Maximum Estrada Index of Bicyclic Graphs*

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Abstract Let $G$ be a simple graph of order $n$, let $\lambda_1(G), \lambda_2(G), \ldots, \lambda_n(G)$ be the eigenvalues of the adjacency matrix of $G$. The Estrada index of $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i(G)}$. In this paper we determine the unique graph with maximum Estrada index among bicyclic graphs with fixed order.

Keywords: Bicyclic graphs; Estrada index; eigenvalues

MR Subject Classifications: 05C50

1 Introduction

Let $G$ be a simple graph of order $n$ and let $A(G)$ be its adjacency matrix. The eigenvalues of $G$ are referred to the eigenvalues of $A(G)$, denoted by $\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_n(G)$. The Estrada index $EE(G)$ of the graph $G$ is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i(G)}$. The Estrada index was first introduced by Estrada [7] in 2000. It was found useful in biochemistry and complex networks, see [8, 9, 10, 11, 12]. Recently the Estrada index has been received a lot of attention in mathematics itself. Many bounds have been established for the Estrada index in [13, 15, 16, 14, 17]. Briefly, for a class $S$ of graphs, a graph $G \in S$ is called Estrada maximal if $EE(G) \geq EE(H)$ for any $H \in S$. The Estrada maximal trees subject to one or more graph parameters have been characterized; see [2, 4, 13, 16]. The unique Estrada maximal unicyclic graph was also determined in [6]. So, naturally the next problem is to characterize the Estrada maximal graph among all bicyclic graphs of fixed order. In this paper, we focus on this problem and determine the unique Estrada maximal graphs among all bicyclic graphs of fixed order.

A bicyclic graph $G = (V, E)$ is a connected simple graph which satisfies $|E| = |V| + 1$. There are two basic bicyclic graphs: $\infty$-graph and $\theta$-graph. More concisely, 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 $P_l$ of length $l - 1$ (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 $p, q, l$ respectively with common end vertices, where $p, q, l \geq 1$ and at most one of them is 1. Observe that any bicyclic graph $G$ is obtained from an $\infty$-graph or a $\theta$-graph $G_0$ (possibly) by attaching trees to some of its vertices. We call $G_0$ the kernel of $G$.

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2 Preliminaries and Lemmas

Let $M_k(G)$ be the $k$-th spectral moment of a graph $G$ of order $n$, i.e., $M_k(G) = \sum_{i=1}^{n} \lambda_i^k(G)$. It is well known that $M_k(G)$ is equal to the number of closed walks of length $k$ in $G$. The following result reveals the connection between the spectral moments and Estrada index:

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

For any vertices $u$, $v$ and $w$ (not necessary be distinct) in $G$, we denote by $M_k(G; u, v)$ the number of walks in $G$ with length $k$ from $u$ to $v$, and by $M_k(G; u, v, [w])$ the number of walks in $G$ with length $k$ from $u$ to $v$ which go through $w$. Denote by $W_k(G; u, v)$ a walk of length $k$ from $u$ to $v$ in $G$, and by $W_k(G; u, v, [w])$ the set of all such walks. Clearly $M_k(G; u, v) = |W_k(G; u, v)|$.

Let $G_1$ and $G_2$ be two graphs with $u_1, v_1 \in V(G_1)$ and $u_2, v_2 \in V(G_2)$. We write $(G_1; u_1, v_1) \preceq (G_2; u_2, v_2)$ if $M_k(G_1; u_1, v_1) \leq M_k(G_2; u_2, v_2)$ for any positive integer $k$. If, in addition, $M_k(G_1; u_1, v_1) < M_k(G_2; u_2, v_2)$ for at least one positive integer $k$, then we write $(G_1; u_1, v_1) \prec (G_2; u_2, v_2)$. Surely $(G_1; u_1, v_1) = (G_2; u_2, v_2)$ implies $M_k(G_1; u_1, v_1) = M_k(G_2; u_2, v_2)$ for any positive integer $k$.

**Lemma 2.1** \[ \text{Let } G \text{ be a graph containing two vertices } u, v. \text{ Suppose that } w_i \in V(G) \text{ and } uw_i \notin E(G), vw_i \notin E(G) \text{ for } i = 1, 2, \ldots, k. \text{ Let } E_u = \{uw_i, i = 1, 2, \ldots, k\} \text{ and } E_v = \{vw_i, i = 1, 2, \ldots, k\}. \text{ Let } G_u = G + E_u \text{ and } G_v = G + E_v. \text{ If } (G; u, u) \prec (G; v, v) \text{ and } (G; u, w_i) \leq (G; v, w_i) \text{ for } 1 \leq i \leq k, \text{ then } EE(G_u) < EE(G_v). \]

The **coalescence** of two vertex-disjoint connected graphs $G, H$, denoted by $G(u) \circ H(w)$, where $u \in V(G)$ and $w \in V(H)$, is obtained by identifying the vertex $u$ of $G$ with the vertex $w$ of $H$. A graph is called **nontrivial** if it contains at least two vertices.

**Lemma 2.2** \[ \text{Let } G \text{ be a connected graph containing two vertices } u, v, \text{ and let } H \text{ be a nontrivial connected graph containing a vertex } w. \text{ If } (G; u, u) \succ (G; v, v), \text{ then } EE(G(u) \circ H(w)) > EE(G(u) \circ H(w)). \]

**Lemma 2.3** \[ \text{Let } H_1 \text{ be a nontrivial connected graph containing a vertex } w, \text{ and let } H_2 \text{ be a connected graph of order at least 3 containing an pendant edge } uv, \text{ where } v \text{ is a pendant vertex. Then } EE(H_1(u) \circ H_2(u)) > EE(H_1(w) \circ H_2(w)). \]

**Lemma 2.4** \[ \text{Let } H_1 \text{ be a connected graph containing two vertices } u, v, \text{ and let } H_2 \text{ be a connected graph disjoint to } H_1, \text{ which contains a vertex } w. \text{ Let } H'_2 \text{ be a copy of } H_2, \text{ containing the vertex } w' \text{ corresponding to } w \text{ of } H_2. \text{ Let } G = (H_1(u) \circ H_2(w))(v) \circ H'_2(w'). \text{ If there exists an automorphism } \sigma \text{ of } H_1 \text{ such that it interchanges } u \text{ and } v, \text{ then } (G; u, u) = (G; v, v) \text{ and } (G; u, t) = (G; v, \sigma(t)) \text{ for any vertex } t \text{ distinct to } u. \]

Furthermore, if letting $H_1$ be obtained from $H_1$ by adding some edges incident with $v$ but not $u$, letting $H'_2$ be obtained from $H'_2$ by adding some vertices or edges such that the resulting graph is connected, and letting $G$ be obtained from $G$ by replacing $H_1$ with $H_1'$ or $H'_2$ with $H_2'$, then $(G; u, u) \prec (G; v, v)$ and $(G; u, t) \prec (G; v, \sigma(t))$ for any vertex $t$ distinct to $u$.

**Proof.** Surely $\sigma$ induces an automorphism of $G$, and also induces a 1-1 map from $W_k(G; x, y)$ to $W_k(G; \sigma(x), \sigma(y))$ for any $x, y$ and $k$. The first assertion follows.

Now we prove the second assertion. Note that

$$M_k(\tilde{G}; u, u) = M_k(\tilde{G}; v; u, u) + M_k(\tilde{G}; u, u, [v]), M_k(G; u, v) = M_k(\tilde{G}; u; v, v) + M_k(\tilde{G}; v, v, [u]);$$

where $\tilde{G}$ is the graph obtained from $G$ by replacing $G$ with its line graph $L(G)$, and $M_k(\tilde{G}; u, v)$ denotes the $k$-th spectral moment of $\tilde{G}$ with respect to vertices $u$ and $v$. For any positive integer $k$, $M_k(\tilde{G}; u, v)$ is the number of closed walks of length $k$ from $u$ of $G$ to $v$ of $\tilde{G}$ which go through $w$. If $\tilde{G}$ is a connected graph, then $M_k(\tilde{G}; u, v)$ is the number of closed walks of length $k$ from $u$ of $G$ to $v$ of $\tilde{G}$ which go through $w$. Hence, $M_k(\tilde{G}; u, v) = M_k(G; u, v)$. The second assertion follows from the first assertion.


and

\[ M_k(\bar{G} - v; u, u) = M_k((\bar{H}_1 - v)(u) \circ H_2(w); u, u) = M_k((H_1 - v)(u) \circ H_2(w); u, u) = M_k((H_1 - u)(v) \circ H'_2(w); v, v), \]

where the last equality holds as \( \sigma \) induces an isomorphism between \((H_1 - v)(u) \circ H_2(w)\) and \((H_1 - u)(v) \circ H'_2(w)\) and interchanges \(u\) and \(v\). However,

\[ M_k(G - u; v, v) = M_k((\bar{H}_1 - u)(v) \circ H'_2(w); v, v). \]

Since \(H_1\) is a proper subgraph of \(\bar{H}_1\) or \(H'_2\) is a proper subgraph of \(\bar{H}'_2\), we have

\[ M_k(G - v; u, u) \leq M_k(G - u; v, v) \]

with strict inequality for at least one \(k\).

For each walk \(W \in W_k(G; u, u, [v])\), write it as \(W = W_1W_2\), where \(W_1\) is the longest subwalk of \(W\) from \(u\) to \(v\), and \(W_2\) is the remaining section from \(v\) to \(u\). Define a map \(f : W_k(G; u, u, [v]) \to W_k(G; v, v, [u])\) by \(f(W) = W_2W_1\). One can verify \(f\) is an injection, and hence \(M_k(G; u, u, [v]) \leq M_k(G; v, v, [u])\). So we proved \((G; u, u) \prec (G; v, v)\). The proof of \((G; u, t) \prec (G; v, \sigma(t))\) can be argued in a similar way. □

Denote by \(N_G(v)\) the set of neighbors of a vertex \(v\) in a graph \(G\), and by \(d_G(v)\) the cardinality of the set \(N_G(v)\).

**Corollary 2.5** Let \(G\) be a unicyclic graph obtained from a cycle \(C\) by attaching some trees on its vertices. Assume \(u, w\) are two adjacent vertices on the cycle \(C\) such that the tree attached at \(u\) is a star centered at \(v\) with one of its pendant vertices identified with \(u\), and the tree attached at \(w\) is a star with its center identified with \(w\); see Fig. 2.1. If \(d_G(w) \geq d_G(v) + 1\), then

(i) \((G; w, w) \succ (G; v, v)\);

(ii) \((G; w, t) \succ (G; v, t)\) for any \(t \notin (N_G(v) \cup N_G(w) \cup \{w\}) \setminus V(C)\).

![Fig. 2.1. An illustration of the graph G in Corollary 2.5](image)

**Proof.** Let \(G'\) be the graph obtained from \(G\) by deleting the edge on the cycle incident to \(w\) except \(uw\), and deleting \(d_G(w) - d_G(v) - 1\) pendant vertices of \(w\). Then there exists an automorphism of \(G'\) which interchanges \(v\) and \(w\) together with their pendant vertices, and preserves all other vertices. Now the assertion follows from the second result of Lemma 2.1. □

**Corollary 2.6** Let \(G\) be obtained from \(\theta(2, 2, 1)\) by attaching some pendant edges at the vertices of its cycles. Let \(u, v, w, t\) be the vertices as shown in Fig. 2.2.

(i) If \(d_G(w) > 2\) and \(d_G(t) = 2\), then \((G; w, w) \succ (G; t, t)\);

(ii) If \(d_G(u) > 3\), \(d_G(v) = 3\) and \(d_G(x) = 2\) for any \(x \in V(G) \setminus \{u, v, w\}\), then \((G; u, u) \succ (G; v, v)\);

(iii) If \(d_G(u) > 3\), \(d_G(v) = 3\) and \(d_G(x) = 2\) for any \(x \in V(G) \setminus \{u, v, w\}\), then \((G; u, u) \succ (G; w, w)\).
Lemma 2.7 Let \( G = \theta(p, q, l) \) and let \( u, v \) be the two vertices of \( G \) with degree 3 respectively. Then \( (G; u, u) = (G; v, v) \triangleright (G; w, w) \) for any vertex \( w \) distinct to \( u \) and \( v \).

**Proof.** Let \( P_{p+1}, P_{q+1}, P_{l+1} \) be respectively the induced paths of \( G \) joining \( u \) and \( v \). Define an automorphism \( \sigma \) of the graph \( G \) as follows: \( \sigma \) interchanges \( u \) and \( v \), and for each vertex \( x \) of the path \( \sigma(p+1) \) (respectively, \( P_{q+1}, P_{l+1} \)), \( \sigma(x) \) is also on \( P_{p+1} \) (respectively, \( P_{q+1}, P_{l+1} \)) such that the distance between \( x \) and \( u \) along this path is equal to that between \( \sigma(x) \) and \( v = \sigma(u) \). The automorphism \( \sigma \) naturally induces a map from \( W_k(G; s, t) \) to \( W_k(G; \sigma(s), \sigma(t)) \), such that \( \sigma(W_k(G; s, t)) = W_k(G; \sigma(s), \sigma(t)) \) for any \( K \) and \( s, t \in V(G) \), where each vertex \( x \) of \( W_k(G; s, t) \) is mapped to \( \sigma(x) \). In particular, \( \sigma \) is a 1-1 map from \( W_k(G; u, u) \) to \( W_k(G; v, v) \) for any \( k \), and hence \( (G; u, u) = (G; v, v) \).

To prove \( (G; u, u) \triangleright (G; w, w) \) for any vertex \( w \) distinct to \( u \) and \( v \), we only consider the case when \( w \) lies on the internal part of the path \( P_{l+1} \). The other cases can be proved in a similar way. Denote \( C_{ij} \) the cycle made by \( P_{i+1} \) and \( P_{j+1} \), where \( i \not= j \), and \( i, j \) is one of \( p, q, l \). One can easily see that \( M_k(C_{ij}; u, u) = M_k(C_{ij}; w, w) \). Thus it suffices to consider the closed walks of length \( k \) from \( u \) to \( w \) that pass though at least one edge of \( P_{l+1} \). Suppose that \( W_k(G; w, w) \) is such a walk. We decompose the walk \( W_k(G; w, w) \) into three parts \( W_1, W_2, W_3 \) in a unique way, where \( W_1 \) starts at \( w \) and goes along the path \( P_{l+1} \) as far as possible, whose terminal point must be \( u \) or \( v \); \( W_2 \) starts at the terminal point of \( W_1 \), takes the first step and the last step on edges of \( C_{pq} \), and \( W - W_2 \) contains no edges of \( C_{pq} \), whose terminal point must be \( u \) or \( v \); \( W_3 = W - W_1W_2 \).

Now we construct a map \( g \) from \( W_k(G; w, w) \) to \( W_k(G; u, u) \) in the following way. If \( W_2 \) is a \( u - u \) walk or \( u - v \) walk, \( g(W_1W_2W_3) = W_2W_3W_1 \); if \( W_2 \) is a \( v - u \) walk, \( g(W_1W_2W_3) = W_3W_1W_2 \); if \( W_2 \) is a \( v - v \) walk, \( g(W_1W_2W_3) = \sigma(W_3W_1W_2) \). By directly checking we find that \( g \) is an injection. Thus \( M_k(G; u, u) \geq M_k(G; w, w) \) for any \( k \). Obviously, \( M_2(G; u, u) = 3 > 2 = M_2(G; w, w) \). This completes the proof.

\[ \square \]

### 3 Main results

Denote by \( G_{\infty}(n; p, q) \) the set of all bicyclic graphs of order \( n \) which contains an \( \infty \)-graph as a kernel with two cycles having length \( p, q \) respectively. Denote by \( G_{\theta}(n; p, q) \) the set of all bicyclic graphs of order \( n \) which contains \( \theta(p', q', l') \) as kernel, where \( p' \geq q' \geq l' \) and \( p' + l' = p, q' + l' = q \). We first investigate some properties of Estrada maximal graphs in \( G_{\infty}(n; p, q) \) or \( G_{\theta}(n; p, q) \), and show that any Estrada maximal graph in \( G_{\infty}(n; p, q) \) will have a smaller Estrada index than some graph in \( G_{\theta}(n; p, q) \). Finally we determine the unique Estrada maximal graph among all bicyclic graphs of fixed order.
Lemma 3.1 If $G$ is an Estrada maximal graph among all bicyclic graphs of order $n$, then $G$ is obtained from its kernel by attaching some pendant edges.

Proof. Assume to the contrary, there exists a pendant edge $G$ not attached to its kernel. Then there is a cut edge $uw$ of $G$ such that $G - uw$ has two components $G_1, G_2$, where $G_1$ contains the vertex $u$ and the kernel of $G$, and $G_2$ is a nontrivial tree containing the vertex $w$. Removing $G_2$ at $w$ and attaching it to $u$, by Lemma 2.1 we will arrive at a new bicyclic graph but with larger Estrada index, a contradiction. □

Theorem 3.2 If $G$ is an Estrada maximal graph in $G_\infty(n; p, q)$, then $G$ is obtained from $\infty(p, q, 1)$ by attaching some pendant edges.

Proof. Suppose $G$ is the Estrada maximal graph in $G_\infty(n; p, q)$, and contains $\infty(p, q, l)$ as its kernel. By Lemma 3.1 $G$ is obtained from $\infty(p, q, l)$ by attaching some pendant edges. We assert $l = 1$. Otherwise, let $P_1(l > 1)$ be the path connecting $C_p$ and $C_q$, and let $v_1v_2$ be the starting edge of $P_1$, where $v_1 \in V(C_p)$. Write $G = G_1(v_1) \circ G_2(v_1)$, where $G_1$ contains $C_p$, and $G_2$ contains $C_q$ and the vertex $v_1$ as a pendant vertex. Removing $G_1$ at $v_1$ and attaching it to $v_2$, we will arrive at a graph $G' \in G_\infty(n; p, q)$.

However, by Lemma 2.3 $EE(G') > EE(G)$, a contradiction.

Theorem 3.3 If $G$ is an Estrada maximal graph in $G_\theta(n; p, q)$, then $G$ is obtained from $\theta(p - 1, q - 1, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges.

Proof. Suppose $G$ is an Estrada maximal graph in $G_\theta(n; p, q)$, and contains $\theta(p', q', l')$ as its kernel, where $p' \geq q' \geq l'$ and $p' + l' = p, q' + l' = q$. By Lemma 3.1 $G$ is obtained from $\theta(p', q', l')$ by attaching some pendant edges. If $l' = 1$, or $l' = 2$ and $p' = q' = 2$, the result follows. Now assume $l' \geq 2$ and $p' \geq 3$. Let $u, v, w, t$ be the vertices of $\theta(p', q', l')$ as shown in the left graph of Fig. 3.1. Without loss of generality, assume $d_G(u) \geq d_G(v)$. Deleting the edge $tv$ and adding a new edge $tw$, we will arrive at a new graph $\tilde{G}$ whose kernel is $\theta(p' - 1, q' - 1, l')$ as shown in the right graph in Fig. 3.1. Consider the unicyclic graph $G - tv$. By Lemma 2.3 $(G - tv; w, w) \succeq (G - tv; v, v)$ and $(G - tv; w, t) \succeq (G - tv; v, t)$. So, by Lemma 2.1 $EE(\tilde{G}) > EE(G)$, a contradiction.

Fig. 3.1. An illustration of the proof of Theorem 3.3

Lemma 3.4 Let $G$ be a bicyclic graph which is obtained from $\infty(p, q, 1)$ by attaching some pendant edges to its vertices. Then there exists a bicyclic graph $\tilde{G}$ whose kernel is $\theta(p - 1, q - 1, 1)$ such that $EE(\tilde{G}) > EE(G)$.

Proof. Let $v, w, t$ be the vertices of $\infty(p, q, 1)$ as shown in Fig. 3.2, where $d_G(w) \geq d_G(v)$. Deleting the edge $tv$ and adding a new edge $tw$, we will arrive at a new graph $\tilde{G}$ whose kernel is $\theta(p - 1, q - 1, 1)$ as shown in Fig. 3.2. Consider the unicyclic graph $G - tv$. By Lemma 2.3 $(G - tv; w, w) \succeq (G - tv; v, v)$ and $(G - tv; w, t) \succeq (G - tv; v, t)$. So, by Lemma 2.1 $EE(\tilde{G}) > EE(G)$, a contradiction. □
Denote by $G_1$ the bicyclic graph of order $n$ obtained from $\theta(2, 2, 1)$ by attaching $n - 4$ pendant edges to one of its vertices of degree 3, and by $G_2$ the bicyclic graph of order $n$ obtained from $\theta(2, 2, 2)$ by attaching $n - 5$ pendant edges to one of its vertices of degree 3.

**Lemma 3.5** Let $G$ be an Estrada maximal graph among all bicyclic graphs of order $n$. Then $G$ is either $G_1$ or $G_2$.

**Proof.** By Theorem 3.2 and Lemma 3.4 $G$ must contains a $\theta$-graph as its kernel. By Lemma 3.3 $G$ is obtained from $\theta(p, q, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges. Assume $G$ contains $\theta(p, q, 1)$ as its kernel, where $p \geq q$ and $p \geq 3$. Let $v, w, t$ be the vertices of $\theta(p, q, 1)$ as shown in Fig. 3.3, where $d_G(w) \geq d_G(v)$. Deleting the edge $tv$ and adding a new edge $tw$, we will arrive at a new graph $G$ whose kernel is $\theta(p - 1, q - 1, 2)$ as shown in Fig. 3.3. By a similar discussion to the proof of Lemma 3.4, we have $EE(G) > EE(G)$, a contradiction. So $G$ is obtained from $\theta(2, 2, 1)$ or $\theta(2, 2, 2)$ by attaching some pendant edges.

We next show all the pendant edges of $G$ are attached at a unique vertex $\theta(2, 2, 1)$ or $\theta(2, 2, 2)$ with degree 3, and hence $G$ is exactly $G_1$ or $G_2$. We only prove the case of $G$ having $\theta(2, 2, 2)$ as the kernel; the other case can be discussed in a similar way. Let $v_i, i = 1, 2, \ldots, 5$, be the vertices of $\theta(2, 2, 2)$ as shown in the last graph in Fig. 3.3. Assume each $v_i$ is attached to $m_i$ pendant edges in the graph $G$, for $i = 1, 2, \ldots, 5$, where $m_i \geq 0$ and $\sum_{i=1}^{5} m_i = n - 5$.

Denote $G = G(m_1, m_2, m_3, m_4, m_5)$. If at least two of $m_3, m_4, m_5$ are nonzero, say $m_3 > 0, m_4 > 0$, by Corollary 2.6(i), $(G(m_1, m_2, m_3, 0, m_5; v_3, v_5)) = (G(m_1, m_2, m_3, 0, m_5; v_4, v_4))$, and by Lemma 2.2 removing all the pendant edges of $G(m_1, m_2, m_3, m_4, m_5)$ at $v_4$ and attaching them to $v_3$, we will get a graph $G(m_1, m_2, m_3 + m_4, 0, m_5)$ with a larger Estrada index, a contradiction. So, at least two of $m_3, m_4, m_5$ are zero, say $m_4 = m_5 = 0$. Then $G = G(m_1, m_2, m_3, 0, 0)$.

If both $m_1, m_2$ are nonzero, by Corollary 2.6(ii), $(G(m_1, 0, m_3, 0, v_1, v_1)) = (G(m_1, 0, m_3, 0; v_2, v_2))$, and by Lemma 2.2 removing all the pendant edges of $G(m_1, m_2, m_3, 0, 0)$ at $v_2$ and attaching them to $v_1$, we will arrive at graph $G(m_1 + m_2, 0, m_3, 0, 0)$ with a larger Estrada index, also a contradiction. So at least one of $m_1, m_2$ is zero, say $m_2 = 0$, i.e. $G = G(m_1, 0, m_3, 0, 0)$. By Lemmas 2.7 and 2.6 $(G(m_1, 0, m_3, 0, 0; v_1, v_1)) = (G(m_1, 0, 0, 0, v_3, v_3))$ whether or not $m_1 = 0$. If $m_3 > 0$, by a similar discussion we get $EE(G(m_1 + m_3, 0, 0, 0)) > EE(G(m_1, 0, m_3, 0, 0))$, a contradiction. So $G = G(m_1, 0, 0, 0, 0)$, and the result follows. \(\square\)

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<th>$\theta(p - 1, q - 1, 2)$</th>
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Fig. 3.3. An illustration of proof of Lemma 3.5

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![Fig. 3.2. An illustration of proof of Lemma 3.4](image4.png)
Finally we determine which is larger between $EE(G_1)$ and $EE(G_2)$. Denote by $\phi(G, x)$ the characteristic polynomial of the adjacency matrix of a graph $G$.

**Lemma 3.6** Let $G$ be a graph containing a vertex $v$, and let $C(v)$ be the set of cycles containing $v$. Then

$$\phi(G, x) = x\phi(G - v, x) - \sum_{w \in N_C(v)} \phi(G - v - w, x) - 2\sum_{Z \in C(v)} \phi(G - V(Z), x).$$

**Proposition 3.7** $EE(G_1) > EE(G_2)$ for $n \geq 5$.

**Proof.** By Proposition 3.6, $\phi(G_1, x) = x^{n-4}f(x)$, $\phi(G_2, x) = x^{n-4}g(x)$, where

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

By a direct calculation, $EE(G_1) > EE(G_2)$ when $5 \leq n \leq 22$. Now assume $n \geq 23$. Since $f(\sqrt{n-1}) = -6 - 4\sqrt{n-1} < 0$, $\lambda_1(G_1) > \sqrt{n-1}$. On the other hand, as $g(x)$ is increasing for $x > \sqrt{\frac{n+1}{2}}$, $g\left(\sqrt{n-\frac{3}{2}}\right) = \frac{3}{2} - \frac{4n}{3} > 0$ when $n \geq 23$, which implies $\lambda_1(G_2) < \sqrt{n-\frac{3}{2}}$ when $n \geq 23$.

Let $u, v$ be the vertices of $G_1$ and $G_2$ both with maximal degree, respectively. The graph $G_1 - u$ has eigenvalues $\pm \sqrt{2}$ and 0 with multiplicity $n - 3$, and the graph $G_2 - v$ has eigenvalues $\pm \sqrt{3}$ and 0 with multiplicity $n - 3$. By interlacing property of the eigenvalues of $A(G_1 - u)$ and $A(G_1)$ (or see [1]), $\lambda_i(G_1) \geq \lambda_i(G_1 - u)$ for $i = 2, 3, \ldots, n - 1$. So

$$EE(G_1) = \sum_{i=1}^{n} e^{\lambda_i(G_1)} > e^{\lambda_1(G_1)} + \sum_{i=2}^{n-1} e^{\lambda_i(G_1 - u)} > e^{\sqrt{n-1}} + (n-3) + e^{-\sqrt{3}}.$$

Similarly, by the fact $\lambda_i(G_2) \leq \lambda_{i-1}(G_2 - v)$ for $i = 2, 3, \ldots, n$,

$$EE(G_2) \leq e^{\lambda_1(G_2)} + \sum_{i=2}^{n} e^{\lambda_i(G_2 - v)} < e^{\sqrt{n-\frac{3}{2}}} + e^{\sqrt{3}} + (n-3) + e^{-\sqrt{3}}.$$

Noting that $e^{\sqrt{n-1}} > e^{\sqrt{n-\frac{3}{2}}} + e^{\sqrt{3}}$ for $n \geq 23$, so we get the result.

By Lemma 3.6 and Proposition 3.7 we get the main result of this paper.

**Theorem 3.8** Let $G$ be a bicyclic graph of order $n$. Then $EE(G) \leq EE(G_1)$, with equality if and only if $G = G_1$.

**References**


