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# On the signless Laplacian Estrada index of bicyclic graphs

Kun Wang [a], Wenjie Ning [b,*], Mei Lu [c]

[a] School of Mathematical Sciences, Anhui University, Hefei 230601, China
[b] College of Science, China University of Petroleum (East China), Qingdao 266580, China
[c] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, China

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ABSTRACT

The signless Laplacian Estrada index of a graph 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 determine the unique bicyclic graph with maximum *SLEE* and the unique bipartite bicyclic graph with maximum *SLEE*, respectively.



## 1. Introduction

In this paper, a graph means a simple undirected graph. Let $G = (V, E)$ be a graph with $n$ vertices and $m$ edges. Let $N_G(v)$ be the set of vertices adjacent to $v$ in $G$. The *degree* of $v$ in $G$, denoted by $d_G(v)$, is equal to $|N_G(v)|$. A vertex of degree one is called a *pendent vertex*. The edge incident with a pendent vertex is known as a *pendent edge*.

Let $A(G)$ be the adjacency matrix of $G$ and $D(G) = \mathrm{diag}(d_1, d_2, \ldots, d_n)$ be the diagonal matrix of vertex degrees. Then the signless Laplacian matrix of $G$ is $Q(G) = D(G) + A(G)$ and the Laplacian matrix of $G$ is $L(G) = D(G) - A(G)$. It is obvious that $A(G)$, $Q(G)$ and $L(G)$ are real symmetric matrices. Thus their eigenvalues are real numbers. We denote the eigenvalues of $A(G)$, $Q(G)$ and $L(G)$ by $\lambda_1, \lambda_2, \ldots, \lambda_n, q_1, q_2, \ldots, q_n$ and $\mu_1, \mu_2, \ldots, \mu_n$, respectively.

For a graph $G$, the *Estrada index* of $G$ is defined as

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i}.$$

It was first proposed as a measure of the degree of folding of a protein [6] and has found multiple applications in a large variety of problems, including those in biochemistry and in complex networks, see [7–11]. Fath-Tabar et al. [12] generalized it to the *Laplacian Estrada index*, which is defined as

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i}.$$

* Corresponding author.
*E-mail addresses:* wangkun26@163.com (K. Wang), ningwenjie-0501@163.com (W. Ning), mlu@math.tsinghua.edu.cn (M. Lu).

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Various mathematical properties of $EE$ and $LEE$ have been discussed by several authors (see [3,15,16,19–21]). Ayyaswamy et al. [1] defined the *signless Laplacian Estrada index* of a graph $G$ as

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

and established some lower and upper bounds for $SLEE$ in terms of the number of vertices and number of edges. Although $SLEE(G) = LEE(G)$ for a bipartite graph $G$, it is still chemically interesting for fullerenes, fluoranthenes and other non-alternant conjugated species, in which $SLEE$ and $LEE$ differ.

Estimating bounds for $SLEE$ is of great interest, and many results have been obtained. Gao and Liu in [13] gave some sharp lower bounds for $SLEE$ in terms of the $k$-degree and the first Zagreb index. Gutmann et al. in [14] determined the graphs having maximum $SLEE$ among graphs with fixed order and vertex frustration index. Ellahi et al. in [4,17] found the unique graphs with maximum $SLEE$ among graphs with given number of cut edges, cut vertices, pendent vertices, vertex connectivity, edge connectivity and diameter. They also characterized the unicyclic graphs with the first two largest and smallest $SLEE$ in [5]. Moreover, they in [18] showed that there are exactly two graphs having maximum $SLEE$ among all tricyclic graphs. In this paper, we determine the unique bicyclic graph with maximum $SLEE$ and the unique bipartite bicyclic graph with maximum $SLEE$, respectively.

A *bicyclic graph* $G = (V, E)$ is a connected graph with $|E| = |V|+1$. Obviously, there are two basic bicyclic graphs: $\infty$-graph and $\theta$-graph. An $\infty$-*graph*, denoted by $\infty(p, q, l)$, is obtained from two vertex-disjoint cycles $C_p$ and $C_q$ by connecting one vertex of $C_p$ and one of $C_q$ with a path of length of $l - 1$ (in the case of $l = 1$, identifying the above two vertices); and a $\theta$-*graph*, denoted by $\theta(p, q, l)$, is a union of three internally disjoint paths $P_{p+1}, P_{q+1}, P_{l+1}$ of length $p, q, l$ resp. with common end vertices, where $p, q, l \geq 1$ and at most one of them is 1. Notice that any bicyclic graph $G$ is obtained from an $\infty$-graph or a $\theta$-graph $G_0$ by attaching trees to some of its vertices. The graph $G_0$ is called the *kernel* of $G$.

This paper is organized as follows. In Section 2, we introduce some lemmas that will be used later. In Section 3, we characterize the unique graph with maximum $SLEE$ among all bicyclic graphs with fixed order. In Section 4, we characterize the unique bipartite bicyclic graph with the largest $SLEE$.

## 2. Lemmas

Let $T_k(G)$ be the $k$th signless Laplacian spectral moment of the graph $G$ defined as $T_k(G) = \sum_{i=1}^{n} q_i^k$. Obviously, we have $T_k(G) = tr(Q^k)$. By the Taylor expansion of the exponential function $e^x$, we have

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

**Definition 1** (*[2]*). A semi-edge walk of length $k$ in a graph $G$, 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 for any $i = 1, 2, \ldots, k$, the vertices $v_i$ and $v_{i+1}$ are end-vertices (not necessarily distinct) of the edge $e_i$. We say that $W$ starts at $v_1$ and terminates at $v_{k+1}$. If $v_1 = v_{k+1}$, then we say $W$ is a closed semi-edge walk.

**Theorem 2** (*[2]*). *Let $Q$ be the signless Laplacian matrix of a graph $G$. The $(i, j)$-entry of the matrix $Q^k$ is equal to the number of semi-edge walks of length $k$ starting at vertex $i$ and terminating at vertex $j$.*

Let $G$ and $H$ be two graphs with $x, y \in V(G)$ and $u, v \in V(H)$. Let $SW_k(G; x, y)$ be the set of all semi-edge walks of length $k$ in $G$, which starts at $x$ and terminates at $y$, and let $|SW_k(G; x, y)| = T_k(G; x, y)$. If $T_k(G; x, y) \leq T_k(H; u, v)$ for all nonnegative $k$, then we write $(G; x, y) \preceq_s (H; u, v)$. If $(G; x, y) \preceq_s (H; u, v)$ and there exists some $k_0$ such that $T_{k_0}(G; x, y) < T_{k_0}(H; u, v)$, then we write $(G; x, y) \prec_s (H; u, v)$.

Let $SW_k(G; x, x) = SW_k(G; x)$, $T_k(G; x, x) = T_k(G; x)$ and $(G; u, u) = (G; u)$.

The *coalescence* of two vertex-disjoint connected graphs $G$ and $H$, denoted by $G(u) \circ H(w)$, where $u \in V(G)$ and $w \in V(H)$, is obtained from $G$ and $H$ by identifying the vertex $u$ of $G$ with the vertex $w$ of $H$.

**Lemma 3** (*[4]*). *Let $G$ be a graph with $u, v, w_1, w_2, \ldots, w_r \in V(G)$. Suppose that $E_v = \{e_1 = vw_1, \ldots, e_r = vw_r\}$ and $E_u = \{e'_1 = uw_1, \ldots, e'_r = uw_r\}$ where $e_i, e'_i \notin E(G)$, for $i = 1, 2, \ldots, r$. Let $G_u = G + E_u$ be the graph obtained from $G$ by adding all edges in $E_u$ and $G_v = G + E_v$ be the graph obtained from $G$ by adding all edges in $E_v$, respectively. 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 $SLEE(G_v) < SLEE(G_u)$.*

**Lemma 4** (*[18]*). *Let $G$ be a graph and $u, v \in V(G)$. If $N_G(v) \subseteq N_G(u) \cup \{u\}$, then $(G; v) \preceq_s (G; u)$, and $(G; w, v) \preceq_s (G; w, u)$ for each $w \in V(G) \setminus \{v\}$. Moreover, if $d_G(v) < d_G(u)$, then $(G; v) \prec_s (G; u)$.*

By Lemmas 3 and 4, we easily obtain the following two corollaries.

**Corollary 5.** *Let $H_1$ and $H_2$ be two graphs with $u, v \in V(H_1)$ and $w \in V(H_2)$. Let $G_v = H_1(v) \circ H_2(w)$ and $G_u = H_1(u) \circ H_2(w)$. If $(H_1; v) \prec_s (H_1, u)$, then $SLEE(G_v) < SLEE(G_u)$.*

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