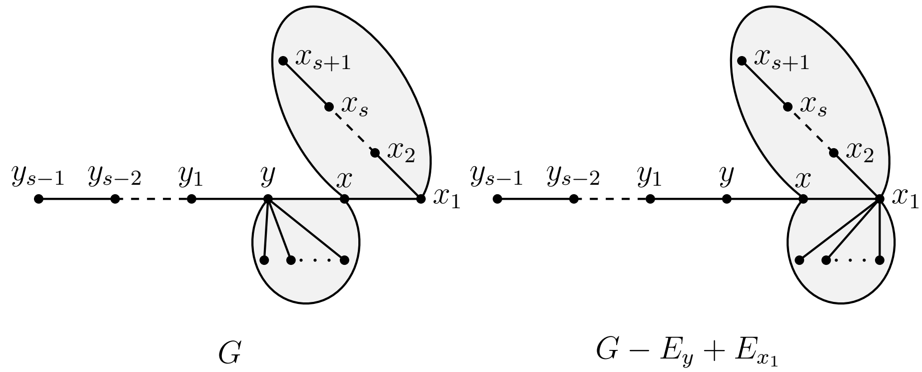

Figure 4. An illustration of graphs in Lemma 4.1.

and $i = 0, 1, \ldots, s-1$. The map $f : A_k \to B_k$, defined by the rule $f(W_1W_2W_3) = W_1'W_2W_3'$, is injective, and thus, $|A_k| \le |B_k|$. Therefore, $|SW_k(G'; y)| \le |SW_k(G'; x_1)|$ and for some $k = k_0$ the inequality is strict. Hence, $(G'; y) \prec_s (G'; x_1)$.

Let $w \in N_{H_1}(y) \setminus \{x\}$ and $W \in SW_k(G'; w, y)$. We can decompose W uniquely to W_1W_2, such that $W_1 \in SW_{k_1}(G'; w, x)$ is as long as possible. Let W_2' be obtained from W_2 by replacing each y_i with x_{i+1}, where $W_2 \in SW_{k_2}(G'; x, y)$, $k = k_1 + k_2$, and $i = 0, 1, \ldots, s-1$. The map $g_{w,k} : SW_k(G'; w, y) \to SW_k(G'; w, x_1)$, defined by the rule $g_{w,k}(W_1W_2) = W_1W_2'$, is injective. Thus, $|SW_k(G'; w, y)| \le |SW_k(G'; w, x_1)|$ for each k. Therefore, $(G'; w, y) \preceq_s (G'; w, x_1)$ for each $w \in N_{H_1}(y) \setminus \{x\}$. □

Now, we get to the most important proof of this section.

Proof of Theorem 1.2. Since $P_n = G_n^{n-2}$ is the unique graph with $n-2$ cut vertices, the case $r = n-2$ is obvious. If $r = 0$, then by Lemma 2.1, $K_n = G_n^0$ is the unique graph on n vertices with the greatest signless Laplacian spectral moments, and also maximum $SLEE$. Let $1 \le r \le n-3$ and G be a graph with the greatest signless Laplacian spectral moments among all graphs on n vertices with r cut vertices. First, we prove that G is connected, for if G is not connected and x is a cut vertex of G, then x is also a cut vertex of a component, say G_1 of G. Let G_2 be another component of G. If G_2 has a cut vertex, say y, then set $G' = G + \{xy\}$. If G_2 has no cut vertex, then suppose that G' is the graph obtained from G by attaching x to each vertex of G_2. It is easy to show that in both cases G' is a graph with r cut vertices and $G \prec_s G'$, a contradiction. Thus, G is connected.

By Lemma 2.1, every block of G is complete. Let x be a cut vertex contained in at least 3 blocks, say B_1, B_2 and B_3. Assume that B_1 and B_3 are disjointed if the vertex x is removed. Let G' be the graph obtained from G by attaching each vertex of B_1 to each vertex of B_2. Obviously, G' has r cut vertices, and by Lemma 2.1 $G \prec_s G'$, a contradiction. Thus, each cut vertex of G is contained in exactly two blocks. Suppose that G has at least one block with at least 3 vertices. Otherwise, since each block of G has 2 vertices, G is a tree with maximum degree 2. Thus, $G \cong P_n$ and $r = n-2$, a contradiction. Let P_s be a pendent path with minimum length in G at x. Obviously, x lies in a block of G, say B, with at least 3 vertices. Note that if $s = 1$, then x is not a cut vertex.

For each $y \in V(B)$, let H_y be the component of $G - E(B)$ which contains y. Obviously, $H_x = P_s$. Let $y \in V(B)$ such that $y \neq x$. Let H be the component of $G - \big(E(H_x) \cup E(H_y)\big)$ containing y. We have $G \cong \big(H(x) \circ H_x(x)\big)(y) \circ H_y(y)$. Suppose that H_y is not a path. Since P_s has minimum length, there is a pendent path on at least s vertices at a vertex in H_y, say z, where $z \neq y$. Thus, H_y contains a path on at least $s+2$ vertices with an end vertex y. Note that since H_y is not a path, we can choose some vertices of H_y and construct the path of length at least $s+2$ with an end vertex y. By Lemma 4.1, we may get another graph on n vertices with r cut vertices, which has greater signless Laplacian spectral moments, a contradiction. Therefore, H_y is a pendent path, say P_t at y. Bearing in mind the choice of P_s, we have $t \geq s$. If $t \geq s+2$, then by Lemma 4.1, we can obtain another graph on n vertices with r cut vertices, which has greater signless Laplacian spectral moments than G, a contradiction. Therefore, for each $y \in V(B)$, $H_y \cong P_s$ or P_{s+1}. Hence, $G \cong G_n^r$. □

5. Concluding Remarks

In this paper and [10], we have studied the **Q**-spectral moments and signless Laplacian Estrada index ($SLEE$) of graphs. More precisely, we have determined graphs with greatest **Q**-spectral moments, thus maximum $SLEE$, through the set of all n-vertex graphs with a given parameter, namely, the number of cut edges, cut vertices, pendent vertices, (vertex) connectivity, edge connectivity, and diameter.

It would be of interest to investigate the behavior of these quantities on other classes of graphs such as chemical, c-cyclic, cactus graphs and linear polymers. Also, one might continue our work, by considering some other given parameters and finding their corresponding extremal graphs.

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