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MINIMAL ESTRADA INDEX OF THE TREES
WITHOUT PERFECT MATCHINGS

WEN-HUAN WANG† AND CHUN-XIANG ZHAI‡

Abstract. Trees possessing no Kekulé structures (i.e., perfect matching) with the minimal Estrada index are considered. Let $T_n$ be the set of the trees having no perfect matchings with $n$ vertices. When $n$ is odd and $n \geq 5$, the trees with the smallest and the second smallest Estrada indices among $T_n$ are obtained. When $n$ is even and $n \geq 6$, the tree with the smallest Estrada index in $T_n$ is deduced.

Key words. Estrada indices, Perfect matching, Trees.

AMS subject classifications. 05C05, 05C35.

1. Introduction. Let $G$ be a simple graph with a vertex set $V(G)$, where $|V(G)| = n$. Let $A(G)$ be the adjacency matrix of $G$ and $I$ the identity matrix of order $n$. Let $\Phi(G, \lambda) = \det[\lambda I - A(G)]$ be the characteristic polynomial of $G$ [3]. The $n$ roots of $\Phi(G, \lambda) = 0$ are denoted by $\lambda_1 \geq \cdots \geq \lambda_n$. Since $A(G)$ is a real symmetric matrix, $\lambda_1, \ldots, \lambda_n$ are all real numbers. The Estrada index (EI) of $G$, is defined by [9]

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

According to Estrada, the EI is useful to characterize the degree of folding of a protein chain, and to account for the contribution of amino acids to folding [9, 13, 14]. Later, the EI was extended to measure the centrality of complex network [10, 11], extended atomic branching [12], and the carbon-atom skeleton [18]. For a comprehensive survey of the index, one can refer to [16]. Since its inception in 2000, several analogous graph invariants, such as the Laplacian and signless Laplacian Estrada indices [1, 20] based respectively on the eigenvalues of Laplacian and signless Laplacian matrices, the resolvent Estrada indices [2, 17] based on the resolvent of the adjacency matrix, and the skew Estrada index of oriented graphs [15], have been considered.

A walk $W$ of length $k$ in $G$ is any sequence of vertices and edges of $G$, namely $W = v_0, e_1, v_1, e_2, \ldots, v_{k-1}, e_k, v_k$ such that $e_i$ is the edge joining vertices $v_{i-1}$ and $v_i$ for every $i = 1, 2, \ldots, k$. If $v_0 = v_k$, then the walk $W$ is closed and is referred to as the $(v_0, v_0)$-walk of length $k$. For $k \geq 0$, we denote $M_k(G) = \sum_{i=1}^{n} \lambda_i^k$ and refer to $M_k(G)$ as the $k$-th spectral moment of $G$. It is well known that $M_k(G)$ is equal to the number of the closed walks of length $k$ in $G$ [3]. From the Taylor expansion of $e^{\lambda_i}$, $EE(G)$ in (1.1) can be rewritten as

\begin{equation}
EE(G) = \sum_{k=0}^{\infty} \frac{M_k(G)}{k!}.
\end{equation}
In particular, if \( G \) is a bipartite graph, then \( M_{2k+1}(G) = 0 \) for \( k \geq 0 \). Hence, we have

\[
EE(G) = \sum_{k=0}^{\infty} \frac{M_{2k}(G)}{(2k)!}.
\]

Let \( G_1 \) and \( G_2 \) be bipartite graphs of order \( n \). If \( M_{2k}(G_1) \geq M_{2k}(G_2) \) holds for each positive integer \( k \), then \( EE(G_1) \geq EE(G_2) \) and we write \( G_1 \succeq G_2 \). If \( G_1 \succeq G_2 \) and there is at least one positive integer \( k_0 \) such that \( M_{2k_0}(G_1) > M_{2k_0}(G_2) \), then \( EE(G_1) > EE(G_2) \) and we write \( G_1 \succ G_2 \). If \( G_1 \succeq G_2 \) and \( G_2 \succeq G_1 \), then we write \( G_1 \sim G_2 \).

Within groups of isomers, it was found that the EI increases with the rising extend of branching of the carbon-atom skeleton \([18, 21]\). Therefore, the ordering of graphs with extremal Estrada indices (EIs) is of practical importance and theoretical interest in the subject of graph theory. In graph theory, a connected acyclic graph is called a tree. Therefore, the topological properties of acyclic molecules agree with those of trees. Based on the above relationship obtained from (1.3), a number of results have been reached for the graphs with the extremal EIs. For the general trees, and the trees with given parameters, such as the trees with a given matching number, the trees with a fixed diameter, the trees with a given number of pendant vertices, and the trees with a given maximum degree, etc., one can refer to \([4, 5, 6, 8, 21, 27]\). For the characterization of the unicyclic graphs, the bicyclic graphs and the tricyclic graphs, etc., one can refer to \([7, 22, 23, 25, 28]\).

Recall that conjugated molecules in chemistry may be classified into two groups: Kekuléan and non-Kekuléan molecules, depending on whether or not they possess the Kekulé structures, which are perfect matchings in the molecular graph corresponding to the carbon atom skeleton of a conjugated unsaturated hydrocarbon \([19]\). In the set of trees with perfect matchings, Wang \([24]\) obtained the trees with the largest and the second largest EIs. Zhai and Wang \([26]\) deduced the trees with the smallest and the second smallest EIs. However, the trees with the extremal EIs in the set of trees without perfect matchings remains unknown. For simplicity, \( \mathcal{P}M \) stands for “perfect matching”. Let \( \mathcal{T}_n \) be the set of the trees with \( n \) vertices having no \( \mathcal{P}M \). In this paper, for completeness, in \( \mathcal{T}_n \), we will investigate the ordering of trees in terms of their minimal EIs. Thus, we characterize the acyclic non-Kekuléan \( \pi \)-electron systems with the minimal EIs.

2. Transformations for studying the Estrada indices. Let \( v \in V(G) \), and \( d_G(v) \) be the degree of \( v \) of \( G \). A pendent path at \( v \) of \( G \) is a path in \( G \) connecting vertex \( v \) and a pendent vertex such that all internal vertices (if exist) in this path have degree two and \( d_G(v) \geq 3 \). Lemmas 2.1 and 2.2 are simply quoted.

**Lemma 2.1.** \([21]\) Let \( w \) be a vertex of the nontrivial connected graph \( G \). For non-negative integers \( p \) and \( q \), let \( G(p, q) \) denote the graph obtained from \( G \) by attaching at \( w \) pendant paths \( P \cong wu_1u_2\cdots u_p \) and \( Q \cong wu_1u_2\cdots u_q \) of lengths \( p \) and \( q \), respectively. If \( p \geq q \geq 1 \), then \( EE(G(p, q)) > EE(G(p + 1, q - 1)) \).

Let the coalescence \( G(u) \cdot H(v) \) be the graph obtained from \( G \) and \( H \) by identifying \( u \) of \( G \) with \( v \) of \( H \). Let \( P_n \) be a path with \( n \) vertices.

**Lemma 2.2.** \([6]\) Let \( u \) be a non-isolated vertex of a simple graph \( H \). Let \( H_1 \cong H(u) \cdot P_n(v_1) \) (as shown in Figure 1(a)) and \( H_2 \cong H(u) \cdot P_n(v_1) \) (as shown in Figure 1(b)), where \( P_n \equiv v_1v_2\cdots v_n \). As \( n \geq 3 \) and \( k \geq 2 \), we have \( M_{2k}(H_2) > M_{2k}(H_1) \).

To obtain our results, Lemma 2.3 is introduced as follows.
Lemma 2.3. Let $G_1$ be a connected graph, $u \in V(G_1)$ and $|V(G_1)| \geq 2$. Let $G_2$ be a tree with $n \geq 3$ vertices, $G_2 \not\cong P_n$ and $v \in V(G_2)$. Let $G \cong G_1(u) \cdot G_2(v)$ (as shown in Figure 2(a)) and $G' \cong G_1(u) \cdot P_n(v)$ (as shown in Figure 2(b)), where $P_n \cong v_2 \cdots v_n$. We have $EE(G) > EE(G')$.

Proof. Let $G$ be the graph as shown in Figure 2(a). Two cases are considered as follows.

Case (i). $d_{G_2}(v) = 1$.

In $G$, since $G_2 \not\cong P_n$, we can choose one vertex (denoted by $w$) of $G_2$ such that $d_{G_2}(w) \geq 3$ and there are $(d_{G_2}(w) - 1)$ pendent paths attached at $w$. By using Lemma 2.2 $(d_{G_2}(w) - 2)$ times on $w$ in $G$, we get a new graph $H$ satisfying $d_H(w) = 2$ and $G \succ H$. By using the same procedure on all the vertices in $G_2$ which have degrees three or more, we can obtain a graph $G'$ such that $H \succeq G'$, where $G'$ is the graph as shown in Figure 2(b). Thus, we get $G \succ G'$.

Case (ii). $d_{G_2}(v) \geq 2$.

Subcase (ii.i). $d_{G_2}(v) \geq 2$ and all the vertices in $V(G_2) \setminus \{v\}$ have degrees 2 or 1.

Obviously, $G$ is the graph obtained from $G_1$ by attaching $d_{G_2}(v)$ pendent paths at $u$ of $G_1$. By using Lemma 2.2 $(d_{G_2}(v) - 1)$ times on $v$ in $G$, we have $G \succ G'$.

Subcase (ii.ii). $d_{G_2}(v) \geq 2$ and there exist $k \geq 1$ vertices in $V(G_2) \setminus \{v\}$ having degrees three or more.

In $G$, we can choose one vertex (denoted by $s$) of $V(G_2) \setminus \{v\}$ such that $d_{G_2}(s) \geq 3$ and there are $(d_{G_2}(s) - 1)$ pendent paths attached at $s$. By using Lemma 2.2 $(d_{G_2}(s) - 2)$ times on $s$ of $G$, we get a new graph $H$ satisfying $d_H(s) = 2$ and $G \succ H$. In $G$, by using the same procedure on all the vertices in $G_2$ which have degrees three or more (except for $v$), we can obtain a graph $H'$ such that $H \succeq H'$, where $H'$ is the graph obtained from $G_1$ by attaching $d_{G_2}(v)$ pendent paths at $u$ in $G_1$. By using Lemma 2.2 $(d_{G_2}(v) - 1)$ times on $v$ in $H'$, we get $H' \succ G'$. Thus, $G \succ G'$.
3. Ordering of the trees in $\overline{T}_n$ according to their minimal Estrada indices for odd $n$. Let $lT_b^r$ be the tree obtained by attaching three pendant paths of length $l$, $r$ and $b$ at a common vertex $u$, where $l + r + b + 1 = n$. For example, $lT_b^r$ is shown in Figure 3.

For a tree $T$ with $n$ vertices, if $n$ is odd, then $T$ has no PM, namely $T \in \overline{T}_n$. We have $\overline{T}_2 = \emptyset$, $\overline{T}_3 = \{P_3\}$, and $\overline{T}_4 = \{1T_1^1\}$. Next, in $\overline{T}_n$, when $n$ is odd and $n \geq 5$, we obtain the trees with the smallest and the second smallest EIs in Theorem 3.1.

**Theorem 3.1.** Let $T \in \overline{T}_n \setminus \{P_n, 1T_{n-3}^1\}$ and $n$ be odd, where $n \geq 5$. We have $EE(T) > EE(1T_{n-3}^1) > EE(P_n)$.

**Proof.** Let $n$ be odd and $n \geq 5$. By Lemma 2.1, we obtain $1T_{n-3}^1 \succ P_n$. Let $T \in \overline{T}_n \setminus \{P_n, 1T_{n-3}^1\}$. Next, we prove

$$T \succ 1T_{n-3}^1.$$ (3.4)

Since $T \not\cong P_n$, $T$ has at least one vertex having a degree three or more. We consider two cases as follows.

**Case (i).** Only one vertex of $T$ (denoted by $u$) has a degree three or more.

In this case, all the degrees of the vertices in $V(T) \setminus \{u\}$ are 2 or 1. Namely, $T$ is the tree obtained by attaching $d_T(u)$ pendant paths at a common vertex $u$. By using Lemma 2.2 ($d_T(u) - 3$) times on $u$ in $T$, we get $T \succ 1T_b^r$, where $T \sim 1T_b^r$ holds if and only if $T \cong 1T_b^r$. Since $1T_b^r$ has $n \geq 5$ vertices, where $n$ is odd, $1T_b^r \in \overline{T}_n$.

Suppose $r \geq l \geq 1$. By applying Lemma 2.1 ($l - 1$) times, we obtain $1T_b^r \succ l-1 T_b^{r+1} \succ \cdots \succ l T_b^{l+r-1}$. Without loss of generality, let $b \geq l + r - 1$. By using Lemma 2.1 ($n - b - 3$) times again, we have $1T_b^{l+r-1} \succ 1T_{b+1}^{l+r-2} \succ \cdots \succ 1T_{n-3}^1$. Therefore, we get $1T_b^r \succ 1T_{n-3}^1$.

**Case (ii).** There exist $k \geq 2$ vertices in $T$ having degrees three or more.

In this case, we can choose one vertex (denoted by $w$) in $T$ such that $d_T(w) \geq 3$ and there are $(d_T(w) - 1)$ pendant paths attached at $w$. By using Lemma 2.2 ($d_T(w) - 2$) times on $w$ in $T$, we obtain a new tree $T'' \in \overline{T}_n$ (since $n$ is odd) satisfying $d_{T''}(w) = 2$ and $T \succ T''$. By using the same procedure, we can obtain a tree $T''' \in \overline{T}_n$ (since $n$ is odd) such that $T' \succ T'''$, where $T'''$ has only one vertex having a degree three or more and all the other vertices in $T'''$ having degrees 2 or 1. Furthermore, by the proof of case (i), we have $T''' \succ 1T_{n-3}^1$. Therefore, we obtain $T \succ 1T_{n-3}^1$.

By the combination of the proofs of cases (i) and (ii), we get (3.4).

Next, in Section 4, among $\overline{T}_n$, when $n$ is even, we will deduce the tree with the minimal EI by using a different method. The reason is given in the following remark.
Remark 3.2. In Lemma 2.2, if $H_2$ (as shown in Figure 1(b)) has even number of vertices and has no $PM$, then $H_1$ (as shown in Figure 1(a)) may have a $PM$. Therefore, in $T_n$, if $n$ is even, then Lemma 2.2 can not be used to obtain the ordering of the trees according to their minimal EIs.

4. Trees with the minimal Estrada index in $T_n$ for even $n$. In this section, among $T_n$, when $n$ is even, we will investigate the tree with the minimal EI in $T_n$. Since the trees in $T_n$ have no $PM$, we get $P_n \notin T_n$. Let $\bar{T}_n = T_n \cup T_n^2$, where $\bar{T}_n$ is the subset of $T_n$, in which each tree has only one vertex having degree 3 and all the other vertices having degrees 2 or 1, and $T_n^2$ is the subset of $T_n$, in which each tree has at least two vertices having degrees three or more or only one vertex having a degree four or more.

In $T_n$, we have $l + r + b + 1 = n$. If $n$ is even, then only one of $l$, $r$ and $b$ is odd or all of $l$, $r$ and $b$ are odd. Therefore, if $^lT_n^r \in T_n$ and $n$ is even, then $l$, $r$ and $b$ must be all odd. Otherwise, if only one of $l$, $r$ and $b$ is odd, then $^lT_n^r$ has a $PM$. By the definition of $\bar{T}_n$, we get that $\bar{T}_n = \{^lT_n^r | l, r, b$ are all positive odd numbers$\}$.

Let $G$ in Lemma 2.1 be $P_{b+1}$. By using Lemma 2.1, we can obtain Corollary 4.1.

\textbf{Corollary 4.1.} $^lT_n^r \succeq l^2 T_n^{r+2} \succ \ldots \succ \lceil (n-r)/2 \rceil T_n^{r-2} \succ \ldots \succ 1 T_n^{n-b-2}$, where $r \geq l$ and $l, r, b$ are all positive odd numbers.

Let $G$ in Lemma 2.1 be $P_{l+1}$. By using Lemma 2.1, we get Corollaries 4.2 and 4.3.

\textbf{Corollary 4.2.} $^lT_n^r \succ l T_n^{r+2} \succ \ldots \succ l T_n^{r-2} \succ \ldots \succ l T_n^3 \succ T_n^2 \succ T_n^1$, where $b \geq r$ and $l, r, b$ are all positive odd numbers.

\textbf{Corollary 4.3.} $^lT_n^r \succ l T_n^{r+2} \succ \ldots \succ l T_n^{r-2} \succ \ldots \succ l T_n^3 \succ T_n^2 \succ T_n^1$, where $r \geq b$ and $l, r, b$ are all positive odd numbers.

By Corollaries 4.2 and 4.3, we get Corollary 4.4.

\textbf{Corollary 4.4.} $^lT_n^r \succeq l T_n^3 \succ T_n^{l-4} \succ T_n^{l-2}$, with $^lT_n^r \sim l T_n^{l-4}$ if and only if $r = 3$ or $b = 3$, where $r, b \geq 3$ and $l, r, b$ are all positive odd numbers.

Remark 4.5. By the definition of $^lT_n^r$, if $l$, $r$, $b$ are all positive odd numbers, then all the graphs in Corollaries 4.1–4.4 have no $PM$.

For $n$ is even, let $\bar{T}_n^1 = \bar{T}_n^{1,1} \cup \bar{T}_n^{1,2}$, where $\bar{T}_n^{1,1} = \{^lT_n^r | r \geq 1, b \geq l = 1 \}$ and $\bar{T}_n^{1,2} = \{^lT_n^r | b \geq 3, r \geq l \geq 3 \}$.

From Corollary 4.2 (let $l = 1$), we obtain, in Theorem 4.6, the complete ordering of the trees in $\bar{T}_n^{1,1}$ in terms of their minimal EIs.

\textbf{Theorem 4.6.} For $^lT_n^r \in \bar{T}_n^{1,1}$, we have the ordering as follows.

(i) For $n = 4t$ with $t \geq 1$, $^lT_n^{2t-1} \succ l T_n^{2t-3} \succ \ldots \succ l T_n^3 \succ T_n^1$.

(ii) For $n = 4t + 2$ with $t \geq 1$, $^lT_n^{2t-2} \succ l T_n^{2t-4} \succ \ldots \succ l T_n^3 \succ T_n^1$.

From Corollaries 4.1 and 4.4, we get Theorem 4.7 as follows.
THEOREM 4.7. Let \( l T_b^r \in \mathcal{T}^1_n \setminus \{3 T^3_{n-7}\} \), \( n \) be even and \( n \geq 10 \). We have

\[
l T_b^r \geq 3 T^3_{n-7} \geq 1 T^5_{n-7} \geq 1 T^3_{n-5} \geq 1 T^1_{n-3},
\]

with \( l T^3_{n-5} \sim 1 T^3_{n-5} \) if and only if \( n = 10 \).

Proof. Let \( n \) be even and \( n \geq 10 \). It follows from Corollary 4.1 that \( 3 T^3_{n-7} \geq 1 T^5_{n-7} \). Since \( n - 7 \geq 3 \), by Corollary 4.4 (let \( l = 1 \)), we obtain \( l T^3_{n-7} \geq 1 T^5_{n-5} \) with \( l T^3_{n-7} \sim 1 T^3_{n-5} \) if and only if \( n = 10 \). Since \( n - 5 \geq 5 \), by Corollary 4.4 (let \( l = 1 \)) again, we get \( l T^3_{n-5} \geq 1 T^1_{n-3} \). Namely, we have \( 3 T^3_{n-7} \geq 1 T^5_{n-7} \geq 1 T^3_{n-5} \geq 1 T^1_{n-3} \).

Next, let \( l T_b^r \in \mathcal{T}^1_n \setminus \{3 T^3_{n-7}\} \). We will prove

\[
l T_b^r \geq 3 T^3_{n-7}.
\]

By the definition of \( \mathcal{T}^1_n \), in \( l T_b^r \), we have \( b \geq 3 \) and \( r \geq 3 \). By Corollary 4.1, we obtain \( l T_b^r \geq l-2 T_b^{r+2} \geq \ldots \geq 3 T_b^{l+r-3} \). Since \( l+r-3 \geq 3 \) and \( b \geq 3 \), by Corollary 4.4 (let \( l = 3 \)), we get \( 3 T_b^{l+r-3} \geq 3 T^3_{n-7} \) with \( 3 T_b^{l+r-3} \sim 3 T^3_{n-7} \) if and only if \( 3 T_b^{l+r-3} \geq 3 T^3_{n-7} \). Therefore, if \( l T_b^r \not\geq 3 T^3_{n-7} \), then we have \( l T_b^r \not\geq 3 T^3_{n-7} \). Namely, (4.5) holds. Theorem 4.7 is thus proved.

Next, we consider the tree with the minimal EI in \( \mathcal{T}^2_n \). By the definition of \( \mathcal{T}^2_n \), we have \( \mathcal{T}^2_n = \emptyset \) when \( n = 4 \). In \( \mathcal{T}^2_n \), we assume that \( n \) is even and \( n \geq 6 \). To obtain the tree with the minimal EI in \( \mathcal{T}^2_n \), we first give some definitions and proposition and then introduce Lemma 4.9.

Let \( T \in \mathcal{T}^2_n \). For two vertices \( u, v \in V(T) \), let \( d(u, v) \) be the distance between \( u \) and \( v \). Let \( V_p(T) = \{ v \in V(T) \mid d_T(v) = 1 \} \) and \( \mathcal{A}(T) = \{ w \in V(T) \mid d_T(w) \geq 3 \} \). For a given vertex \( w \in \mathcal{A}(T) \), let

\[
P_w(T) = \{ v \in V_p(T) \mid d(v, w) < d(v, x), \text{for any } x \in \mathcal{A}(T) \setminus \{ w \} \}.
\]

For example, let \( T \) be the tree as shown in Figure 4. We have \( \mathcal{A}(T) = \{ w_1, w_2, w_3 \} \), \( P_{w_1}(T) = \{ v_1, v_2 \} \), \( P_{w_2}(T) = \{ v_3, v_4, v_5 \} \), and \( P_{w_3}(T) = \{ v_6, v_7 \} \). For any \( v \in V_p(T) \), there exists a vertex \( w \in \mathcal{A}(T) \) such that \( v \in P_w(T) \). For any \( w \in \mathcal{A}(T) \), there exists at least one vertex \( v \in P_w(T) \), namely \( |P_w(T)| \geq 1 \).

For \( w \in \mathcal{A}(T) \), let \( S_w = \{ w \} \cup P_w(T) \cup Q_w(T) \), where \( Q_w(T) \) is the set of vertices lying on the pendent paths between \( v \) of \( P_w(T) \) and \( w \) (other than \( v \) and \( w \)) for all \( v \in P_w(T) \). For example, for \( T \) in Figure 4, \( S_{w_1} = \{ w_1, v_1, v_2 \} \), \( S_{w_2} = \{ w_2, s_1, v_3, v_4, v_5 \} \), and \( S_{w_3} = \{ w_3, s_2, s_3, v_6, v_7 \} \). We denote by \( T[S_w] \) the induced subtree of \( T \), where the vertex set of \( T[S_w] \) is \( S_w \), and the edge set of \( T[S_w] \) is the set of those edges of \( T \) that have both ends in \( S_w \). We say that the induced subtree \( T[S_w] \) is the pendent subtree attached at \( w \). For example, for \( T \) in Figure 4, \( T[S_{w_1}], T[S_{w_2}] \) and \( T[S_{w_3}] \) are the three pendent subtrees attached at \( w_1 \), \( w_2 \) and \( w_3 \), respectively. By the definition of \( T[S_w] \), we get that \( d_T(S_w)(w) \geq 3 \) and all the degrees of the vertices in \( V(T[S_w]) \setminus \{ w \} \) are 2 or 1.
Let $|\mathcal{A}(T)|$ be the number of vertices in $\mathcal{A}(T)$. When $|\mathcal{A}(T)| \geq 2$, let $\mathcal{A}(T) = \{w_1, w_2, \ldots, w_t\}$, where $t \geq 2$. In $\mathcal{A}(T)$, when $t \geq 2$, we can choose two vertices (denoted by $w_1$ and $w_2$) such that

$$d(w_1, w_2) = \max \{d(w_i, w_j) | w_i, w_j \in \mathcal{A}(T), 1 \leq i < j \leq t\}. \tag{4.6}$$

**Proposition 4.8.** Let $T \in \mathcal{T}_n^2$. For $|\mathcal{A}(T)| \geq 2$, let $w_1$ and $w_2$ be the two vertices as defined in (4.6).

(i) There exist two pendent subtrees $T[S_{w_1}]$ and $T[S_{w_2}]$ attached at $w_1$ and $w_2$, respectively.

(ii) $|P_{w_1}(T)| \geq 2$ and $|P_{w_2}(T)| \geq 2$.

**Proof.** (i) Let $T \in \mathcal{T}_n^2$ and $w_1$ and $w_2$ be the two vertices as defined in (4.6). We can choose one vertex $u \in V(T)$ ($u$ can be $w_2$) such that $u$ is adjacent to $w_1$ and $T - w_1 u = T_1' \cup T_2'$, where $T_1'$ and $T_2'$ are the two components of $T - w_1 u$ which contain $w_1$ and $w_2$, respectively. Suppose that there exists a vertex (let it be $x$, $x \neq w_1$) in $T_1'$ which has a degree three or more. Then $d(x, w_2) = d(x, w_1) + d(w_1, w_2) > d(w_1, w_2)$, which contradicts the definition of $w_1$ and $w_2$. Thus, all the vertices of $T_1'$ (except for $w_1$) have degrees 2 or 1. Namely, $T_1'$ is the pendant subtree attached at $w_1$. Similarly, we can get that there exists a pendant subtree attached at $w_2$. Thus, we get Proposition 4.8(iii).

(ii) Since $d_T(w_1) \geq 3$, we get $d_{T_1'}(w_1) \geq 2$. Furthermore, since $T_1'$ is the pendant subtree attached at $w_1$, we get $|P_{w_1}(T)| \geq 2$. Similarly, we can get $|P_{w_2}(T)| \geq 2$. Thus, we get Proposition 4.8(ii). \[\square\]

**Lemma 4.9.** Let $T \in \mathcal{T}_n^2$, $n$ be even, and $n \geq 6$. We get that there exists a tree $T_b^1 \in \mathcal{T}_n^1$ such that $EE(T) > EE(T_b^1)$.

**Proof.** Let $T \in \mathcal{T}_n^2$, $n$ be even, and $n \geq 6$. By the definition of $\mathcal{T}_n^2$, we have $|\mathcal{A}(T)| \geq 1$. We prove Lemma 4.9 by induction on $|\mathcal{A}(T)|$.

(I) $|\mathcal{A}(T)| = 1$.

Since $T \in \mathcal{T}_n^2$ and $|\mathcal{A}(T)| = 1$, by the definition of $\mathcal{T}_n^2$, in $T$, there is only one vertex (let it be $w$) having a degree four or more and all the other vertices of $T$ have degrees 2 or 1. Namely, $T$ is a starlike
tree obtained from \( w \) by attaching \( d_T(w) \geq 4 \) pendent paths at \( w \). Let the lengths of the \( d_T(w) \) pendent paths be \( r_1, r_2, \ldots, r_{d_T(w)} \), where \( \sum_{i=1}^{d_T(w)} r_i = n - 1 \). Let \( \mathcal{R} = \{ r_i \mid r_i \text{ is odd, } 1 \leq i \leq d_T(w) \} \). Since \( n \) is even, \( |\mathcal{R}| \) must be odd number. Furthermore, since \( T \) has no \( \mathcal{P} \mathcal{M} \), \( |\mathcal{R}| \geq 3 \). Otherwise, if \( |\mathcal{R}| = 1 \), then \( T \) has a \( \mathcal{P} \mathcal{M} \). Therefore, we can choose \( r_s, r_t \in \mathcal{R} \), where \( 1 \leq s, t \leq d_T(w) \). By employing Lemma 2.2 on \( w \) in \( T \) \( (d_T(w) - 3) \) times, we get \( T \succ^* T_{n-r_s-r_t-1}^r \) since \( d_T(w) \geq 4 \). Since \( r_s \) and \( r_t \) are odd numbers and \( n \) is even, \( n - r_s - r_t - 1 \) is odd number. Therefore, \( r_s T_{n-r_s-r_t-1}^r \in \mathcal{T}_n \). Thus, we get Lemma 4.9 when \( |\mathcal{A}(T)| = 1 \).

(II). When \( |\mathcal{A}(T)| = k \) and \( k \geq 1 \), we suppose there exists a tree \( T_0^r \in \mathcal{T}_n \) such that \( T \succ^l T_0^r \).

(III). When \( |\mathcal{A}(T)| = k + 1 \) and \( k \geq 1 \), next, we will prove that Lemma 4.9 holds.

Let \( \mathcal{A}'(T) = \{ w_i \in \mathcal{A}(T) \mid |P_{w_i}(T)| \geq 2, 1 \leq i \leq t \} \). Obviously, \( \mathcal{A}'(T) \subseteq \mathcal{A}(T) \). Let \( \mathcal{A}'(T) = \{ w_1, w_2, \ldots, w_h \} \). By Proposition 4.8(ii), in \( \mathcal{A}'(T) \), \( h \geq 2 \). For \( w_i \) \( (1 \leq i \leq h) \) in \( \mathcal{A}'(T) \), let \( \mathcal{T}_S = \{ T[S_{w_1}], T[S_{w_2}], \ldots, T[S_{w_h}] \} \).

Next, when \( |\mathcal{A}(T)| = k + 1 \) with \( k \geq 1 \), we consider two cases according to the trees in \( \mathcal{T}_S \) having \( \mathcal{P} \mathcal{M} \) or not.

Case (i). There exists at least one pendent subtree in \( \mathcal{T}_S \) having \( \mathcal{P} \mathcal{M} \).

Let \( T \) be the graph as shown in Figure 5(a). Let \( T[S_w] \) be the pendent subtree in \( \mathcal{T}_S \) having a \( \mathcal{P} \mathcal{M} \). Since \( T \) has no \( \mathcal{P} \mathcal{M} \), we get that \( T_0 \) has no \( \mathcal{P} \mathcal{M} \). By employing Lemma 2.3 on \( T \) (namely, transformation \( \alpha \) in Figure 5), we can get a new tree \( T_1 \) (as shown in Figure 5(b)) such that \( T \succ T_1 \). Obviously, \( |\mathcal{A}(T_1)| = |\mathcal{A}(T)| - 1 = k \) and \( T_1 \) has no \( \mathcal{P} \mathcal{M} \) since \( T_0 \) has no \( \mathcal{P} \mathcal{M} \). By the induction, we can get that there exists a tree \( T_1^r \in \mathcal{T}_n \) such that \( T_1 \succeq^l T_1^r \). Therefore, we obtain \( T \succ^l T_1^r \).

Case (ii). All the pendent subtrees in \( \mathcal{T}_S \) do not have \( \mathcal{P} \mathcal{M} \).

Let \( T \) be the tree as shown in Figure 6(a). Let \( w_1 \) and \( w_2 \) be the two vertices as defined in (4.6). By Proposition 4.8, we get that there exist two pendent subtrees \( T[S_{w_1}] \) and \( T[S_{w_2}] \) attached at \( w_1 \) and \( w_2 \), respectively, and \( |P_{w_1}(T)|, |P_{w_2}(T)| \geq 2 \).

Subcase (ii.1). \( |V(T[S_{w_1}])| \equiv 1 \) (mod 2) or \( |V(T[S_{w_2}])| \equiv 1 \) (mod 2).

Without loss of generality, we assume \( |V(T[S_{w_1}])| \equiv 1 \) (mod 2).

In \( T \), if the induced graph \( T[V(T_0')] \cup V(T[S_{w_2}]) \cup \{w_1\} \) has no \( \mathcal{P} \mathcal{M} \), then by employing Lemma 2.3 on \( T \) (namely, transformation \( \beta \) in Figure 6), we can get a new tree \( T_2 \) (as shown in Figure 6(b)) having no \( \mathcal{P} \mathcal{M} \) such that \( T \succ T_2 \). Since \( |\mathcal{A}(T_2)| = |\mathcal{A}(T)| - 1 = k \), by the induction, we get \( T_2 \succeq^l T_0^r \). Therefore, \( T \succ^l T_0^r \), where \( T_0^r \in \mathcal{T}_n \).

In \( T \), if the induced graph \( T[V(T_0')] \cup V(T[S_{w_2}]) \cup \{w_1\} \) has \( \mathcal{P} \mathcal{M} \), then \( w_1 \) (as shown in Figure 6(a)) is saturated with another vertex in \( T[V(T_0')] \cup V(T[S_{w_2}]) \cup \{w_1\} \). Since \( T \) has no \( \mathcal{P} \mathcal{M} \), we can deduce that, in \( T[S_{w_1}] \), there exist at least one vertex (except for \( w_1 \)) which is unsaturated. By employing Lemma 2.3 on \( T \) (namely, transformation \( \gamma \) in Figure 6), we can get a new tree \( T_3 \) (as shown in Figure 6(c)) such that \( T \succ T_3 \), where \( T_3 \) has no \( \mathcal{P} \mathcal{M} \). Since \( |\mathcal{A}(T_3)| = 1 \), by the proof for (I) with \( |\mathcal{A}(T)| = 1 \), we get \( T_3 \succeq^l T_0^r \). Thus, \( T \succ^l T_0^r \), where \( T_0^r \in \mathcal{T}_n \).
Subcase (ii.ii). \( |V(T[S_{w_1}])| \equiv 0 \pmod{2} \) and \( |V(T[S_{w_2}])| \equiv 0 \pmod{2} \).

By employing Lemma 2.3 on \( T \) (namely, transformation \( \gamma \) in Figure 6), we get a new tree \( T_3 \) (as shown in Figure 6(c)) such that \( T \succ T_3 \), where \( T_3 \) has no \( PM \) since \( T[S_{w_1}] \) has no \( PM \). Obviously, \( |A(T_3)| = 1 \).

By the proof for (I) with \( |A| \), in Figure 6(a), we get a new tree \( T_3 \) (as shown in Figure 6(c)) such that \( T \succ T_3 \). Therefore, we get \( T \succ T_3 \), where \( T_3 \in T_n \).

By the combination of the proofs of cases (i) and (ii), we get that Lemma 4.9 holds when \( |A(T)| = k + 1 \).

Therefore, by the proofs of (I)–(III) and the induction on \( |A(T)| \), we obtain Lemma 4.9.

**Remark 4.10.** In the proof for case (ii) of Lemma 4.9, if \( u = w_2 \) or \( v = u, w_2 \) and \( v \) are shown in Figure 6(a), then we can check that the technique used in case (ii) of Lemma 4.9 remains valid.

By Theorem 4.6, Theorem 4.7 and Lemma 4.9, we obtain the tree with the minimal EI in \( T_n \) when \( n \) is even.

**Theorem 4.11.** Let \( T \in T_n \), \( n \) be even and \( n \geq 4 \). We have \( EE(T) \geq EE(T^1_{n-3}) \), with the equality if and only if \( T \equiv T^1_{n-3} \).

**Proof.** Let \( T \in T_n \), \( n \) be even and \( n \geq 4 \). For \( n = 4 \), \( T \equiv T^1_1 \). Let \( n \geq 6 \). For \( T \in T^1_{n-1} \), obviously, \( T \equiv T^1_6 \). For \( T \in T^2_{n-1} \), by Lemma 4.9, there exists a tree \( T^r_6 \in T^1_n \) such that \( T \succ T^r_6 \). Furthermore, by Theorems 4.6 and 4.7, we obtain Theorem 4.11.

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**References**


Minimal Estrada Index of the Trees Without Perfect Matchings


